

Supplementary Information for

Bismuth halide perovskite derivatives for direct X-ray detection

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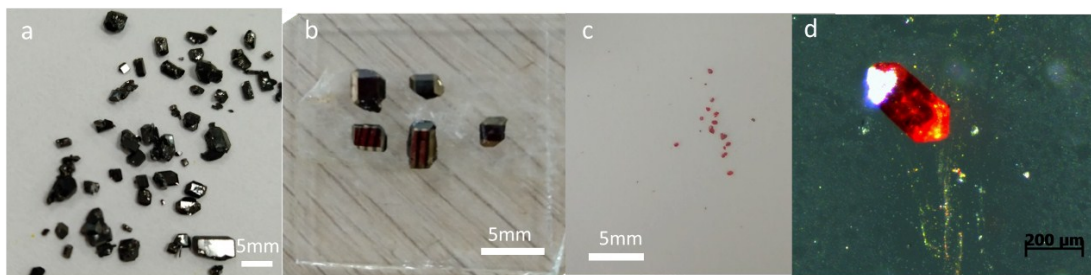


Figure S1 (a) The photo of as-grown black single crystals ((DMEDA)Bi₅). (b) The photo of selected black single crystals (the yellow stripes on the surface of the black single crystals are Au electrodes used for different tried device structures). (c) The photo of as-grown red single crystals ((DMEDA)_{1.5}Bi₆). (d) The embodiment microscope picture of one selected red single crystal with relatively regular shape. The scale sizes are provided in the corresponding pictures.

Table S1 Bond lengths for (DMEDA)Bi₅ and (DMEDA)_{1.5}Bi₆

| (DMEDA)Bi ₅ | | | (DMEDA) _{1.5} Bi ₆ | | |
|--|---------------------|------------|---|--------------------|------------|
| Atom | Atom | Length (Å) | Atom | Atom | Length (Å) |
| Bi(01) | I(002) | 2.9984(14) | Bi(1) | I(2) ¹ | 2.9770(7) |
| Bi(01) | I(003) | 3.1589(13) | Bi(1) | I(2) ² | 2.9770(7) |
| Bi(01) | I(004) | 2.9430(9) | Bi(1) | I(2) | 2.9770(7) |
| Bi(01) | I(004) ¹ | 2.9430(9) | Bi(1) | I(1) ² | 3.1988(7) |
| Bi(01) | I(005) | 3.2106(6) | Bi(1) | I(1) | 3.1987(7) |
| Bi(01) | I(005) ² | 3.2106(6) | Bi(1) | I(1) ¹ | 3.1988(7) |
| N(1) | C(3) | 1.505(19) | N(1) | C(2) | 1.457(19) |
| N(1) | C(4) | 1.52(2) | N(1) | C(1A) | 1.60(3) |
| N(2) | C(5) | 1.548(19) | C(1A) | C(1A) ³ | 1.517(19) |
| N(2) | C(11) | 1.50(2) | | | |
| C(3) | C(5) | 1.50(2) | | | |
| ¹ +X,1/2-Y,+Z; ² 1-X,1/2+Y,1-Z | | | ¹ 1+Y-X,1-X,+Z; ² 1-Y,+X-Y,+Z; ³ 4/3-X,2/3-X+Y,7/6-Z | | |

Table S2 Bond Angles for (DMEDA)BiI₅ and (DMEDA)_{1.5}BiI₆

| (DMEDA) BiI ₅ | | | | (DMEDA) _{1.5} BiI ₆ | | | |
|--|--------|---------------------|------------|---|-------|-------------------|-----------|
| Atom | Atom | Atom | Angle (°) | Atom | Atom | Atom | Angle (°) |
| I(002) | Bi(01) | I(003) | 175.52(4) | I(2) ¹ | Bi(1) | I(2) ² | 95.31(2) |
| I(002) | Bi(01) | I(005) ¹ | 89.44(3) | I(2) ¹ | Bi(1) | I(2) | 95.31(2) |
| I(002) | Bi(01) | I(005) | 89.44(3) | I(2) ² | Bi(1) | I(2) | 95.31(2) |
| I(003) | Bi(01) | I(005) ¹ | 87.20(3) | I(2) | Bi(1) | I(1) | 86.82(2) |
| I(003) | Bi(01) | I(005) | 87.20(3) | I(2) ¹ | Bi(1) | I(1) | 174.57(3) |
| I(004) ² | Bi(01) | I(002) | 92.46(3) | I(2) ² | Bi(1) | I(1) ¹ | 174.57(3) |
| I(004) | Bi(01) | I(002) | 92.46(3) | I(2) ¹ | Bi(1) | I(1) ² | 89.45(2) |
| I(004) | Bi(01) | I(003) | 90.61(3) | I(2) ² | Bi(1) | I(1) | 89.45(2) |
| I(004) ² | Bi(01) | I(003) | 90.61(3) | I(2) | Bi(1) | I(1) ² | 174.57(3) |
| I(004) ² | Bi(01) | I(004) | 93.71(4) | I(2) | Bi(1) | I(1) ¹ | 89.45(2) |
| I(004) ² | Bi(01) | I(005) ¹ | 174.18(3) | I(2) ¹ | Bi(1) | I(1) ¹ | 86.82(2) |
| I(004) ² | Bi(01) | I(005) | 91.70(2) | I(2) ² | Bi(1) | I(1) ² | 86.82(2) |
| I(004) | Bi(01) | I(005) ¹ | 91.70(2) | I(1) ² | Bi(1) | I(1) ¹ | 88.21(2) |
| I(004) | Bi(01) | I(005) | 174.18(3) | I(1) ² | Bi(1) | I(1) | 88.21(2) |
| I(005) | Bi(01) | I(005) ¹ | 82.814(19) | I(1) | Bi(1) | I(1) ¹ | 88.21(2) |
| Bi(01) | I(005) | Bi(01) ³ | 180.0 | C(2) | N(1) | C(1A) | 123.7(13) |
| C(3) | N(1) | C(4) | 112(2) | C(1A) ³ | C(1A) | N(1) | 99(2) |
| C(5) | N(2) | C(11) | 111.8(19) | | | | |
| N(1) | C(3) | C(5) | 115(2) | | | | |
| N(2) | C(5) | C(3) | 111.9(19) | | | | |
| ¹ 1-X,1/2+Y,1-Z; ² 1-X,1/2-Y,+Z; ³ 1-X,-Y,1-Z | | | | ¹ 1+Y-X,1-X,+Z; ² 1-Y,+X-Y,+Z; ³ 4/3-X,2/3-X+Y,7/6-Z | | | |