

Supplementary Materials: Hybrid Gold-Based Perovskite Derivatives: Synthesis, Properties, and Prospects in Photovoltaics

Chang Liu^{1,2,3,4}, Xifeng Fu^{1,4,5}, Zi-Ang Nan⁵, Zilong Zhang^{2,3}, Lingyi Meng^{1,2,4,5}, Peng Gao^{1,2,3,4*}

1 College of Chemistry and Materials Science, Fujian Normal University, Fuzhou 350007, China

2 CAS Key Laboratory of Design and Assembly of Functional Nanostructures, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China

3 Laboratory for Advanced Functional Materials, Xiamen Institute of Rare Earth Materials, Haixi Institute, Chinese Academy of Sciences Xiamen 361021, China

4 Fujian College, University of Chinese Academy of Sciences, Fuzhou, 350002, China

5 Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China

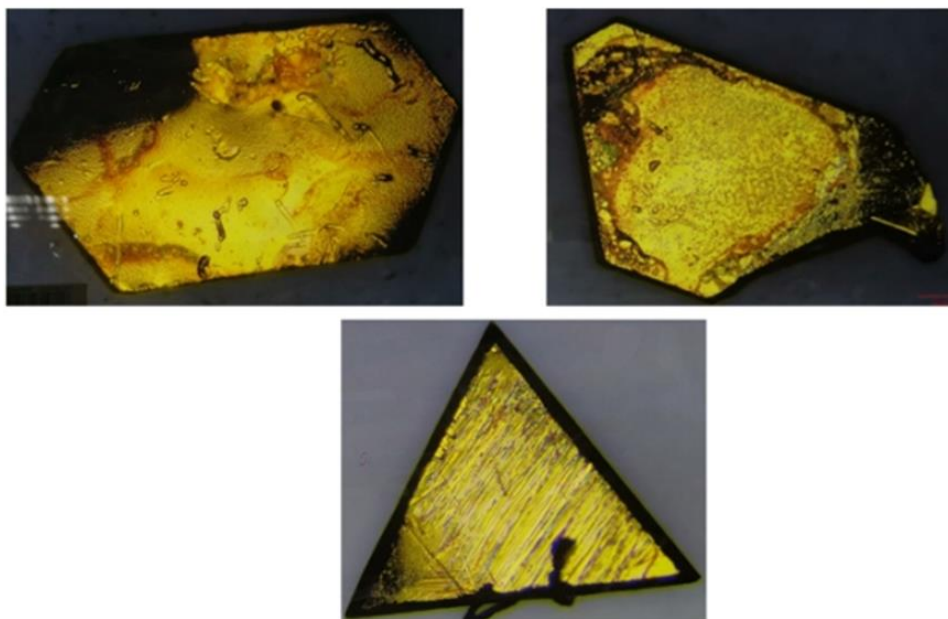


Figure S1. The elemental gold produced by decomposition of products at high temperatures under optical microscope (100 \times).

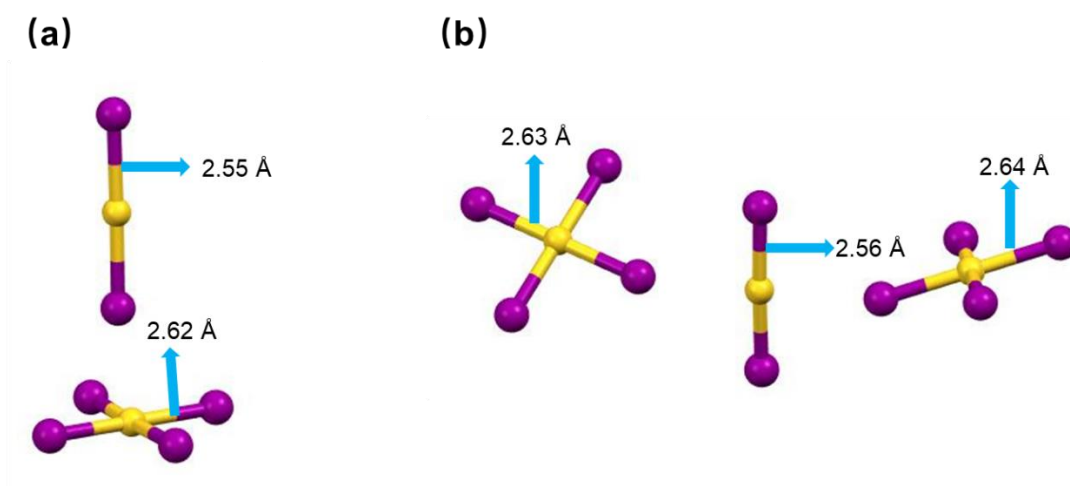


Figure S2. (a, b) The length of the Au-I bonds in the **3AMP** and **3AMPY** structures.

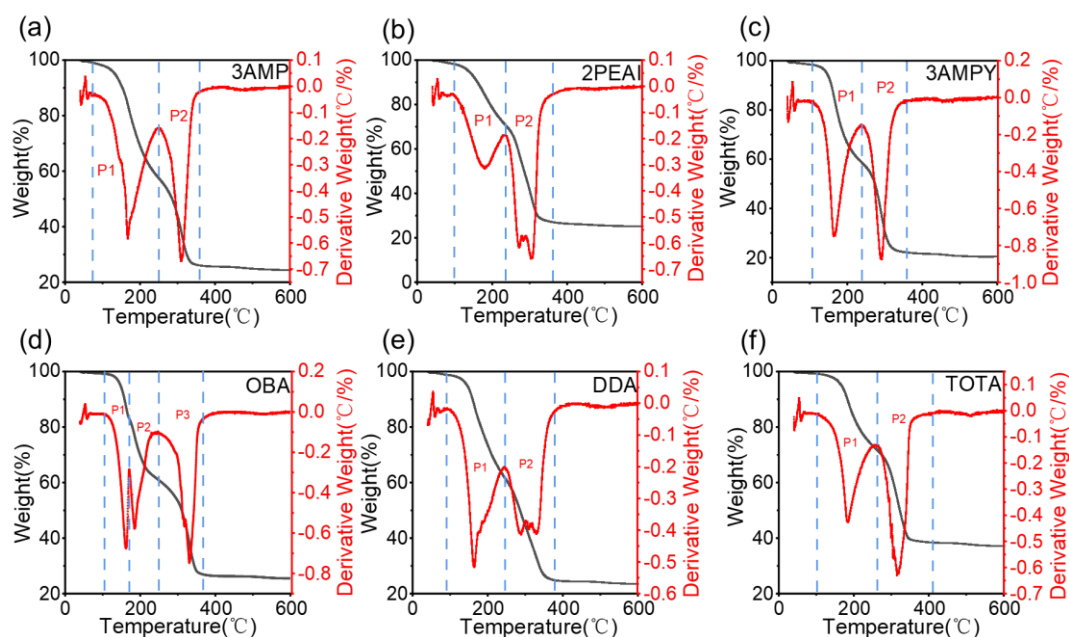


Figure S3. (a-f) The thermogravimetric analysis (TGA) curves of gold-based perovskite derivatives.

Table S1. Crystal structure information of 2PEAI, 3AMP and 3AMPY

	2PEAI	3AMP	3AMPY
Empirical formula	$C_8H_{12}AuI_4N$	$C_6H_{14}Au_2I_6N_2$	$C_6H_8Au_2I_6N_2$
Formula weight	699.85	2396.06	1265.49
Temperature [K]	200.00	200.00	200.00
Crystal system	monoclinic	monoclinic	triclinic
Space group (number)	$P2_1/c$ (14)	Cm (8)	$P\bar{1}$ (2)
a [Å]	6.0259(4)	19.084(2)	8.3376(3)
b [Å]	25.4258(13)	8.3142(9)	9.3799(3)
c [Å]	9.2683(6)	13.762(2)	14.0131(5)
α [°]	90	90	90.1030(10)
β [°]	92.634(2)	111.702(5)	103.457(2)
γ [°]	90	90	115.3170(10)
Volume [Å ³]	1418.53(15)	2028.8(4)	957.03(6)
Z	4	2	2
ρ_{calc} [gcm ⁻³]	3.277	3.922	4.391
μ [mm ⁻¹]	16.865	23.471	24.972
$F(000)$	1220	1991	1072
Crystal colour	Black	Black	Black
Radiation	MoK α	MoK α	MoK α

	2PEAI	3AMP	3AMPY
	($\lambda=0.71073$ Å)	($\lambda=0.71073$ Å)	($\lambda=0.71073$ Å)
2 θ range [°]	6.77 to 52.92 (0.80 Å)	5.83 to 64.20 (0.67 Å)	5.56 to 77.48 (0.57 Å)
Index ranges	$-7 \leq h \leq 7$ $-31 \leq k \leq 31$ $-11 \leq l \leq 11$	$-28 \leq h \leq 28$ $-12 \leq k \leq 12$ $-19 \leq l \leq 20$	$-14 \leq h \leq 14$ $-16 \leq k \leq 16$ $-24 \leq l \leq 24$
Reflections collected	29709	21707	79993
Independent reflections	2903 $R_{\text{int}} = 0.0991$ $R_{\text{sigma}} = 0.0430$	7061 $R_{\text{int}} = 0.0480$ $R_{\text{sigma}} = 0.0577$	10929 $R_{\text{int}} = 0.0583$ $R_{\text{sigma}} = 0.0420$
Completeness to $\theta = 25.242^\circ$	99.2 %	99.4 %	99.9 %
Data / Restraints / Parameters	2903/0/119	7061/50/215	10929/0/150
Absorption correction	0.5256/0.7454 (none)	0.4910/0.7463 (none)	0.5219/0.7476 (none)
$T_{\text{min}}/T_{\text{max}}$ (method)			
Goodness-of-fit on F^2	1.089	1.731	1.074
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0812$ $wR_2 = 0.2163$	$R_1 = 0.1602$ $wR_2 = 0.4277$	$R_1 = 0.0341$ $wR_2 = 0.0651$
Final R indexes [all data]	$R_1 = 0.1049$ $wR_2 = 0.2361$	$R_1 = 0.1876$ $wR_2 = 0.4592$	$R_1 = 0.0788$ $wR_2 = 0.0813$
Largest peak/hole [$\text{e}\text{\AA}^{-3}$]	8.70/−8.28	15.29/−10.61	2.96/−3.02

Table S2. Crystal structure information of OBA, DDA and TOTA

	OBA	DDA	TOTA
Empirical formula	$\text{C}_4\text{H}_{14}\text{Au}_2\text{I}_8\text{N}_2\text{O}$	$\text{C}_{18}\text{H}_{54}\text{Au}_4\text{I}_{22}\text{N}_6\text{O}_6$	$\text{C}_{10}\text{H}_{26}\text{AuI}_7\text{N}_2\text{O}_3$
Formula weight	1515.30	1853.23	1307.59
Temperature [K]	200.00	200.00	200.0
Crystal system	monoclinic	triclinic	monoclinic
Space group (number)	$P2_1/c$ (14)	$P\bar{1}$ (2)	$P2_1/n$ (14)
a [Å]	15.7263(8)	8.1710(5)	9.1421(5)
b [Å]	8.8418(4)	10.8475(8)	24.0782(12)
c [Å]	17.2007(8)	20.3167(14)	12.9102(6)
α [°]	90	80.611(3)	90
β [°]	98.458(2)	85.264(3)	102.001(2)
γ [°]	90	73.480(3)	90

	OBA	DDA	TOTA
Volume [\AA^3]	2365.7(2)	1702.1(2)	2779.7(2)
<i>Z</i>	4	2	4
ρ_{calc} [gcm^{-3}]	4.254	3.616	3.124
μ [mm^{-1}]	22.820	16.003	13.077
<i>F</i> (000)	2568	1602	2296
Crystal colour	Black	Black	Black
Crystal shape	Polyhedron	Polyhedron	Irregular
Radiation	MoK $_{\alpha}$	MoK $_{\alpha}$	MoK $_{\alpha}$
	($\lambda=0.71073$ \AA)	($\lambda=0.71073$ \AA)	($\lambda=0.71073$ \AA)
2 θ range [$^{\circ}$]	5.11 to 62.07 (0.69 \AA)	3.96 to 62.27 (0.69 \AA)	4.86 to 54.48 (0.78 \AA)
Index ranges	$-22 \leq h \leq 22$ $-12 \leq k \leq 12$ $-24 \leq l \leq 24$	$-11 \leq h \leq 11$ $-15 \leq k \leq 15$ $-29 \leq l \leq 29$	$-11 \leq h \leq 10$ $-30 \leq k \leq 30$ $-16 \leq l \leq 16$
Reflections collected	48868	66940	33809
Independent reflections	7557 $R_{\text{int}} = 0.0650$ $R_{\text{sigma}} = 0.0468$	10882 $R_{\text{int}} = 0.0895$ $R_{\text{sigma}} = 0.0653$	6168 $R_{\text{int}} = 0.1162$ $R_{\text{sigma}} = 0.0785$
Completeness to $\theta = 25.242^{\circ}$	99.9 %	99.4 %	99.9 %
Data / Restraints /Parameters	7557/0/131	10882/0/251	6168/0/210
Absorption correction	0.5926/0.7462	0.5196/0.7462	0.5805/0.7455
T _{min} /T _{max} (method)	(none)	(none)	(none)
Goodness-of-fit on F^2	1.084	1.053	1.043
Final <i>R</i> indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0477$ $wR_2 = 0.1139$	$R_1 = 0.0668$ $wR_2 = 0.2725$	$R_1 = 0.0545$ $wR_2 = 0.1304$
Final <i>R</i> indexes [all data]	$R_1 = 0.0964$ $wR_2 = 0.1450$	$R_1 = 0.1464$ $wR_2 = 0.3746$	$R_1 = 0.1066$ $wR_2 = 0.1649$
Largest peak/hole [$\text{e}\text{\AA}^{-3}$]	10.22/−3.11	7.22/−3.08	9.21/−2.70