Electronic Supplementary Material (ESI) for Dalton Transactions.


# Supporting Information

## Broadband White-Light Emission from Supramolecular Piperazinium-based Lead Halide Perovskites Linked by Hydrogen Bonds

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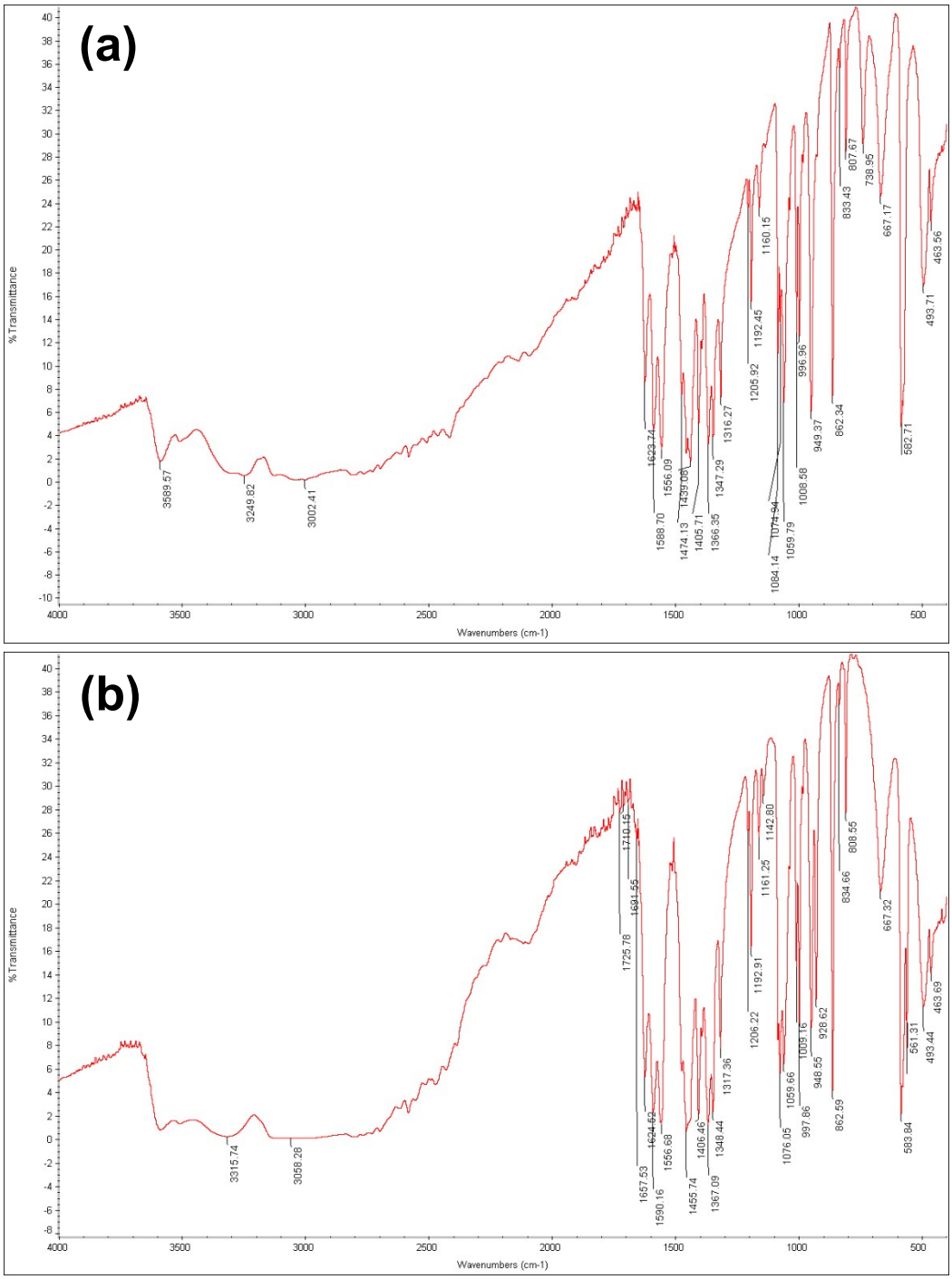


**Figure S1**. FT-IR of (a) $(pip)_2PbBr_6$ and (b) $(pip)_2Pb_4Cl_{12}$ perovskites

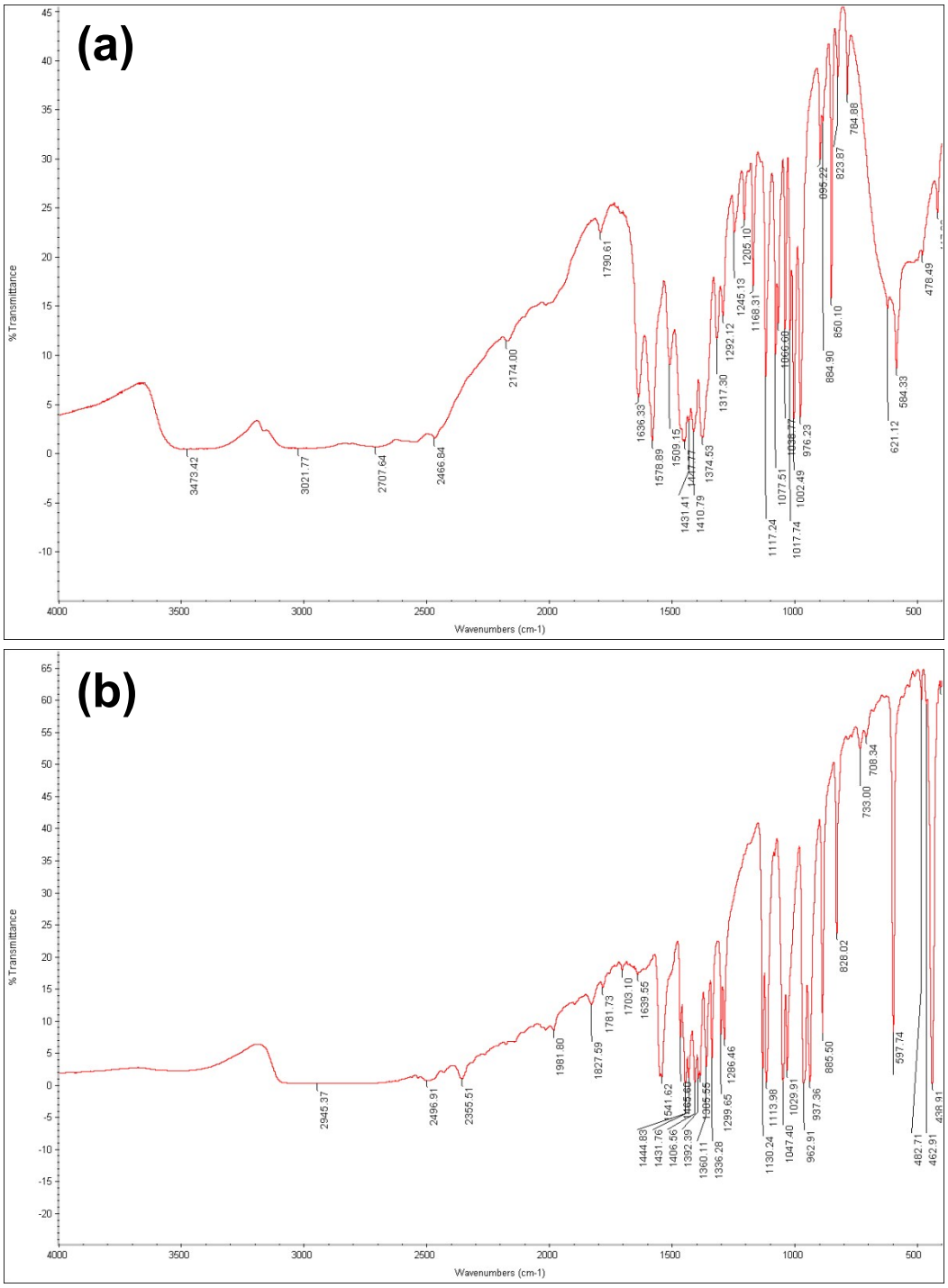


**Figure S2**. FT-IR of (a) $(1mpz)_2PbBr_6$ and (b) $(2,5\text{-}dmpz)_{0.5}PbBr_3 \cdot 2((CH_3)_2SO)$

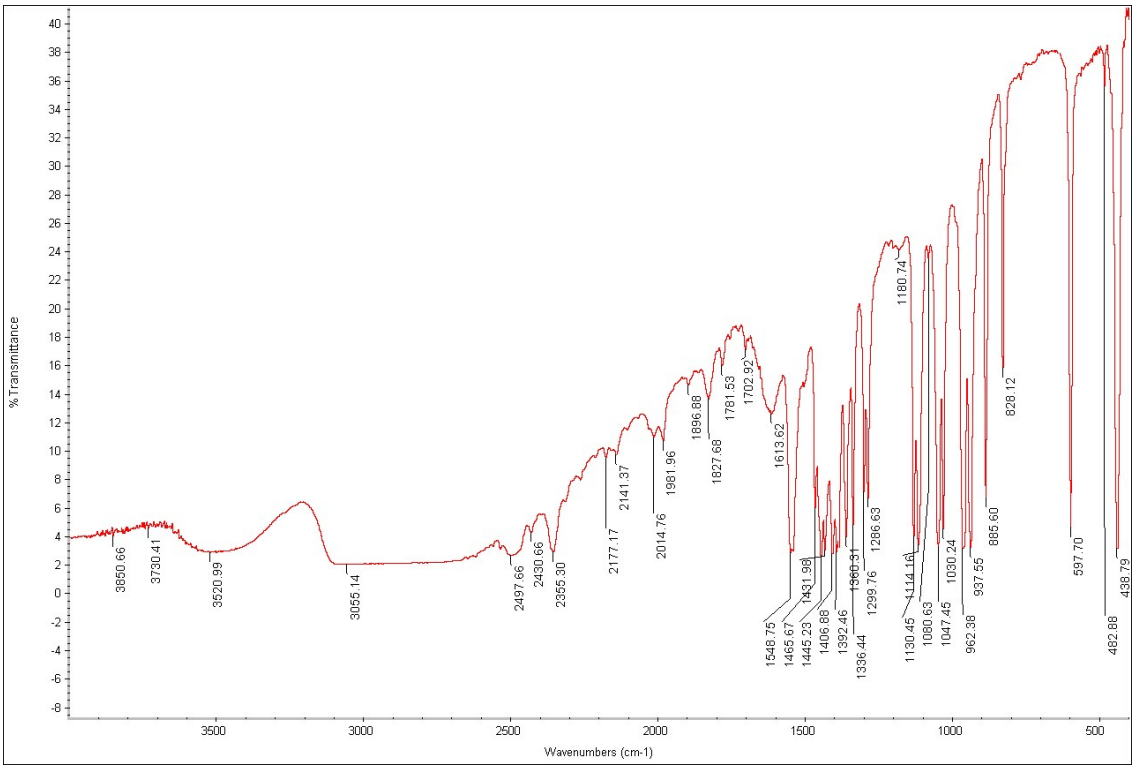


**Figure S3**. FT-IR of (2,5-dmpz) $PbBr_3 \cdot (CH_3)_2SO$ perovskite

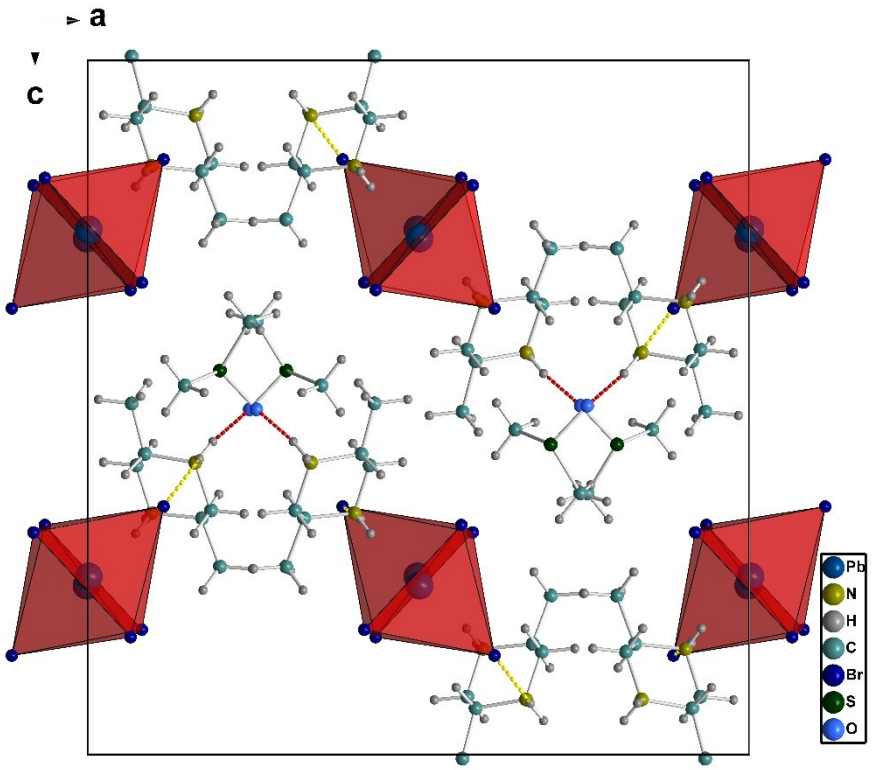


**Figure S4**. Hydrogen geometry in the (2,5-dmpz) $PbBr_3 \cdot (CH_3)_2SO$ perovskite. The dashed yellow and red lines indicate the hydrogen bond of $[PbBr_3]^-$ octahedra and 2,5-dmpz dication, and the hydrogen bond of 2,5-dmpz dication and DMSO solvent molecule, respectively.

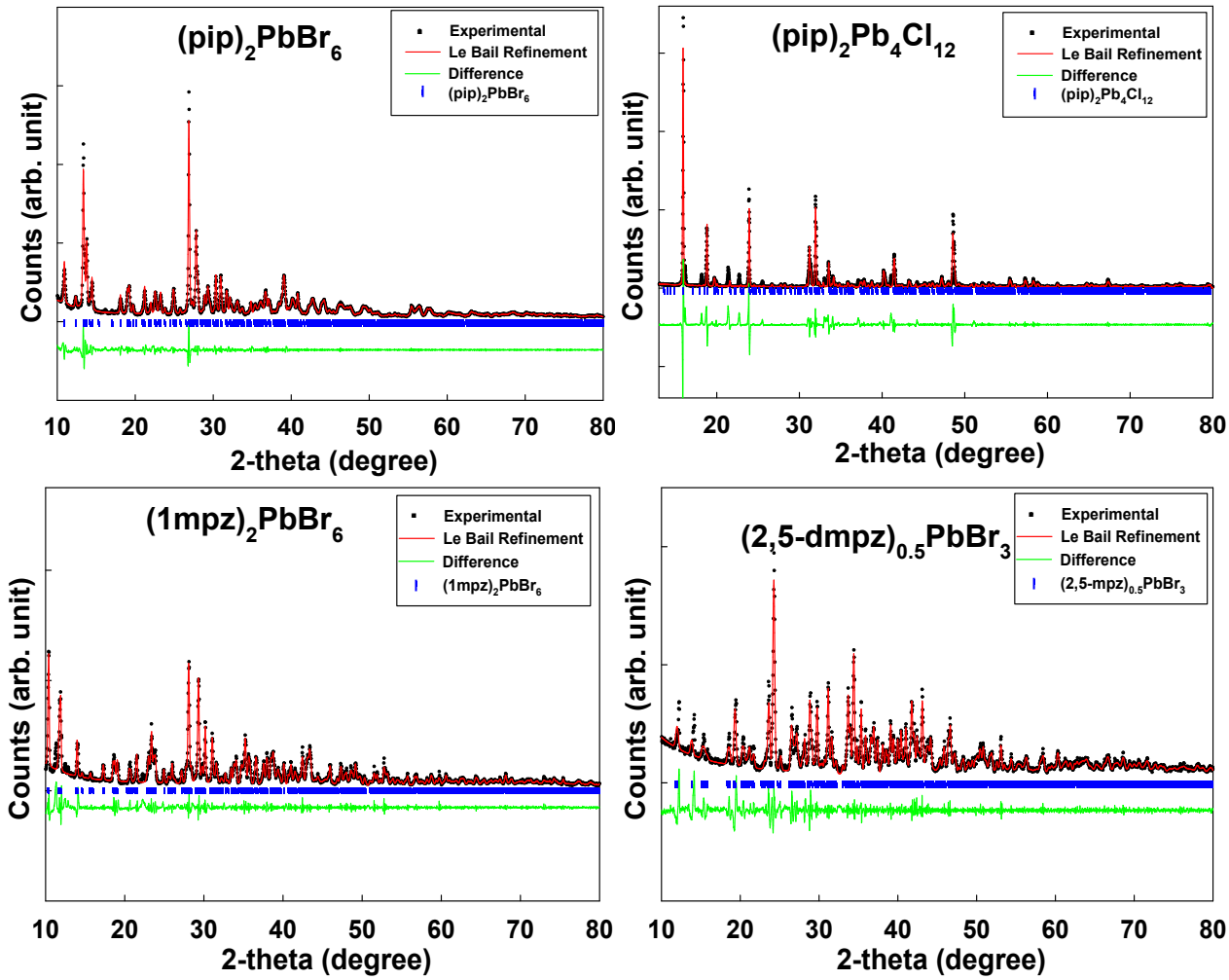


**Figure S5**. The experimental and theoretical XRD pattern for the crystal structure of the $(pip)_2PbBr_6$, $(pip)_2Pb_4Cl_{12}$, $(1mpz)_2PbBr_6$, and $(2,5\text{-}dmpz)_{0.5}PbBr_3$ perovskites.

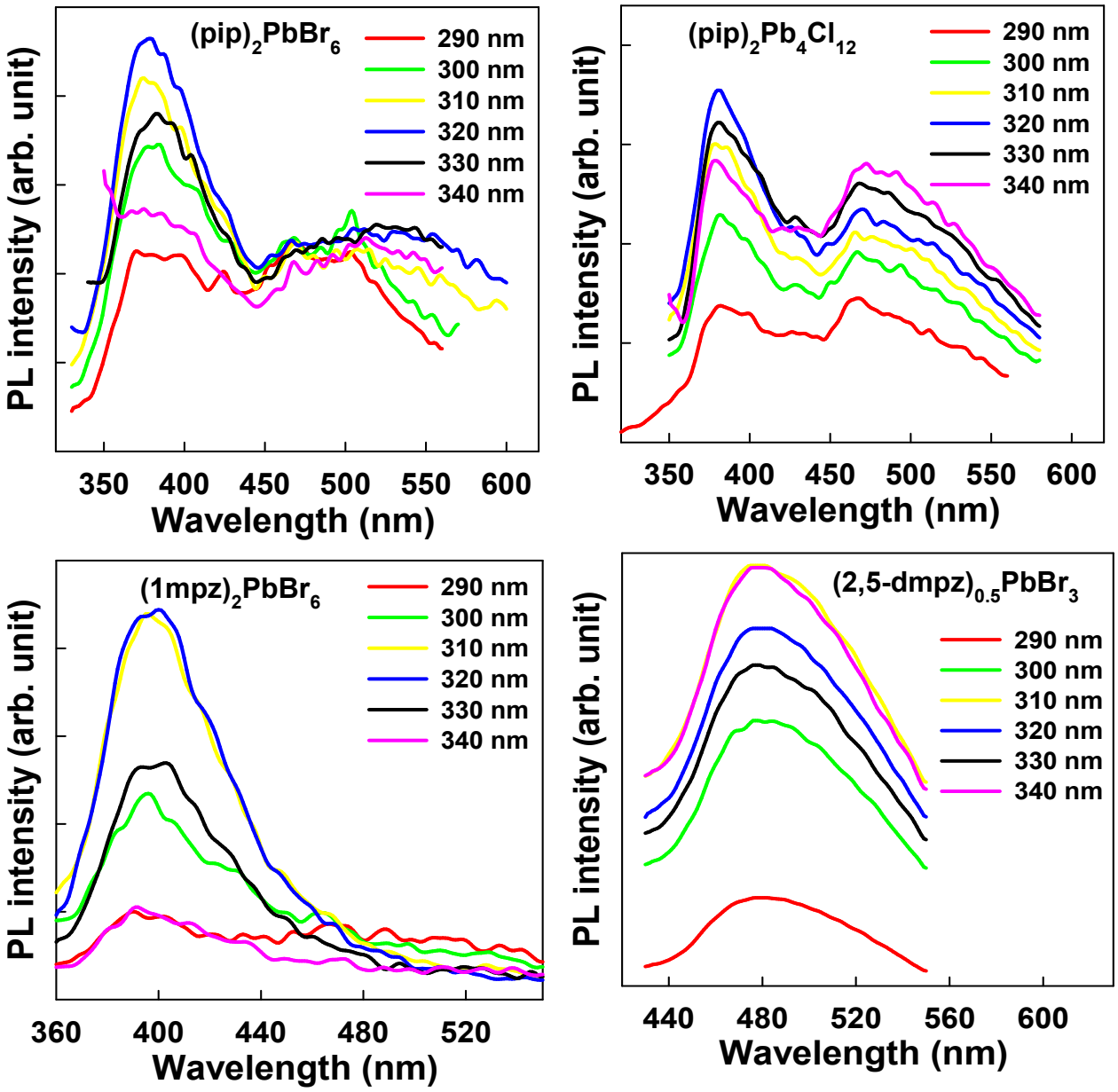


**Figure S6**. Excitation dependent PL spectra of the $(pip)_2PbBr_6$, $(pip)_2Pb_4Cl_{12}$, $(1mpz)_2PbBr_6$, and $(2,5\text{-}dmpz)_{0.5}PbBr_3$ perovskites.

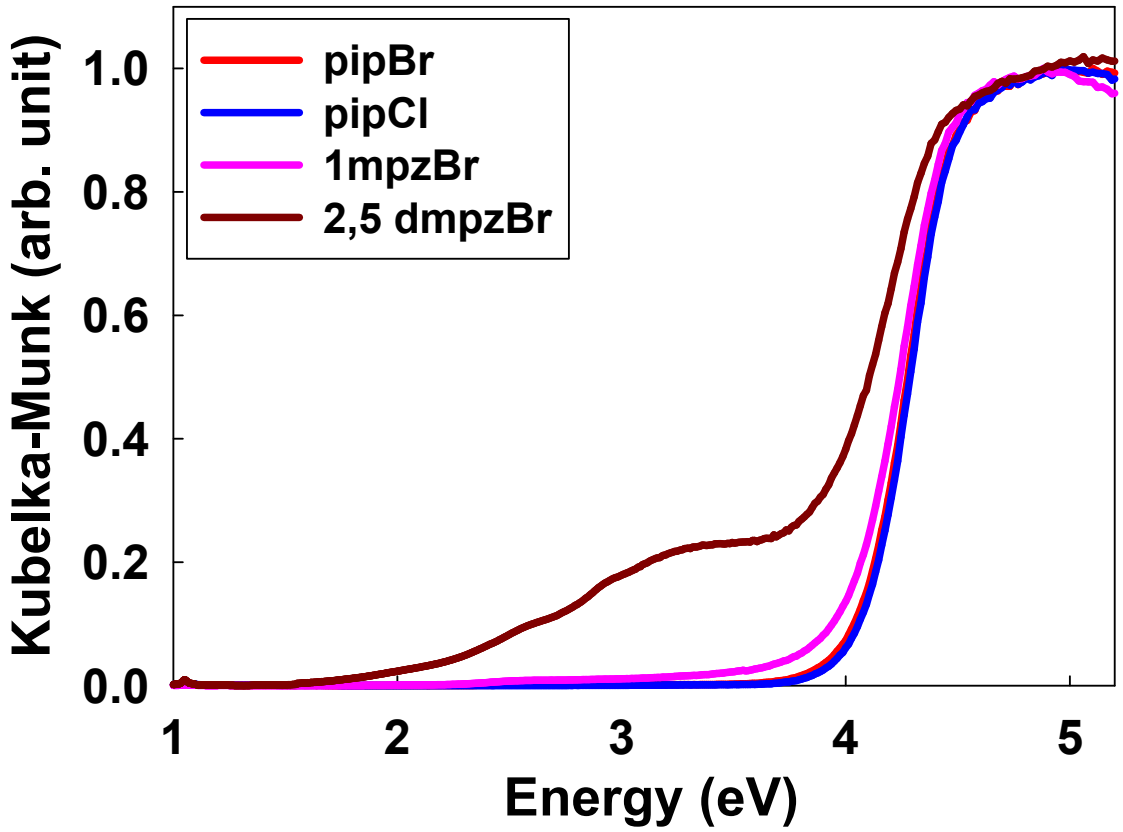


**Figure S7**. Optical absorption spectra for the three diammonium salts, pipBr, pipCl, 1mpzBr and 2,5 dmpzBr.

**Table S1**. Hydrogen bonds for $(pip)_2PbBr_6$.

| D-H···A | D-H/Å | H···A/Å | D···A/Å | <(DHA)/° | Symmetry transformations |
|---|---|---|---|---|---|
| N(1)-H(1B)···Br(2) | 0.89 | 2.80 | 3.476(10) | 133.8 | -x+3/2, y-1/2, -z+1/2 |
| N(1)-H(1B)···Br(3) | 0.89 | 3.10 | 3.712(7) | 127.6 | -x+3/2, y-1/2, -z+1/2 |
| N(1)-H(1B)···Br(3) | 0.89 | 3.10 | 3.712(7) | 127.6 | -x+3/2, y-1/2, z-1/2 |
| N(1)-H(1C)···Br(1) | 0.89 | 2.97 | 3.668(8) | 136.4 | -x+3/2, y+1/2, -z+1/2 |
| N(1)-H(1C)···Br(1) | 0.89 | 2.97 | 3.668(8) | 136.4 | -x+3/2, y+1/2, z-1/2 |
| N(5)-H(5B)···Br(1) | 0.89 | 2.88 | 3.503(7) | 128.7 | x, y+1, z |
| N(5)-H(5B)···Br(1) | 0.89 | 2.88 | 3.503(7) | 128.7 | x, y+1, -z+1 |
| N(5)-H(5C)···Br(3) | 0.89 | 2.86 | 3.544(8) | 135.1 | – |
| N(5)-H(5C)···Br(3) | 0.89 | 2.86 | 3.544(8) | 135.1 | x, y, -z+1 |

**Table S2**. Hydrogen bonds for $(pip)_2Pb_4Cl_{12}$

| D-H···A | D-H/Å | H···A/Å | D···A/Å | <(DHA)/° | Symmetry transformations |
|---|---|---|---|---|---|
| N(2)-H(2C)···Cl(14) | 0.89 | 2.88 | 3.676(18) | 149.9 | – |
| N(3)-H(3C)···Cl(6) | 0.89 | 2.74 | 3.47(3) | 140.4 | – |
| N(3)-H(3C)···Cl(09) | 0.89 | 2.08 | 2.53(3) | 110.1 | – |
| N(4)-H(4C)···Cl(2) | 0.89 | 2.82 | 3.50(3) | 134.7 | -x+y, -x, z |
| N(4)-H(4C)···Cl(09) | 0.89 | 2.94 | 3.543(17) | 126.2 | -x+y, -x, z |
| N(4)-H(4C)···Cl(13) | 0.89 | 2.97 | 3.423(14) | 113.3 | x-1/3, y-2/3, z+1/3 |
| N(4)-H(4D)···Cl(10) | 0.89 | 2.81 | 3.32(2) | 118.5 | x-1/3, y-2/3, z+1/3 |

**Table S3**. Hydrogen bonds for $(1mpz)_2PbBr_6$

| D-H···A | D-H/Å | H···A/Å | D···A/Å | <(DHA)/° | Symmetry transformations |
|---|---|---|---|---|---|
| N(1)-H(1B)···Br(2) | 0.89 | 2.63 | 3.373(7) | 140.9 | -x+1/2, y+1, -z+1/2 |
| N(1)-H(1C)···Br(1) | 0.89 | 2.50 | 3.302(6) | 150.7 | – |

**Table S4**. Hydrogen bonds for $(2,5\text{-dmpz})_{0.5}PbBr_3 \cdot 2((CH_3)_2SO)$

| D-H···A | D-H/Å | H···A/Å | D···A/Å | <(DHA)/° | Symmetry transformations |
|---|---|---|---|---|---|
| N(2)-H(2A)···O(1) | 0.89 | 1.95 | 2.741(10) | 146.9 | – |
| N(2)-H(2B)···O(2) | 0.89 | 1.89 | 2.768(13) | 170.9 | – |

**Table S5**. Bond lengths [Å] and angles [°] for $(pip)_2PbBr_6$ at 293(2) K with estimated standard deviation in parenthesis.

| Label | Distances (Å) | Label | Angles (°) |
|---|---|---|---|
| Pb(1)-Br(2) | 2.8906(12) | Br(2)-Pb(1)-Br(3)#1 | 86.28(3) |
| Pb(1)-Br(3)#1 | 2.9329(10) | Br(2)-Pb(1)-Br(3) | 86.27(3) |
| Pb(1)-Br(3) | 2.9329(10) | Br(3)#1-Pb(1)-Br(3) | 86.53(5) |
| Pb(1)-Br(1) | 3.0716(11) | Br(2)-Pb(1)-Br(1) | 92.07(3) |
| Pb(1)-Br(1)#1 | 3.0716(11) | Br(3)#1-Pb(1)-Br(1) | 95.01(3) |
| Pb(1)-Br(4) | 3.2377(7) | Br(3)-Pb(1)-Br(1) | 177.66(3) |
| C(1)-N(1) | 1.472(10) | Br(2)-Pb(1)-Br(1)#1 | 92.07(3) |
| C(1)-C(2) | 1.571(12) | Br(3)#1-Pb(1)-Br(1)#1 | 177.66(3) |
| N(6)-C(4)#2 | 1.499(10) | Br(3)-Pb(1)-Br(1)#1 | 95.01(3) |
| N(6)-C(4) | 1.499(10) | Br(1)-Pb(1)-Br(1)#1 | 83.39(4) |
| C(2)-N(2) | 1.460(9) | Br(2)-Pb(1)-Br(4) | 176.66(3) |
| C(3)-C(3)#3 | 1.434(16) | Br(3)#1-Pb(1)-Br(4) | 91.291(19) |
| C(3)-N(5) | 1.506(9) | Br(3)-Pb(1)-Br(4) | 91.292(19) |
| C(4)-C(4)#4 | 1.484(19) | Br(1)-Pb(1)-Br(4) | 90.43(2) |
| Pb(1)-Br(2) | 2.8906(12) | Br(1)#1-Pb(1)-Br(4) | 90.43(2) |
| Pb(1)-Br(3)#1 | 2.9329(10) | Pb(1)-Br(4)-Pb(1)#5 | 180.0 |
| Pb(1)-Br(3) | 2.9329(10) | N(1)-C(1)-C(2) | 110.0(7) |
| Pb(1)-Br(1) | 3.0716(11) | C(4)#2-N(6)-C(4) | 110.0(9) |
| Pb(1)-Br(1)#1 | 3.0716(11) | N(2)-C(2)-C(1) | 109.2(7) |
| Pb(1)-Br(4) | 3.2377(7) | C(3)#3-C(3)-N(5) | 111.5(6) |
| C(1)-N(1) | 1.472(10) | C(4)#4-C(4)-N(6) | 111.5(7) |
| C(1)-C(2) | 1.571(12) | C(1)-N(1)-C(1)#2 | 111.6(9) |
| N(6)-C(4)#2 | 1.499(10) | C(2)-N(2)-C(2)#2 | 114.2(8) |
| N(6)-C(4) | 1.499(10) | C(3)#1-N(5)-C(3) | 112.4(8) |
| C(2)-N(2) | 1.460(9) | | |
| C(3)-C(3)#3 | 1.434(16) | | |
| C(3)-N(5) | 1.506(9) | | |
| C(4)-C(4)#4 | 1.484(19) | | |

Symmetry transformations used to generate equivalent atoms: #1 x, y, -z+1; #2 x, y, -z; #3 -x+1, -y+2, z; #4 -x+1, -y+1, z; #5 -x+1,-y+1,-z+1

**Table S6**. Bond lengths [Å] and angles [°] for $(pip)_2Pb_4Cl_{12}$ at 293(2) K with estimated standard deviation in parenthesis.

| Label | Distances (Å) | Label | Angles (°) |
|---|---|---|---|
| Pb(1)-Cl(4) | 2.773(5) | Cl(4)-Pb(1)-Cl(3) | 88.11(18) |
| Pb(1)-Cl(3) | 2.825(5) | Cl(4)-Pb(1)-Cl(09) | 81.22(17) |
| Pb(1)-Cl(09) | 2.905(5) | Cl(3)-Pb(1)-Cl(09) | 79.16(12) |
| Pb(1)-Cl(1) | 3.016(3) | Cl(4)-Pb(1)-Cl(1) | 81.37(15) |
| C(1)-C(2) | 1.473(13) | Cl(3)-Pb(1)-Cl(1) | 78.62(14) |
| C(1)-N(1) | 1.489(13) | Cl(09)-Pb(1)-Cl(1) | 152.09(11) |
| N(1)-C(4) | 1.462(13) | Pb(1)#1-Cl(1)-Pb(1)#2 | 95.42(14) |
| Pb(2)-Cl(6) | 2.727(5) | Pb(1)#1-Cl(1)-Pb(1) | 95.41(14) |
| Pb(2)-Cl(09) | 2.799(5) | Pb(1)#2-Cl(1)-Pb(1) | 95.41(14) |
| Pb(2)-Cl(3) | 2.893(5) | C(2)-C(1)-N(1) | 108.6(15) |
| Pb(2)-Cl(5) | 3.063(4) | C(4)-N(1)-C(1) | 107.7(15) |
| C(2)-N(2) | 1.485(13) | Cl(6)-Pb(2)-Cl(09) | 87.03(17) |
| N(2)-C(3) | 1.479(13) | Cl(6)-Pb(2)-Cl(3) | 79.87(17) |
| C(3)-C(4) | 1.461(13) | Cl(09)-Pb(2)-Cl(3) | 79.80(13) |
| Pb(3)-Cl(9) | 2.786(5) | Cl(6)-Pb(2)-Cl(5) | 82.01(12) |
| Pb(3)-Cl(10) | 2.795(5) | Cl(09)-Pb(2)-Cl(5) | 77.10(16) |
| Pb(3)-Cl(12) | 3.010(5) | Cl(3)-Pb(2)-Cl(5) | 151.22(14) |
| Pb(3)-Cl(8) | 3.010(4) | C(1)-C(2)-N(2) | 117.8(15) |
| Pb(3)-Cl(7) | 3.084(4) | C(3)-N(2)-C(2) | 106.9(16) |
| N(3)-C(5) | 1.458(14) | C(4)-C(3)-N(2) | 114.8(15) |
| N(3)-C(8) | 1.469(13) | Cl(9)-Pb(3)-Cl(10) | 88.4(2) |
| Pb(4)-Cl(13) | 2.728(5) | Cl(9)-Pb(3)-Cl(12) | 79.56(19) |
| Pb(4)-Cl(12) | 2.785(5) | Cl(10)-Pb(3)-Cl(12) | 80.50(13) |
| Pb(4)-Cl(10) | 2.999(5) | Cl(9)-Pb(3)-Cl(8) | 82.66(14) |
| Pb(4)-Cl(14) | 3.064(5) | Cl(10)-Pb(3)-Cl(8) | 76.71(16) |
| N(4)-C(7) | 1.465(14) | Cl(12)-Pb(3)-Cl(8) | 151.35(15) |
| N(4)-C(6) | 1.467(13) | Cl(9)-Pb(3)-Cl(7) | 72.91(11) |
| C(5)-C(6) | 1.467(14) | Cl(10)-Pb(3)-Cl(7) | 138.25(16) |
| C(7)-C(8) | 1.479(13) | Cl(12)-Pb(3)-Cl(7) | 129.56(14) |
| | | Cl(8)-Pb(3)-Cl(7) | 64.33(16) |
| | | Pb(1)-Cl(3)-Pb(2) | 97.71(14) |
| | | C(5)-N(3)-C(8) | 114.4(19) |
| | | Cl(13)-Pb(4)-Cl(12) | 87.36(19) |
| | | Cl(13)-Pb(4)-Cl(10) | 78.74(18) |
| | | Cl(12)-Pb(4)-Cl(10) | 80.86(14) |
| | | Cl(13)-Pb(4)-Cl(14) | 82.78(12) |

| | |
|---|---|
| Cl(12)-Pb(4)-Cl(14) | 74.94(18) |
| Cl(10)-Pb(4)-Cl(14) | 150.08(17) |
| C(3)-C(4)-N(1) | 110(2) |
| C(7)-N(4)-C(6) | 111.0(16) |
| Pb(2)-Cl(5)-Pb(2)#3 | 93.57(18) |
| Pb(2)-Cl(5)-Pb(2)#4 | 93.57(18) |
| Pb(2)#3-Cl(5)-Pb(2)#4 | 93.57(18) |
| N(3)-C(5)-C(6) | 133(3) |
| N(4)-C(6)-C(5) | 105.4(16) |
| Pb(3)#5-Cl(7)-Pb(3)#6 | 92.81(15) |
| Pb(3)#5-Cl(7)-Pb(3) | 92.80(15) |
| Pb(3)#6-Cl(7)-Pb(3) | 92.80(15) |
| N(4)-C(7)-C(8) | 138.0(18) |
| Pb(3)#5-Cl(8)-Pb(3) | 95.77(16) |
| Pb(3)#5-Cl(8)-Pb(3)#6 | 95.77(16) |
| Pb(3)-Cl(8)-Pb(3)#6 | 95.76(16) |
| N(3)-C(8)-C(7) | 105.8(14) |
| Pb(2)-Cl(09)-Pb(1) | 98.01(13) |
| Pb(3)-Cl(10)-Pb(4) | 95.83(17) |
| Pb(4)-Cl(12)-Pb(3) | 95.80(16) |
| Pb(4)-Cl(14)-Pb(4)#7 | 93.7(2) |
| Pb(4)-Cl(14)-Pb(4)#8 | 93.7(2) |
| Pb(4)#7-Cl(14)-Pb(4)#8 | 93.6(2) |

Symmetry transformations used to generate equivalent atoms: #1 -x+y, -x+1, z;  #2 -y+1, x-y+1, z;  #3 -y, x-y, z;  #4 -x+y, -x, z;  #5 -x+y+1, -x+2, z;  #6 -y+2, x-y+1, z;  #7 -y+1, x-y, z;  #8 -x+y+1, -x+1, z

**Table S7**. Bond lengths [Å] and angles [°] for $(1mpz)_2PbBr_6$ at 293(2) K with estimated standard deviation in parenthesis.

| Label | Distances (Å) | Label | Angles (°) |
|---|---|---|---|
| Pb(1)-Br(1) | 2.9707(8) | Br(1)-Pb(1)-Br(1)#1 | 91.43(4) |
| Pb(1)-Br(1)#1 | 2.9708(8) | Br(1)-Pb(1)-Br(3) | 90.41(3) |
| Pb(1)-Br(3) | 3.0209(10) | Br(1)#1-Pb(1)-Br(3) | 84.34(3) |
| Pb(1)-Br(3)#1 | 3.0209(10) | Br(1)-Pb(1)-Br(3)#1 | 84.35(3) |
| Pb(1)-Br(2) | 3.0605(8) | Br(1)#1-Pb(1)-Br(3)#1 | 90.41(3) |
| Pb(1)-Br(2)#1 | 3.0605(8) | Br(3)-Pb(1)-Br(3)#1 | 172.49(4) |
| C(1)-N(2) | 1.472(14) | Br(1)-Pb(1)-Br(2) | 173.92(2) |
| C(2)-N(2) | 1.470(9) | Br(1)#1-Pb(1)-Br(2) | 93.53(3) |
| C(2)-C(3) | 1.516(11) | Br(3)-Pb(1)-Br(2) | 93.58(3) |
| C(3)-N(1) | 1.502(13) | Br(3)#1-Pb(1)-Br(2) | 92.10(3) |
| C(4)-N(1) | 1.480(10) | Br(1)-Pb(1)-Br(2)#1 | 93.53(3) |
| C(4)-C(5) | 1.497(10) | Br(1)#1-Pb(1)-Br(2)#1 | 173.92(2) |
| C(5)-N(2) | 1.496(10) | Br(3)-Pb(1)-Br(2)#1 | 92.10(3) |
| | | Br(3)#1-Pb(1)-Br(2)#1 | 93.58(3) |
| | | Br(2)-Pb(1)-Br(2)#1 | 81.75(3) |
| | | N(2)-C(2)-C(3) | 109.1(6) |
| | | N(1)-C(3)-C(2) | 110.6(6) |
| | | N(1)-C(4)-C(5) | 110.8(6) |
| | | N(2)-C(5)-C(4) | 111.9(6) |
| | | C(4)-N(1)-C(3) | 112.0(6) |
| | | C(2)-N(2)-C(1) | 109.5(8) |
| | | C(2)-N(2)-C(5) | 110.2(6) |
| | | C(1)-N(2)-C(5) | 118.2(11) |

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, y, -z+1/2

**Table S8**. Bond lengths [Å] and angles [°] for $(2,5\text{-dmpz})_{0.5}PbBr_3 \cdot 2((CH_3)_2SO)$ at 293(2) K with estimated standard deviation in parenthesis.

| Label | Distances (Å) | Label | Angles (°) |
|---|---|---|---|
| Pb(1)-O(1) | 2.681(7) | O(1)-Pb(1)-Br(2) | 170.22(18) |
| Pb(1)-Br(2) | 2.8569(13) | O(1)-Pb(1)-Br(3) | 79.33(15) |
| Pb(1)-Br(3) | 2.8822(12) | Br(2)-Pb(1)-Br(3) | 94.65(4) |
| Pb(1)-Br(1) | 2.8957(12) | O(1)-Pb(1)-Br(1) | 82.09(16) |
| N(2)-C(3) | 1.474(11) | Br(2)-Pb(1)-Br(1) | 90.36(4) |
| N(2)-C(4) | 1.506(13) | Br(3)-Pb(1)-Br(1) | 90.89(4) |
| N(2)-H(2A) | 0.8900 | C(3)-N(2)-C(4) | 111.7(7) |
| N(2)-H(2B) | 0.8900 | C(3)-N(2)-H(2A) | 109.3 |
| C(3)-C(4)#1 | 1.497(12) | C(4)-N(2)-H(2A) | 109.3 |
| C(3)-H(3A) | 0.9700 | C(3)-N(2)-H(2B) | 109.3 |
| C(3)-H(3B) | 0.9700 | C(4)-N(2)-H(2B) | 109.3 |
| C(4)-C(5) | 1.534(14) | H(2A)-N(2)-H(2B) | 107.9 |
| C(4)-H(4) | 0.9800 | N(2)-C(3)-C(4)#1 | 110.6(7) |
| C(5)-H(5A) | 0.9600 | N(2)-C(3)-H(3A) | 109.5 |
| C(5)-H(5B) | 0.9600 | C(4)#1-C(3)-H(3A) | 109.5 |
| C(5)-H(5C) | 0.9600 | N(2)-C(3)-H(3B) | 109.5 |
| S(1)-O(1) | 1.521(7) | C(4)#1-C(3)-H(3B) | 109.5 |
| S(1)-C(1S) | 1.761(15) | H(3A)-C(3)-H(3B) | 108.1 |
| S(1)-C(2S) | 1.775(14) | C(3)#1-C(4)-N(2) | 108.8(8) |
| C(1S)-H(1S1) | 0.9600 | C(3)#1-C(4)-C(5) | 110.8(9) |
| C(1S)-H(1S2) | 0.9600 | N(2)-C(4)-C(5) | 109.0(8) |
| C(1S)-H(1S3) | 0.9600 | C(3)#1-C(4)-H(4) | 109.4 |
| C(2S)-H(2S1) | 0.9600 | N(2)-C(4)-H(4) | 109.4 |
| C(2S)-H(2S2) | 0.9600 | C(5)-C(4)-H(4) | 109.4 |
| C(2S)-H(2S3) | 0.9600 | C(4)-C(5)-H(5A) | 109.5 |
| S(2)-O(2) | 1.479(10) | C(4)-C(5)-H(5B) | 109.5 |
| S(2)-C(4S) | 1.762(12) | H(5A)-C(5)-H(5B) | 109.5 |
| S(2)-C(3S) | 1.774(15) | C(4)-C(5)-H(5C) | 109.5 |
| C(3S)-H(3S1) | 0.9600 | H(5A)-C(5)-H(5C) | 109.5 |
| C(3S)-H(3S2) | 0.9600 | H(5B)-C(5)-H(5C) | 109.5 |
| C(3S)-H(3S3) | 0.9600 | O(1)-S(1)-C(1S) | 103.8(6) |
| C(4S)-H(4S1) | 0.9600 | O(1)-S(1)-C(2S) | 105.3(6) |
| C(4S)-H(4S2) | 0.9600 | C(1S)-S(1)-C(2S) | 98.0(7) |
| C(4S)-H(4S3) | 0.9600 | S(1)-O(1)-Pb(1) | 120.5(4) |
| | | S(1)-C(1S)-H(1S1) | 109.5 |
| | | S(1)-C(1S)-H(1S2) | 109.5 |
| | | H(1S1)-C(1S)-H(1S2) | 109.5 |

| | |
|---|---|
| S(1)-C(1S)-H(1S3) | 109.5 |
| H(1S1)-C(1S)-H(1S3) | 109.5 |
| H(1S2)-C(1S)-H(1S3) | 109.5 |
| S(1)-C(2S)-H(2S1) | 109.5 |
| S(1)-C(2S)-H(2S2) | 109.5 |
| H(2S1)-C(2S)-H(2S2) | 109.5 |
| S(1)-C(2S)-H(2S3) | 109.5 |
| H(2S1)-C(2S)-H(2S3) | 109.5 |
| H(2S2)-C(2S)-H(2S3) | 109.5 |
| O(2)-S(2)-C(4S) | 108.0(6) |
| O(2)-S(2)-C(3S) | 106.1(7) |
| C(4S)-S(2)-C(3S) | 98.9(7) |
| S(2)-C(3S)-H(3S1) | 109.5 |
| S(2)-C(3S)-H(3S2) | 109.5 |
| H(3S1)-C(3S)-H(3S2) | 109.5 |
| S(2)-C(3S)-H(3S3) | 109.5 |
| H(3S1)-C(3S)-H(3S3) | 109.5 |
| H(3S2)-C(3S)-H(3S3) | 109.5 |
| S(2)-C(4S)-H(4S1) | 109.5 |
| S(2)-C(4S)-H(4S2) | 109.5 |
| H(4S1)-C(4S)-H(4S2) | 109.5 |
| S(2)-C(4S)-H(4S3) | 109.5 |
| H(4S1)-C(4S)-H(4S3) | 109.5 |
| H(4S2)-C(4S)-H(4S3) | 109.5 |

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1

**Table S9**. Bond lengths [Å] and angles [°] for (2,5-dmpz) $PbBr_3 \cdot (CH_3)_2SO$ at 293(2) K with estimated standard deviation in parenthesis.

| Label | Distances (Å) | Label | Angles (°) |
|---|---|---|---|
| Pb(1)-Br(1) | 2.9140(12) | Br(1)-Pb(1)-Br(2) | 86.94(3) |
| Pb(1)-Br(2) | 2.9279(10) | Br(1)-Pb(1)-Br(3) | 93.05(3) |
| Pb(1)-Br(3) | 2.9391(10) | Br(2)-Pb(1)-Br(3) | 91.63(3) |
| Pb(1)-Br(1)#1 | 3.0345(12) | Br(1)-Pb(1)-Br(1)#1 | 172.27(3) |
| Pb(1)-Br(2)#2 | 3.1115(10) | Br(2)-Pb(1)-Br(1)#1 | 86.85(3) |
| N(1)-C(3) | 1.470(11) | Br(3)-Pb(1)-Br(1)#1 | 91.72(3) |
| N(1)-C(4) | 1.474(11) | Br(1)-Pb(1)-Br(2)#2 | 85.67(3) |
| N(1)-H(1A*) | 0.8900 | Br(2)-Pb(1)-Br(2)#2 | 171.93(3) |
| N(1)-H(1B) | 0.8900 | Br(3)-Pb(1)-Br(2)#2 | 92.00(3) |
| C(1)-C(2) | 1.522(12) | Br(1)#1-Pb(1)-Br(2)#2 | 100.24(3) |
| C(1)-H(1A) | 0.9600 | C(3)-N(1)-C(4) | 109.8(7) |
| C(1)-H(1AB) | 0.9600 | C(3)-N(1)-H(1A*) | 109.7 |
| C(1)-H(1AC) | 0.9600 | C(4)-N(1)-H(1A*) | 109.7 |
| N(2)-C(7) | 1.490(11) | C(3)-N(1)-H(1B) | 109.7 |
| N(2)-C(2) | 1.505(11) | C(4)-N(1)-H(1B) | 109.7 |
| N(2)-H(2A) | 0.8900 | H(1A*)-N(1)-H(1B) | 108.2 |
| N(2)-H(2B) | 0.8900 | C(2)-C(1)-H(1A) | 109.5 |
| C(2)-C(3) | 1.511(12) | C(2)-C(1)-H(1AB) | 109.5 |
| C(2)-H(2) | 0.9800 | H(1A)-C(1)-H(1AB) | 109.5 |
| C(3)-H(3A) | 0.9700 | C(2)-C(1)-H(1AC) | 109.5 |
| C(3)-H(3AB) | 0.9700 | H(1A)-C(1)-H(1AC) | 109.5 |
| C(7)-C(4) | 1.513(12) | H(1AB)-C(1)-H(1AC) | 109.5 |
| C(7)-H(7A) | 0.9700 | Pb(1)-Br(1)-Pb(1)#2 | 94.20(3) |
| C(7)-H(7AB) | 0.9700 | Pb(1)-Br(2)-Pb(1)#1 | 92.33(2) |
| C(6)-C(4) | 1.532(12) | C(7)-N(2)-C(2) | 112.7(7) |
| C(6)-H(6A) | 0.9600 | C(7)-N(2)-H(2A) | 109.1 |
| C(6)-H(6AB) | 0.9600 | C(2)-N(2)-H(2A) | 109.1 |
| C(6)-H(6AC) | 0.9600 | C(7)-N(2)-H(2B) | 109.1 |
| C(4)-H(4) | 0.9800 | C(2)-N(2)-H(2B) | 109.1 |
| S(1)-O(1) | 1.524(7) | H(2A)-N(2)-H(2B) | 107.8 |
| S(1)-C(1S) | 1.787(9) | N(2)-C(2)-C(3) | 109.1(7) |
| S(1)-C(2S) | 1.791(10) | N(2)-C(2)-C(1) | 110.3(7) |
| C(1S)-H(1S1) | 0.9600 | C(3)-C(2)-C(1) | 111.6(8) |
| C(1S)-H(1S2) | 0.9600 | N(2)-C(2)-H(2) | 108.6 |
| C(1S)-H(1S3) | 0.9600 | C(3)-C(2)-H(2) | 108.6 |
| C(2S)-H(2S1) | 0.9600 | C(1)-C(2)-H(2) | 108.6 |

| | | | |
|---|---|---|---|
| C(2S)-H(2S2) | 0.9600 | N(1)-C(3)-C(2) | 112.2(7) |
| C(2S)-H(2S3) | 0.9600 | N(1)-C(3)-H(3A) | 109.2 |
| | | C(2)-C(3)-H(3A) | 109.2 |
| | | N(1)-C(3)-H(3AB) | 109.2 |
| | | C(2)-C(3)-H(3AB) | 109.2 |
| | | H(3A)-C(3)-H(3AB) | 107.9 |
| | | N(2)-C(7)-C(4) | 109.8(7) |
| | | N(2)-C(7)-H(7A) | 109.7 |
| | | C(4)-C(7)-H(7A) | 109.7 |
| | | N(2)-C(7)-H(7AB) | 109.7 |
| | | C(4)-C(7)-H(7AB) | 109.7 |
| | | H(7A)-C(7)-H(7AB) | 108.2 |
| | | C(4)-C(6)-H(6A) | 109.5 |
| | | C(4)-C(6)-H(6AB) | 109.5 |
| | | H(6A)-C(6)-H(6AB) | 109.5 |
| | | C(4)-C(6)-H(6AC) | 109.5 |
| | | H(6A)-C(6)-H(6AC) | 109.5 |
| | | H(6AB)-C(6)-H(6AC) | 109.5 |
| | | N(1)-C(4)-C(7) | 109.1(7) |
| | | N(1)-C(4)-C(6) | 111.8(7) |
| | | C(7)-C(4)-C(6) | 109.7(8) |
| | | N(1)-C(4)-H(4) | 108.7 |
| | | C(7)-C(4)-H(4) | 108.7 |
| | | C(6)-C(4)-H(4) | 108.7 |
| | | O(1)-S(1)-C(1S) | 105.9(4) |
| | | O(1)-S(1)-C(2S) | 106.1(4) |
| | | C(1S)-S(1)-C(2S) | 97.3(5) |
| | | S(1)-C(1S)-H(1S1) | 109.5 |
| | | S(1)-C(1S)-H(1S2) | 109.5 |
| | | H(1S1)-C(1S)-H(1S2) | 109.5 |
| | | S(1)-C(1S)-H(1S3) | 109.5 |
| | | H(1S1)-C(1S)-H(1S3) | 109.5 |
| | | H(1S2)-C(1S)-H(1S3) | 109.5 |
| | | S(1)-C(2S)-H(2S1) | 109.5 |
| | | S(1)-C(2S)-H(2S2) | 109.5 |
| | | H(2S1)-C(2S)-H(2S2) | 109.5 |
| | | S(1)-C(2S)-H(2S3) | 109.5 |
| | | H(2S1)-C(2S)-H(2S3) | 109.5 |
| | | H(2S2)-C(2S)-H(2S3) | 109.5 |

Symmetry transformations used to generate equivalent atoms: #1 -x+1, y+1/2, -z+1/2 #2 -x+1, y-1/2, -z+1/2