Crystal structures of the gold NHC complex bis(4-bromo-1,3-diethylimidazol-2-ylidene)gold(I) iodide and its 1:1 adduct with trans-bis(4-bromo-1,3-diethyl-imidazol-2-ylidene)diiodidogold(III) iodide

Rolf Büssing,a Ingo Otta and Peter G. Jonesb*

aInstitut für Medizinische und Pharmazeutische Chemie, Technische Universität Braunschweig, Beethovenstr. 55, D-38106 Braunschweig, Germany, and bInstitut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Hagenring 30, D-38106 Braunschweig, Germany. *Correspondence e-mail: p.jones@tu-bs.de

The first title compound, [Au(C7H11BrN2)2]I, crystallizes in the space group $P\overline{1}$ without imposed symmetry. The cations and anions are linked to form chains by Br...I...Br halogen-bond linkages. The second title compound, [Au(C7H11BrN2)2][AuI2(C7H11BrN2)2]I2, is an adduct of the first and its formally I2-oxidized AuIII analogue. It also crystallizes in space group $P\overline{1}$, whereby both gold atoms occupy inversion centres. The extended structure is a reticular layer involving Br...I...Br and I...I...Au linkages.

1. Chemical context

Gold complexes have been used in medicine since ancient times and have been applied as drugs for the treatment of rheumatoid arthritis since the 1930s. Currently, gold species are being actively investigated in inorganic medicinal chemistry as possible anticancer agents or anti-infectives (Mora et al., 2019). Some of the existing therapeutics have reached the clinical trial stage as a result of drug repurposing efforts. Metal N-heterocyclic carbene (NHC) complexes in general have also proved to be biologically and medicinally active compounds (Ott, 2020); in particular, gold complexes with NHC ligands are often synthesized and investigated because of the high stability of the gold–carbon bonds and the convenient synthetic access to a broad variety of structurally diverse NHC structures (Nahra et al., 2021). We have reported on the synthesis, characterization and biological effects of [bis(4-bromo-1,3-diethyl-imidazol-2-ylidene)gold(I)] iodide (3) (Schmidt et al., 2017a) (Fig. 1). Notably, this complex and related derivatives triggered cytotoxicity against cancer cells, showed a low serum protein binding, and inhibited growth of some pathogenic bacteria. Furthermore, we have recently investigated various gold NHC complexes as antibacterial agents and inhibitors of bacterial thioredoxin reductase (Büssing et al., 2021).
Here we report the structure of 3, together with that of its 1:1 complex (4) with trans-[bis(4-bromo-1,3-diethyl-imidazol-2-ylidene)diiodidogold(III)] iodide, formally its I₂-oxidized AuIII analogue; the latter was formed in small quantities when 3 was recrystallized. Further studies on the bioinorganic and medicinal chemistry of 3 and related derivatives are the subject of ongoing projects.

2. Structural commentary

The structure of the asymmetric unit of 3 is shown in Fig. 2. All atoms lie on general positions in space group P1. Selected intra- and intermolecular dimensions (including contact distances) are presented in Table 1. The gold atom is, as expected, linearly coordinated. The NHC planes subtend an interplanar angle of 78.74 (10)°. The short contact Br₂/C₁/C₁/C₁/I₁ seen in Fig. 2 is one of two such contacts that determine the crystal packing (see next section).

The structure of compound 4 is shown in Fig. 3. Selected metrical parameters for intra- and intermolecular interactions (including contact distances) are presented in Table 2. Both gold atoms lie on inversion centres; the C—Au—C and I—Au—I angles are thus exactly linear, and the NHC planes of both cations are exactly coplanar. The gold(III) centre displays the expected square planar geometry. The Au—C bond is slightly longer than in 3. For further discussion, see Database survey below.

Table 1

| Distance (Å) | Standard Deviation (Å) |
|-------------|------------------------|
| Au—I₁—Cl   | 2.020 (2)              |
| Au—I₁—C₈   | 2.022 (2)              |
| I₁—Br₁i    | 3.5294 (3)             |
| C₁—Au—I₁—C₈| 174.97 (9)             |
| Br₁i—I₁—Br₂| 101.436 (8)            |

Symmetry codes: (i) x, y, z + 1; (ii) −x + 1, −y + 1, −z + 1; (iii) x + 1, y + 1, z.

Table 2

| Distance (Å) | Standard Deviation (Å) |
|-------------|------------------------|
| Au—I₁—C₁   | 2.033 (7)              |
| Au—I₁—Br₂  | 2.018 (7)              |
| I₁—Br₂     | 3.6072 (3)             |
| C₁—Br₁—I₁—C₈| 174.97 (9)             |
| C₁—Br₁—I₁| 114.871 (16)           |

Symmetry codes: (i) −x, −y, −z; (ii) −x + 1, −y + 1, −z; (iii) −x − 2, −y + 2, −z + 1; (iv) x − 1, y − 1, z.
3. Supramolecular features

The packing of compound 3 is shown in Fig. 4. It is dominated by short Br···I contacts (Table 1) that may be considered as halogen bonds (for reviews, see Metrangelo, 2008 and Cavallaro et al., 2016). The C—Br···I angles are approximately linear, whereas Br···I···Br is approximately a right angle. The anions and cations are connected to form chains with overall direction parallel to [11̅1]. The chains are in turn connected in pairs by the contact Au···Br2 [3.8033 (3) Å, operator 1 — x, 1 — y, 1 — z]. Within the double chains, the intercentroid distance between the carbene rings based on N1 and N2 is 3.5265 (14) Å, and between the double chains the intercentroid distance between the rings based on N3 and N4 (operator 1 — x, 2 — y, −z) is 3.6187 (14) Å; these offset contacts may represent π···π interactions.

The packing of compound 4 (Fig. 5) also involves halogen bonds. The cations are connected to form chains parallel to [3̅3̅1] (horizontal in Fig. 5) by contacts between each bromine atom and the iodide I2. As in 3, the C—Br···I angles are approximately linear. The AuIII cations are further connected in the [11̅1] direction (vertical in Fig. 4) by a very short I1···I2 contact and a long I2···Au2 contact. The result is a reticular layer structure parallel to (1̅10), in which the iodide anion I2 is four-coordinate. The angle between the two chain directions is 76.4°. There are no short contacts between ring centroids.

Figure 4
Packing diagram of compound 3 viewed perpendicular to (011). Hydrogen atoms are omitted. Dashed lines indicate halogen bonds or Au···Br interactions. Atom labels correspond to the asymmetric unit.

3.4. Database survey

Using version 2.0.5 of the CSD (Groom et al., 2016), a ConQuest search (Bruno et al., 2002) for bis(carbene)gold(I) cations gave 355 hits, with an average Au—C bond length of 2.023 Å. For AuIII cations of the form [(carbene)2AuX2]+ (X = halogen), only 38 hits were recorded, and only six of these involved iodine as the halogen (refcodes: ANUJIE (Baron et al., 2016), CIVMOK (Jothibasu et al., 2008), MEZZOI (Gil-Rubio et al., 2013), POYHO (Ghosh & Catalano, 2009), XOMFIR and XONCAH (Holtthoff et al., 2019)). XOMFIR presents a rare example of a non-cyclic carbene ligand. The average Au—C and Au—I bond lengths are 2.034 and 2.614 Å, respectively. The Au—C bond lengths of 3 and 4 may thus be considered normal, whereas the Au—I bond of 4 is longer than all those previously reported. It is tempting to suggest that this is associated with the halogen bonding, but MEZZOI and POYHO also display short I···I contacts (3.680 and 3.478 Å, respectively), while XONCAH has a short Au···I contact of 3.438 Å. Short halogen···halogen contacts between AuIII species are relatively frequent; we recently drew attention to such contacts in AuCl4− and AuBr4− salts with protonated amine cations (Döring & Jones, 2016) but we did not include AuI4− salts because these are far more difficult to access.

5. Synthesis and crystallization

We have described the syntheses of compounds 1, 2 (Schmidt et al., 2017b) and 3 (Schmidt et al., 2017a) elsewhere, but give a brief summary here. The reagents were purchased from Sigma—Aldrich, Alfa Aesar or TCI and used without additional purification steps. All reactions were performed without precautions to exclude air or moisture. In the first step, 4-bromoimidazole was reacted with ethyl iodide in the presence of potassium carbonate to yield the bisalkylated imidazolium iodide (1) (Fig. 1). Compound 1 was then transformed in a two-step procedure by reaction with Ag2O and chlorido(dimethylsulfide)gold(I) to the gold(I) NHC complex 2. The biscarbene complex [(NHC)2Au]+ I− (3) was obtained by further reaction of 2 with 1.

Single crystals of complex 3 were obtained by diffusion of n-hexane into a solution of 3 in chloroform/deuterochloroform. A few crystals of the mixed-valence complex 4 also formed, for reasons that are not clear, and the compound was identified by X-ray analysis as reported here.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For both structures, the methyl groups were refined as idealized rigid groups allowed to rotate but not tip (AFIX 137; C—H 0.98 Å, H—C—H 109.5°). The
methylene and NHC ring hydrogens were included using a riding model starting from calculated positions (C—H = 0.99 or 0.95 Å respectively). The \(U_{eq}(H)\) values were fixed at 1.2 (for methylene groups) or 1.5 (for methyl groups) times the \(U_{eq}\) value of the parent carbon atoms.

The asymmetric unit of 3 was chosen to include the short Br\(_2\)−I contact. This means that the iodide lies outside the reference unit cell. Similarly, the asymmetric unit of 4 was chosen as a central I2 anion coordinated by two cations (Fig. 2). The long and narrow shape of this unit means that the centroid of the Au\(^{III}\) cation does not lie within the reference cell. In both cases, this leads to a CheckCIF Alert G.

The large difference peaks close to Au2 and I2 of structure 4 may be a consequence of its moderate crystal quality (some-what irregular and diffuse reflection shapes) and/or residual absorption errors. The peaks can of course be made smaller by cutting the data to a lower \(I > 2\sigma(I)\) reflections (Fig. 2).

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**Computing details**

For both structures, data collection: CrystAlis PRO (Rigaku OD, 2021); cell refinement: CrystAlis PRO (Rigaku OD, 2021); data reduction: CrystAlis PRO (Rigaku OD, 2021); program(s) used to solve structure: SHELXS (Sheldrick, 2008); program(s) used to refine structure: SHELXL2017 (Sheldrick, 2015); molecular graphics: Siemens XP (Siemens, 1994); software used to prepare material for publication: SHELXL2017 (Sheldrick, 2015).

**Bis(4-bromo-1,3-diethylimidazol-2-ylidene)gold(I) iodide (3)**

**Crystal data**

\[
\text{[Au(C}_7\text{H}_{11}\text{BrN}_2\text{)]}_2\text{I}
\]

- \( M_r = 730.04 \)
- Triclinic, \( P\overline{1} \)
- \( a = 8.4676 (2) \) Å
- \( b = 8.8248 (3) \) Å
- \( c = 14.0119 (5) \) Å
- \( \alpha = 76.374 (3)^\circ \)
- \( \beta = 85.320 (2)^\circ \)
- \( \gamma = 85.251 (2)^\circ \)
- \( V = 1011.99 (6) \) Å\(^3\)
- \( Z = 2 \)
- \( F(000) = 672 \)
- \( D_\text{x} = 2.396 \) Mg m\(^{-3}\)
- Mo K\(\alpha\) radiation, \( \lambda = 0.71073 \) Å
- Cell parameters from 47541 reflections
- \( \theta = 2.7–36.4^\circ \)
- \( \mu = 12.74 \) mm\(^{-1}\)
- \( T = 100 \) K
- Block, colourless
- 0.09 \( \times \) 0.06 \( \times \) 0.05 mm

**Data collection**

- XtaLAB Synergy, HyPix diffractometer
- Radiation source: micro-focus sealed X-ray tube
- Detector resolution: 10.0000 pixels mm\(^{-1}\)
- \( \omega\) scans
- Absorption correction: multi-scan
  - (CrystAlisPro; Rigaku OD, 2021)
- \( T_{\text{min}} = 0.751, T_{\text{max}} = 1.000 \)
- 84327 measured reflections
- 9374 independent reflections
- 8185 reflections with \( I > 2\sigma(I) \)
- \( R_{\text{int}} = 0.043 \)
- \( \theta_{\text{max}} = 36.7^\circ, \theta_{\text{min}} = 2.8^\circ \)
- \( h = -14\rightarrow14 \)
- \( k = -14\rightarrow14 \)
- \( l = -22\rightarrow22 \)

**Refinement**

- Refinement on \( F^2 \)
- Least-squares matrix: full
- \( R[F^2 > 2\sigma(F^2)] = 0.023 \)
- \( wR(F^2) = 0.052 \)
- \( S = 1.02 \)
- 9374 reflections
- 203 parameters
- 0 restraints
- Hydrogen site location: inferred from neighbouring sites
- H-atom parameters constrained
\[
w = \frac{1}{\sigma^2(F_o^2) + (0.0219P)^2 + 1.6441P}
\]
\[
\text{where } P = (F_o^2 + 2F_c^2)/3
\]
\[
\Delta \rho_{\text{max}} = 1.53 \text{ e Å}^{-3}
\]
\[
\Delta \rho_{\text{min}} = -2.02 \text{ e Å}^{-3}
\]
\[
(\Delta \sigma)_{\text{max}} = 0.002
\]

**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         | Uiso* / Ueq |
|-----------|-----------|-----------|-------------|
| Au1       | 0.46224 (2) | 0.71713 (2) | 0.23616 (2) | 0.01505 (2) |
| I1        | 0.25568 (2) | -0.12579 (2) | 0.72649 (2) | 0.01947 (3) |
| Br1       | 0.90742 (3) | 0.85910 (3) | -0.11585 (2) | 0.01837 (4) |
| Br2       | 0.22321 (3) | 0.27369 (3) | 0.58678 (2) | 0.02294 (5) |
| N1        | 0.7026 (2) | 0.8013 (2) | 0.06168 (14) | 0.0144 (3) |
| N2        | 0.4687 (2) | 0.7981 (2) | 0.01341 (14) | 0.0151 (3) |
| N3        | 0.3414 (2) | 0.4840 (2) | 0.41402 (14) | 0.0158 (3) |
| N4        | 0.3267 (2) | 0.7110 (2) | 0.44721 (14) | 0.0168 (3) |
| C1        | 0.5490 (3) | 0.7807 (3) | 0.09487 (17) | 0.0152 (4) |
| C2        | 0.7156 (3) | 0.8303 (3) | -0.03991 (16) | 0.0150 (4) |
| C3        | 0.5681 (3) | 0.8289 (3) | -0.07101 (17) | 0.0159 (4) |
| H3        | 0.539432 | 0.845625 | -0.137005 | 0.019* |
| C4        | 0.8329 (3) | 0.7876 (3) | 0.12682 (17) | 0.0190 (4) |
| H4A       | 0.796328 | 0.835665 | 0.182530 | 0.023* |
| H4B       | 0.922392 | 0.845773 | 0.090037 | 0.023* |
| C5        | 0.8904 (3) | 0.6186 (3) | 0.1667 (2) | 0.0268 (5) |
| H5A       | 0.802277 | 0.560658 | 0.203777 | 0.040* |
| H5B       | 0.975985 | 0.614518 | 0.210455 | 0.040* |
| H5C       | 0.930249 | 0.571616 | 0.111832 | 0.040* |
| C6        | 0.3003 (3) | 0.7693 (3) | 0.01381 (19) | 0.0190 (4) |
| H6A       | 0.251033 | 0.845711 | -0.041004 | 0.023* |
| H6B       | 0.244648 | 0.783981 | 0.076250 | 0.023* |
| C7        | 0.2815 (3) | 0.6044 (3) | 0.0029 (2) | 0.0253 (5) |
| H7A       | 0.335813 | 0.590123 | -0.059152 | 0.038* |
| H7B       | 0.168425 | 0.588003 | 0.002906 | 0.038* |
| H7C       | 0.328132 | 0.528699 | 0.057982 | 0.038* |
| C8        | 0.3723 (3) | 0.6350 (3) | 0.37528 (17) | 0.0164 (4) |
| C9        | 0.2739 (3) | 0.4672 (3) | 0.50878 (17) | 0.0175 (4) |
| C10       | 0.2644 (3) | 0.6105 (3) | 0.53014 (17) | 0.0190 (4) |
| H10       | 0.223233 | 0.636119 | 0.589902 | 0.023* |
| C11       | 0.3707 (3) | 0.3610 (3) | 0.35936 (19) | 0.0208 (4) |
| H11A      | 0.380137 | 0.258081 | 0.406376 | 0.025* |
| H11B      | 0.472452 | 0.376079 | 0.319289 | 0.025* |
| C12       | 0.2385 (4) | 0.3624 (3) | 0.2928 (2) | 0.0292 (6) |
| H12A      | 0.137555 | 0.348228 | 0.332223 | 0.044* |
| H12B      | 0.260413 | 0.277190 | 0.258600 | 0.044* |
H12C 0.231993 0.462511 0.244325 0.044*
C13 0.3265 (3) 0.8808 (3) 0.43601 (19) 0.0204 (4)
H13A 0.0407523 0.923764 0.383801 0.024*
H13B 0.354381 0.903198 0.498325 0.024*
C14 0.3265 (4) 0.8808 (3) 0.4096 (3) 0.0367 (7)
H14A 0.0410898 0.949089 0.346040 0.055*
H14B 0.166327 1.070607 0.405280 0.055*
H14C 0.085156 0.913349 0.460390 0.055*

Atomic displacement parameters (Å²)

|     | U¹¹ | U²² | U³³ | U¹² | U¹³ | U²³ |
|-----|-----|-----|-----|-----|-----|-----|
| Au1 | 0.01531 (4) | 0.01589 (4) | 0.01371 (4) | −0.00177 (3) | 0.00196 (3) | −0.00363 (3) |
| I1  | 0.02119 (7) | 0.02104 (7) | 0.01555 (6) | 0.00120 (5) | 0.00096 (5) | −0.00454 (5) |
| Br1 | 0.01523 (10) | 0.02506 (11) | 0.01603 (9) | −0.00645 (8) | 0.00254 (7) | −0.00658 (8) |
| Br2 | 0.03080 (13) | 0.02037 (11) | 0.01701 (10) | −0.00987 (9) | −0.00213 (9) | −0.00004 (8) |
| N1  | 0.0136 (8) | 0.0164 (8) | 0.0137 (8) | −0.0021 (6) | 0.0003 (6) | −0.0045 (6) |
| N2  | 0.0129 (8) | 0.0163 (8) | 0.0155 (8) | −0.0007 (6) | 0.0000 (6) | −0.0031 (7) |
| N3  | 0.0170 (8) | 0.0159 (8) | 0.0149 (8) | −0.0017 (7) | −0.0007 (6) | −0.0040 (7) |
| N4  | 0.0204 (9) | 0.0153 (8) | 0.0148 (8) | −0.0032 (7) | −0.0003 (7) | −0.0035 (7) |
| C1  | 0.0139 (9) | 0.0155 (9) | 0.0165 (9) | −0.0023 (7) | 0.0017 (7) | −0.0046 (7) |
| C2  | 0.0152 (9) | 0.0172 (9) | 0.0128 (8) | −0.0035 (7) | 0.0011 (7) | −0.0038 (7) |
| C3  | 0.0149 (9) | 0.0178 (10) | 0.0153 (9) | −0.0021 (7) | 0.0001 (7) | −0.0045 (8) |
| C4  | 0.0176 (10) | 0.0256 (11) | 0.0157 (9) | −0.0056 (8) | −0.0020 (8) | −0.0070 (8) |
| C5  | 0.0241 (12) | 0.0309 (14) | 0.0253 (12) | 0.0050 (10) | −0.0074 (10) | −0.0065 (10) |
| C6  | 0.0119 (9) | 0.0231 (11) | 0.0217 (10) | −0.0001 (8) | −0.0017 (8) | −0.0049 (9) |
| C7  | 0.0201 (11) | 0.0243 (12) | 0.0330 (13) | −0.0066 (9) | −0.0003 (10) | −0.0081 (10) |
| C8  | 0.0153 (9) | 0.0167 (9) | 0.0169 (9) | −0.0016 (7) | −0.0004 (7) | −0.0036 (8) |
| C9  | 0.0211 (10) | 0.0171 (10) | 0.0136 (9) | −0.0045 (8) | −0.0012 (8) | −0.0011 (8) |
| C10 | 0.0218 (11) | 0.0199 (10) | 0.0151 (9) | −0.0047 (8) | 0.0014 (8) | −0.0037 (8) |
| C11 | 0.0251 (12) | 0.0174 (10) | 0.0212 (11) | −0.0008 (9) | −0.0005 (9) | −0.0075 (9) |
| C12 | 0.0391 (16) | 0.0252 (13) | 0.0264 (13) | −0.0052 (11) | −0.0088 (11) | −0.0085 (10) |
| C13 | 0.0271 (12) | 0.0143 (10) | 0.0200 (10) | −0.0054 (8) | 0.0024 (9) | −0.0042 (8) |
| C14 | 0.0328 (16) | 0.0179 (12) | 0.056 (2) | 0.0019 (11) | −0.0004 (14) | −0.0034 (13) |

Geometric parameters (Å, °)

|     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|
| Au1—C1 | 2.020 (2) | C13—C14 | 1.506 (4) |
| Au1—C8 | 2.022 (2) | C3—H3 | 0.9500 |
| I1—Br1¹ | 3.5294 (3) | C4—H4A | 0.9900 |
| I1—Br2 | 3.6072 (3) | C4—H4B | 0.9900 |
| Au1—Br2² | 3.8033 (3) | C5—H5A | 0.9800 |
| Br1—C2 | 1.869 (2) | C5—H5B | 0.9800 |
| Br2—C9 | 1.861 (2) | C5—H5C | 0.9800 |
| N1—C1 | 1.357 (3) | C6—H6A | 0.9900 |
| N1—C2 | 1.382 (3) | C6—H6B | 0.9900 |
| N1—C4 | 1.468 (3) | C7—H7A | 0.9800 |
| N2—C1 | 1.348 (3) | C7—H7B | 0.9800 |

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| Bond          | Length   | Bond          | Length   |
|---------------|----------|---------------|----------|
| N2—C3         | 1.381 (3) | C7—H7C       | 0.9800   |
| N2—C6         | 1.468 (3) | C10—H10      | 0.9500   |
| N3—C8         | 1.354 (3) | C11—H11A     | 0.9900   |
| N3—C9         | 1.382 (3) | C11—H11B     | 0.9900   |
| N3—C11        | 1.464 (3) | C12—H12A     | 0.9800   |
| N4—C8         | 1.351 (3) | C12—H12B     | 0.9800   |
| N4—C10        | 1.381 (3) | C12—H12C     | 0.9800   |
| N4—C13        | 1.469 (3) | C13—H13A     | 0.9900   |
| C2—C3         | 1.357 (3) | C13—H13B     | 0.9900   |
| C4—C5         | 1.518 (4) | C14—H14A     | 0.9800   |
| C6—C7         | 1.521 (4) | C14—H14B     | 0.9800   |
| C9—C10        | 1.361 (3) | C14—H14C     | 0.9800   |
| C11—C12       | 1.512 (4) |               |          |

| Bond          | Angle     |
|---------------|-----------|
| C1—Au1—C8    | 174.97 (9) |
| Br1—I1—Br2   | 101.436 (8) |
| C2—Br1—I1   | 172.43 (7) |
| C9—Br2—I1   | 162.21 (8) |
| C1—N1—C2    | 109.82 (19) |
| C1—N1—C4    | 123.48 (19) |
| C2—N1—C4    | 126.65 (19) |
| C1—N2—C3    | 111.61 (19) |
| C1—N2—C6    | 124.54 (19) |
| C3—N2—C6    | 123.46 (19) |
| C8—N3—C9    | 110.15 (19) |
| C8—N3—C11   | 123.4 (2)   |
| C9—N3—C11   | 126.4 (2)   |
| C8—N4—C10   | 111.1 (2)   |
| C8—N4—C13   | 124.9 (2)   |
| C10—N4—C13  | 123.7 (2)   |
| N2—C1—N1    | 105.25 (19) |
| N2—C1—Au1   | 127.11 (16) |
| N1—C1—Au1   | 127.41 (17) |
| C3—C2—N1    | 107.77 (19) |
| C3—C2—Br1   | 128.16 (17) |
| N1—C2—Br1   | 124.05 (17) |
| C2—C3—N2    | 105.6 (2)   |
| N1—C4—C5    | 112.1 (2)   |
| N2—C6—C7    | 110.9 (2)   |
| N4—C8—N3    | 105.41 (19) |
| N4—C8—Au1   | 130.27 (17) |
| N3—C8—Au1   | 124.30 (17) |
| C10—C9—N3   | 107.3 (2)   |
| C10—C9—Br2  | 130.48 (18) |
| N3—C9—Br2   | 122.09 (17) |
| C9—C10—N4   | 106.0 (2)   |
| N3—C11—C12  | 111.5 (2)   |
| N4—C13—C14  | 110.6 (2)   |

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### C2—C3—H3

|         | C2—C3—H3 | H13A—C13—H13B | 108.1 |
|---------|-----------|----------------|-------|

### N2—C3—H3

|         | N2—C3—H3 | C13—C14—H14A | 109.5 |
|---------|-----------|---------------|-------|

### N1—C4—H4A

|         | N1—C4—H4A | C13—C14—H14B | 109.5 |
|---------|------------|---------------|-------|

### C5—C4—H4A

|         | C5—C4—H4A | H14A—C14—H14B | 109.5 |
|---------|------------|----------------|-------|

### C1—that is, H4B

|         | C1—that is, H4B | C13—C14—H14C | 109.5 |
|---------|-----------------|---------------|-------|

### C5—that is, H4B

|         | C5—that is, H4B | H14A—C14—H14C | 109.5 |
|---------|-----------------|---------------|-------|

### H4A—that is, H4B

|         | H4A—that is, H4B | H14B—C14—H14C | 109.5 |
|---------|------------------|---------------|-------|

### C3—N2—C1—N1

|         | C3—N2—C1—N1 | C13—N4—C8—N3 | −175.0 (2) |
|---------|--------------|---------------|-----------|

### C6—N2—C1—N1

|         | C6—N2—C1—N1 | C10—N4—C8—Au1 | 177.04 (18) |
|---------|--------------|----------------|------------|

### C3—that is, C1—Au1

|         | C3—that is, C1—Au1 | C13—N4—C8—Au1 | 3.3 (4) |
|---------|---------------------|----------------|--------|

### C6—that is, C1—Au1

|         | C6—that is, C1—Au1 | C9—N3—C8—N4 | 1.3 (3) |
|---------|--------------------|---------------|--------|

### C2—that is, N1—C1—N2

|         | C2—that is, N1—C1—N2 | C11—N3—C8—N4 | 178.8 (2) |
|---------|-----------------------|---------------|----------|

### C4—that is, N1—C1—N2

|         | C4—that is, N1—C1—N2 | C9—N3—C8—Au1 | −177.17 (17) |
|---------|-----------------------|---------------|-----------|

### C2—that is, N1—C1—Au1

|         | C2—that is, N1—C1—Au1 | C11—N3—C8—Au1 | 0.4 (3) |
|---------|------------------------|---------------|--------|

### C4—that is, N1—C1—Au1

|         | C4—that is, N1—C1—Au1 | C8—N3—C9—C10 | −0.8 (3) |
|---------|------------------------|---------------|--------|

### C1—that is, N1—C2—C3

|         | C1—that is, N1—C2—C3 | C11—N3—C9—C10 | −178.3 (2) |
|---------|-----------------------|---------------|----------|

### C4—that is, N1—C2—C3

|         | C4—that is, N1—C2—C3 | C8—N3—C9—Br2 | −177.42 (17) |
|---------|-----------------------|---------------|-----------|

### C1—that is, N1—C2—Br1

|         | C1—that is, N1—C2—Br1 | C11—N3—C9—Br2 | 5.1 (3) |
|---------|------------------------|---------------|--------|

### C4—that is, N1—C2—Br1

|         | C4—that is, N1—C2—Br1 | II—Br2—C9—C10 | −114.8 (3) |
|---------|------------------------|---------------|----------|

### N1—that is, C2—C3—N2

|         | N1—that is, C2—C3—N2 | C11—N3—C9—N3 | 96.4 (3) |
|---------|-----------------------|---------------|---------|

### Br1—that is, C2—C3—N2

|         | Br1—that is, C2—C3—N2 | C9—N3—C10—N4 | 0.0 (3) |
|---------|------------------------|---------------|--------|

### C1—that is, N2—C3—C2

|         | C1—that is, N2—C3—C2 | Br2—C9—C10—N4 | 176.24 (19) |
|---------|-----------------------|---------------|---------|

### C6—that is, N2—C3—C2

|         | C6—that is, N2—C3—C2 | C8—N4—C10—C9 | 0.8 (3) |
|---------|-----------------------|---------------|--------|

### C1—that is, N1—C4—C5

|         | C1—that is, N1—C4—C5 | C13—N4—C10—C9 | 174.6 (2) |
|---------|-----------------------|---------------|---------|

### C2—that is, N1—C4—C5

|         | C2—that is, N1—C4—C5 | C8—N3—C11—C12 | −80.8 (3) |
|---------|-----------------------|---------------|---------|

### C1—that is, N2—C6—C7

|         | C1—that is, N2—C6—C7 | C9—N3—C11—C12 | 96.4 (3) |
|---------|-----------------------|---------------|---------|

### C3—that is, N2—C6—C7

|         | C3—that is, N2—C6—C7 | C8—N4—C13—C14 | 94.0 (3) |
|---------|-----------------------|---------------|---------|

### C10—that is, N4—C8—N3

|         | C10—that is, N4—C8—N3 | C10—N4—C13—C14 | −79.0 (3) |
|---------|-----------------------|---------------|---------|

---

### Hydrogen-bond geometry (Å, °)

| D—H···A   | D—H       | H···A     | D···A     | D—H···A   |
|-----------|-----------|-----------|-----------|-----------|
| C3—H3···I1v | 0.95      | 3.15      | 3.966 (2) | 145       |
| C4—H4···I1v | 0.99      | 3.10      | 3.995 (3) | 151       |
| C6—H6···I1w | 0.99      | 3.21      | 3.955 (3) | 134       |
| C10—H10···I1v | 0.95     | 3.20      | 3.993 (2) | 142       |
| C11—H11···Br2 | 0.99    | 2.79      | 3.265 (3) | 110       |
| C11—H11B···I1v | 0.99    | 3.19      | 3.903 (3) | 130       |
| C12—H12B···Br1vii | 0.98   | 3.06      | 3.831 (3) | 137       |
| C13—H13B···I1v | 0.99     | 3.19      | 4.053 (3) | 146       |

---

Symmetry codes: (i) x−1, y−1, z+1; (ii) −x+1, −y+1, −z+1; (iii) x+1, y+1, z−1.

Symmetry codes: (ii) −x+1, −y+1, −z+1; (iv) x, y+1, z−1; (v) y, y+1, z; (vi) −x+1, −y, −z+1; (vii) −x+1, −y+1, −z. 
Bis(4-bromo-1,3-diethylimidazol-2-ylidene)gold(I) trans-bis(4-bromo-1,3-diethyl-imidazol-2-ylidene)diiodidogold(III) diiodide (4)

Crystal data

\[
\begin{align*}
&[\text{Au(C}_7\text{H}_11\text{BrN}_2)_2][\text{AuI}_2(\text{C}_7\text{H}_11\text{BrN}_2)_2]\text{I}_2 \\
&M_r = 1713.88 \\
&\text{Triclinic, } P\bar{1} \\
&a = 8.0245 (4) \text{ Å} \\
&b = 8.5782 (3) \text{ Å} \\
&c = 15.9814 (6) \text{ Å} \\
&\alpha = 91.228 (3)^\circ \\
&\beta = 96.517 (4)^\circ \\
&\gamma = 92.255 (4)^\circ \\
&V = 1091.77 (8) \text{ Å}^3 \\
&Z = 1 \\
&F(000) = 778 \\
&D_a = 2.607 \text{ Mg m}^{-3} \\
&\text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} \\
&\text{Cell parameters from 24546 reflections} \\
&\theta = 2.6–34.1^\circ \\
&\mu = 13.23 \text{ mm}^{-1} \\
&T = 100 \text{ K} \\
&\text{Plate, brown} \\
&\text{Plate, brown} \\
&0.08 \times 0.03 \times 0.01 \text{ mm} \\
\end{align*}
\]

Data collection

XtaLAB Synergy, HyPix diffractometer

Radiation source: micro-focus sealed X-ray tube

Detector resolution: 10.0000 pixels mm\(^{-1}\)

\(\omega\) scans

Absorption correction: multi-scan

(CrystalPro; Rigaku OD, 2021)

\(\theta_m = 0.703, \theta_m = 1.000\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2\sigma(F^2)] = 0.039\)

\(wR(F') = 0.105\)

\(S = 1.06\)

61886 measured reflections

6378 independent reflections

5409 reflections with \(I > 2\sigma(I)\)

\(R_{int} = 0.048\)

\(\theta_m = 30.0^\circ, \theta_m = 2.7^\circ\)

\(h = -11\rightarrow 11\)

\(k = -12\rightarrow 12\)

\(l = -22\rightarrow 22\)

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\(w = 1/[\sigma(F^2) + (0.0494P)^2 + 12.4607P]\)

where \(P = (F^2 + 2F_c^2)/3\)

\((\Delta\sigma)_{\text{max}} = 0.001\)

\(\Delta\rho_{\text{max}} = 3.97 \text{ e Å}^{-3}\)

\(\Delta\rho_{\text{min}} = -2.66 \text{ e Å}^{-3}\)

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 (Å\(^2\))

\[
\begin{array}{cccccc}
& x & y & z & U_{eq} & U_{eq} \\
\text{Au1} & -0.50000 & 0.50000 & 0.00000 & 0.01890 (8) \\
\text{I1} & -0.36292 (6) & -0.37952 (6) & -0.12916 (3) & 0.02666 (11) \\
\text{Br1} & -0.00401 (10) & -0.09434 (9) & 0.21316 (5) & 0.02965 (16) \\
\text{N1} & -0.2548 (7) & -0.2807 (7) & 0.1082 (4) & 0.0227 (11) \\
\text{N2} & -0.1732 (7) & -0.5172 (7) & 0.1164 (4) & 0.0218 (11) \\
\text{C1} & -0.2957 (9) & -0.4283 (8) & 0.0806 (4) & 0.0199 (12) \\
\text{C2} & -0.1053 (9) & -0.2781 (8) & 0.1624 (4) & 0.0236 (13) \\
\text{C3} & -0.0556 (9) & -0.4261 (8) & 0.1680 (4) & 0.0242 (13) \\
\end{array}
\]

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### Atomic displacement parameters (Å²)

|       | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-------|--------------|--------------|--------------|--------------|--------------|--------------|
| Au1   | 0.02247 (17) | 0.01893 (16) | 0.01489 (15) | −0.00122 (12)| 0.00110 (12) | 0.00024 (12) |
| I1    | 0.0288 (2)   | 0.0301 (2)   | 0.0214 (2)   | −0.00043 (18)| 0.00418 (16) | 0.00327 (17) |
| Br1   | 0.0348 (4)   | 0.0248 (3)   | 0.0272 (3)   | −0.0053 (3)  | −0.0026 (3)  | −0.0047 (3)  |
| N1    | 0.025 (3)    | 0.023 (3)    | 0.020 (3)    | 0.000 (2)    | 0.004 (2)    | −0.002 (2)   |
| N2    | 0.022 (3)    | 0.021 (3)    | 0.021 (3)    | −0.002 (2)   | −0.001 (2)   | −0.003 (2)   |
| C1    | 0.028 (3)    | 0.018 (3)    | 0.013 (3)    | −0.002 (2)   | 0.002 (2)    | −0.001 (2)   |
| Atom | U1  | U2  | U3  | U12 | U13 | U23 |
|------|-----|-----|-----|-----|-----|-----|
| C2   | 0.028 (3) | 0.024 (3) | 0.018 (3) | −0.004 (3) | 0.001 (2) | −0.003 (2) |
| C3   | 0.028 (3) | 0.027 (3) | 0.017 (3) | 0.000 (3) | 0.000 (2) | −0.004 (2) |
| C4   | 0.039 (4) | 0.019 (3) | 0.025 (3) | −0.001 (3) | 0.000 (3) | −0.002 (3) |
| C5   | 0.051 (5) | 0.035 (4) | 0.042 (5) | 0.004 (4) | 0.014 (4) | −0.008 (4) |
| C6   | 0.028 (3) | 0.021 (3) | 0.024 (3) | 0.001 (3) | 0.002 (3) | 0.000 (3) |
| C7   | 0.042 (5) | 0.031 (4) | 0.031 (4) | 0.005 (3) | 0.005 (3) | −0.007 (3) |
| Au2  | 0.02690 (18) | 0.01581 (16) | 0.01892 (16) | 0.00103 (12) | −0.00311 (13) | −0.00180 (12) |
| I2   | 0.0231 (2) | 0.0219 (2) | 0.0252 (2) | −0.00092 (15) | −0.00093 (16) | −0.00113 (16) |
| Br2  | 0.0266 (3) | 0.0199 (3) | 0.0267 (3) | −0.0050 (2) | 0.0032 (3) | −0.0015 (2) |
| N1'  | 0.028 (3) | 0.014 (2) | 0.017 (2) | −0.001 (2) | 0.001 (2) | 0.0007 (19) |
| N2'  | 0.028 (3) | 0.015 (2) | 0.022 (3) | 0.001 (2) | −0.001 (2) | −0.002 (2) |
| C1'  | 0.031 (3) | 0.014 (3) | 0.015 (3) | 0.004 (2) | 0.000 (2) | 0.000 (2) |
| C2'  | 0.024 (3) | 0.020 (3) | 0.022 (3) | 0.000 (2) | 0.005 (2) | 0.000 (2) |
| C3'  | 0.025 (3) | 0.017 (3) | 0.021 (3) | 0.000 (2) | −0.002 (2) | −0.002 (2) |
| C4'  | 0.026 (3) | 0.016 (3) | 0.026 (3) | 0.007 (2) | 0.008 (3) | 0.002 (2) |
| C5'  | 0.031 (4) | 0.019 (3) | 0.039 (4) | 0.008 (3) | 0.010 (3) | 0.001 (3) |
| C6'  | 0.031 (4) | 0.015 (3) | 0.029 (3) | 0.002 (3) | −0.005 (3) | −0.001 (3) |
| C7'  | 0.025 (3) | 0.022 (3) | 0.038 (4) | 0.000 (3) | 0.008 (3) | 0.008 (3) |

**Geometric parameters (Å, †)**

| Bond/Distance | Length/Angle |
|---------------|-------------|
| Au1—C1i       | 2.033 (7)    | N2′—C6′      | 1.459 (9)    |
| Au1—C1        | 2.033 (7)    | C2′—C3′       | 1.519 (9)    |
| Au1—I1i       | 2.6564 (5)   | C4′—C5′       | 1.519 (10)   |
| Au1—I1        | 2.6564 (5)   | C6′—C7′       | 1.519 (11)   |
| I1—I2ii       | 3.5136 (7)   | C3—H3         | 0.9500       |
| Br1—C2        | 1.870 (7)    | C4—H4A        | 0.9900       |
| Br1—I2        | 3.4347 (8)   | C4—H4B        | 0.9900       |
| N1—C1         | 1.347 (8)    | C5—H5A        | 0.9800       |
| N1—C2         | 1.397 (9)    | C5—H5B        | 0.9800       |
| N1—C4         | 1.464 (10)   | C5—H5C        | 0.9800       |
| N2—C1         | 1.351 (9)    | C6—H6A        | 0.9900       |
| N2—C3         | 1.385 (8)    | C6—H6B        | 0.9900       |
| N2—C6         | 1.479 (9)    | C7—H7A        | 0.9800       |
| C2—C3         | 1.348 (10)   | C7—H7B        | 0.9800       |
| C4—C5         | 1.530 (12)   | C7—H7C        | 0.9800       |
| C6—C7         | 1.504 (11)   | C3′—H3′       | 0.9500       |
| Au2—C1'       | 2.018 (7)    | C4′—H4’1      | 0.9900       |
| Au2—C1″ii     | 2.018 (7)    | C4′—H4’2      | 0.9900       |
| I2—Br2        | 3.5575 (8)   | C5′—H5’1      | 0.9800       |
| I2—Au1"      | 4.1539 (5)   | C5′—H5’2      | 0.9800       |
| Br2—C2"      | 1.871 (7)    | C5′—H5’3      | 0.9800       |
| N1′—C1'       | 1.360 (8)    | C6′—H6’1      | 0.9900       |
| N1′—C2"      | 1.383 (9)    | C6′—H6’2      | 0.9900       |
| N1′—C4"      | 1.469 (8)    | C7′—H7’1      | 0.9800       |
| N2′—C1'       | 1.354 (9)    | C7′—H7’2      | 0.9800       |
| N2′—C3"      | 1.386 (9)    | C7′—H7’3      | 0.9800       |
C1′—Au1—C1    180.0     N2—C3—H3    126.7
C1′—Au1—Ii    90.95 (18)     N1—C4—H4A    109.1
C1—Au—Ii    89.05 (18)     C5—C4—H4A    109.1
C1′—Au—Ii    89.05 (18)     N1—C4—H4B    109.1
C1—Au—Ii    90.95 (18)     C5—C4—H4B    109.1
Ii′—Au—Ii    180.0     H4A—C4—H4B    107.8
Au—Iii—I2vii    176.29 (2)     C4—C5—H5A    109.5
C2—Br—I2    179.5 (2)     C4—C5—H5B    109.5
C1—N1—C2    109.5 (6)     H5A—C5—H5B    109.5
C1—N1—C4    124.8 (6)     C4—C5—H5C    109.5
C2—N1—C4    125.3 (6)     H5A—C5—H5C    109.5
C1—N2—C3    110.4 (6)     H5B—C5—H5C    109.5
C1—N2—C6    125.6 (6)     N2—C6—H6A    109.3
C3—N2—C6    124.0 (6)     C7—C6—H6A    109.3
N1—C1—N2    106.2 (6)     N2—C6—H6B    109.3
N1—C1—Au1    126.4 (5)     C7—C6—H6B    109.3
N2—C1—Au1    127.4 (5)     H6A—C6—H6B    107.9
C3—C2—N1    107.2 (6)     C6—C7—H7A    109.5
C3—C2—Br1    129.9 (6)     C6—C7—H7B    109.5
N1—C2—Br1    122.9 (5)     H7A—C7—H7B    109.5
C2—C3—N2    106.6 (6)     C6—C7—H7C    109.5
N1—C4—C5    112.6 (7)     H7A—C7—H7C    109.5
N2—C6—C7    111.8 (6)     H7B—C7—H7C    109.5
C1′—Au2—C1′ivii    180.0     C2′—C3′—H3'    127.0
Br1—I2—Iiiv    97.240 (19)     N2′—C3′—H3'    127.0
Br1—I2—Br2    169.87 (2)     N1′—C4′—H4'1    109.3
Ii′—I2—Br2    72.852 (17)     C5′—C4′—H4'1    109.3
Br1—I2—Au2iv    74.604 (16)     N1′—C4′—H4'2    109.3
Ii′—I2—Au2iv    168.488 (16)     C5′—C4′—H4'2    109.3
Br2—I2—Au2iv    114.871 (16)     H4'1—C4′—H4'2    108.0
C2′—Br2—I2    177.0 (2)     C4′—C5′—H5'1    109.5
C1′—N1′—C2′    110.4 (6)     C4′—C5′—H5'2    109.5
C1′—N1′—C4′    123.3 (6)     H5′1—C5′—H5′2    109.5
C2′—N1′—C4′    126.1 (6)     C4′—C5′—H5’3    109.5
C1′—N2′—C3′    111.4 (6)     H5′1—C5′—H5’3    109.5
C1′—N2′—C6′    124.9 (6)     H5′2—C5′—H5’3    109.5
C3′—N2′—C6′    123.3 (6)     N2′—C6′—H6’1    109.4
N2′—C1′—N1′    104.7 (6)     C7′—C6′—H6’1    109.4
N2′—C1′—Au2    128.9 (5)     N2′—C6′—H6’2    109.4
N1′—C1′—Au2    126.4 (5)     C7′—C6′—H6’2    109.4
C3′—C2′—N1′    107.4 (6)     H6’1—C6′—H6’2    108.0
C3′—C2′—Br2    128.7 (5)     C6′—C7′—H7’1    109.5
N1′—C2′—Br2    123.9 (5)     C6′—C7′—H7’2    109.5
C2′—C3′—N2′    105.9 (6)     H7’1—C7′—H7’2    109.5
N1′—C4′—C5′    111.4 (6)     C6′—C7′—H7’3    109.5
N2′—C6′—C7′    111.0 (6)     H7’1—C7′—H7’3    109.5
C2—C3—H3    126.7     H7’2—C7′—H7’3    109.5

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C2—N1—C1—N2  
C4—N1—C1—N2  
C2—N1—C1—Au1  
C4—N1—C1—Au1  
C3—N2—C1—N1  
C6—N2—C1—N1  
C3—N2—C1—Au1  
C6—N2—C1—Au1  
C1—N1—C2—C3  
C4—N1—C2—C3  
C1—N1—C2—Br1  
C4—N1—C2—Br1  
C1—N2—C3—N2  
Br1—C2—C3—N2  
C1—N2—C3—C2  
C6—N2—C3—C2  
C1—N1—C4—C5  
C2—N1—C4—C5  
C1—N2—C6—C7  
C3—N2—C6—C7  

C3’—N2’—C1’—N1’  
C6’—N2’—C1’—Au2  
C3’—N1’—C1’—N2’  
C6’—N1’—C1’—Au2  
C1’—N1’—C2’—C3’  
C4’—N1’—C2’—C3’  
C1’—N1’—C2’—Br2  
C4’—N1’—C2’—Br2  
N1’—C2’—C3’—N2’  
Br2—C2’—C3’—N2’  
C1’—N2’—C3’—C2’  
C6’—N2’—C3’—C2’  
C1’—N1’—C4’—C5’  
C2’—N1’—C4’—C5’  
C1’—N2’—C6’—C7’  
C3’—N2’—C6’—C7’  

Symmetry codes: (i) −x, −y, −z; (ii) −x, −y, −z; (iii) −x+2, −y+2, −z+1; (iv) x, y−1, z.

Hydrogen-bond geometry (Å, °)

| D—H···A     |  D—H | H···A | D···A | D—H···A |
|-------------|------|------|-------|---------|
| C3—H3···I1v | 0.95 | 3.28 | 3.913 (7) | 126 |
| C3—H3···I2vi| 0.95 | 3.22 | 4.011 (7) | 142 |
| C4—H4.4···I1| 0.99 | 3.28 | 4.002 (7) | 132 |
| C6—H6.4···I1| 0.99 | 3.16 | 3.925 (7) | 136 |
| C6—H6.8···I2vi| 0.99 | 3.11 | 4.064 (7) | 163 |
| C7—H7C···I1v| 0.98 | 3.29 | 4.051 (9) | 136 |
| C3’—H3’···I2vi| 0.95 | 3.08 | 3.916 (7) | 148 |
| C4’—H4’2···I2viii| 0.99 | 3.10 | 3.883 (7) | 137 |
| C7’—H7’1···I2ix| 0.98 | 3.19 | 4.039 (7) | 146 |

Symmetry codes: (i) −x, −y, −z; (v) −x, −y, −z; (vi) x, y−1, z; (vii) x, y+1, z; (viii) −x+1, −y+1, −z+1; (ix) x+1, y+1, z.