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Dimensionally and Structurally Controllable Perovskite Single Crystals: Nickle(II)-Terpyridine-Complex (Ni-Tpy_2) Based Perovskites

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Contents

Experimental section

Materials:

2,2:6,2-terpyridine (Tpy, J&K, >98%), PbI_2 (Aladdin, 99.9%), HI (Aladdin, 55.0 - 58.0%, with ≤1.5 % H_3PO_2 stabilizer), nickel (II) acetate tetrahydrate (Aladdin, 99.9%), acetonitrile (Aladdin, 99.9%).

Growth of $Tpy_2Pb_3I_6$ Single Crystals

0.0233 g Tpy and 0.0693 g PbI_2 were dissolved in a hydrothermal kettle containing 6 mL of HI solvent. The mixture was placed on a heating table, heated to 170 °C and held at this temperature for 3 days to completely dissolve the starting materials. The solution was then cooled from 170 to 110 °C at a rate of 4 °C/h, from 110 °C to 60 °C at a rate of 1 °C/h and last from 60 to 30 °C at a rate of 2 °C/h. Finally, the orange bulk crystal was obtained.

Growth of $[Ni\text{-}Tpy_2]PbI_4$ 0D Single Crystals

0.0233 g Tpy, 0.0125 g Nickel (II) acetate tetrahydrate and 0.0231 g PbI_2 were dissolved in a hydrothermal kettle containing 1mL of water, 2 mL of HI solution and 3 mL of acetonitrile. The cooling process was the same as above. Finally, the red bulk crystal was obtained.

Growth of $[Ni\text{-}Tpy_2]Pb_2I_6$ 1D Single Crystals

0.0233 g Tpy, 0.0125 g Nickel (II) acetate tetrahydrate and 0.0462 g PbI_2 were dissolved in a hydrothermal kettle containing 1mL of water, 2 mL of HI solution and 3 mL of acetonitrile. The cooling process was the same as above. Finally, the orange sheet crystal was obtained.

Growth of $[Ni\text{-}Tpy_2]_2Pb_3I_{10}$ 0D-1D Single Crystals

0.0233 g Tpy, 0.0125 g Nickel (II) acetate tetrahydrate and 0.0347 g PbI_2 were dissolved in a hydrothermal kettle containing 1mL of water, 2 mL of HI solution and 3 mL of acetonitrile. The cooling process was the same as above. Finally, the yellowish lamellar crystal was obtained.

Characterizations

The determination of unit-cell parameters and data collections were performed on XtaLAB Synergy-i using the scan technique with Mo Kα radiation (λ = 0.71073Å), for data collection at a temperature of 100(1) K. The single crystal structure was resolved and refined by SHELXT and OLEX2. [1-3] All H atoms were placed in geometrically calculated positions and refined using a riding model with C—H = 0.97 (methylene) and 0.96 Å (methyl), with Uiso(H) = 1.2Ueq(C) or 1.5 Ueq (methyl C). X-ray photoelectron spectroscopy (XPS) and Ultraviolet photoelectron spectroscopy (UPS) spectra were measured with Thermo K-Alpha+. All XPS spectra were shifted to account for sample charging using inorganic carbon at 284.80 eV as a reference. UPS spectra were used the HeI (21.22eV) emission line. Due to unresolved probable disorder, similarity and rigid-bond restraints were necessary for the anisotropic displacement parameters of the single crystal. UV-vis spectra were measured by placing the corresponding thin films in a double-beam spectrophotometer equipped with an integrating sphere (UV-3600PLUS220/230VC, SHIMADZU). Trap-state density was estimated using SCLC (Space-Charge-Limited Current) method. C-V curve and SCLC curve were measured by an electrochemical workstation (ZAHNER

GIMPS, Germany).

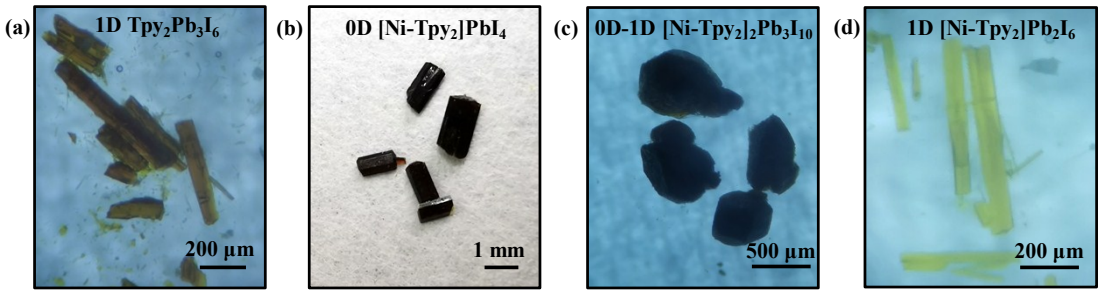

Fig. S1 Morphology of the as-prepared perovskite single crystals.

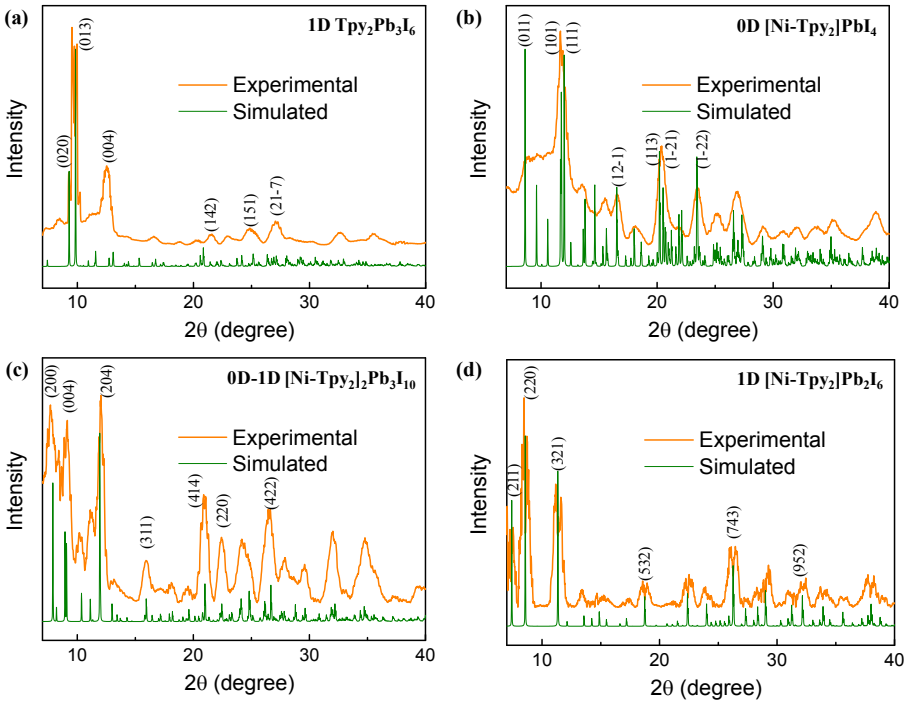

Fig. S2 XRD patterns of as-prepared 1D $Tpy_2Pb_3I_6$, 0D $[Ni\text{-}Tpy_2]PbI_4$, 1D $[Ni\text{-}Tpy_2]Pb_2I_6$ and 0D-1D hybrid $[Ni\text{-}Tpy_2]_2Pb_3I_{10}$ single crystals.

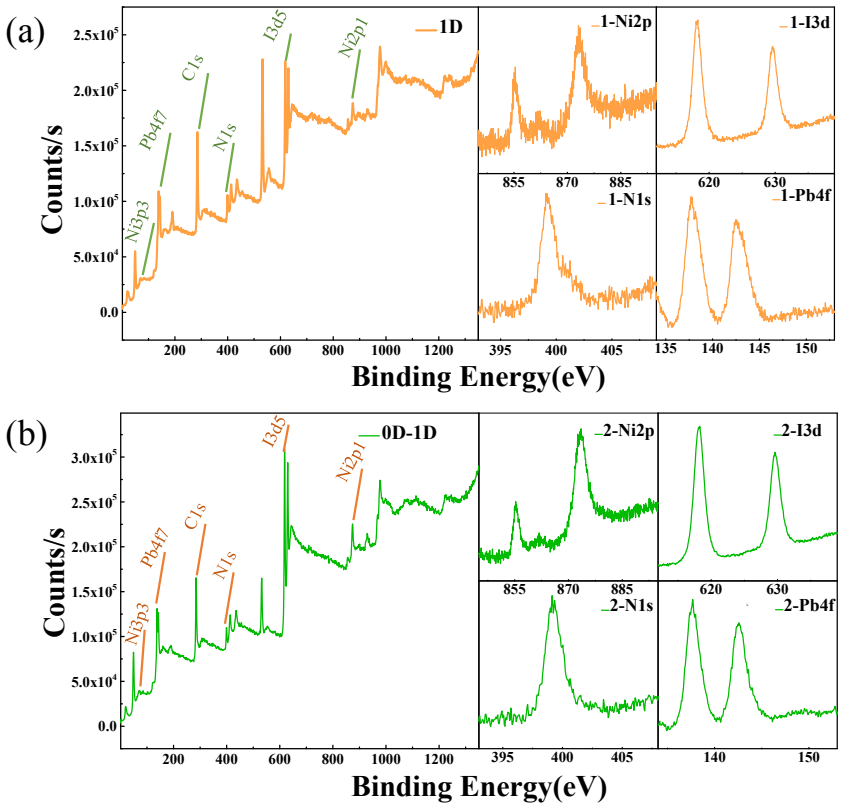

Fig. S3 XPS spectra of (a) 1D [Ni-Tpy$_2$]Pb$_2$I$_6$ and (b) 0D-1D hybrid [Ni-Tpy$_2$]$_2$Pb$_3$I$_{10}$ single crystals.

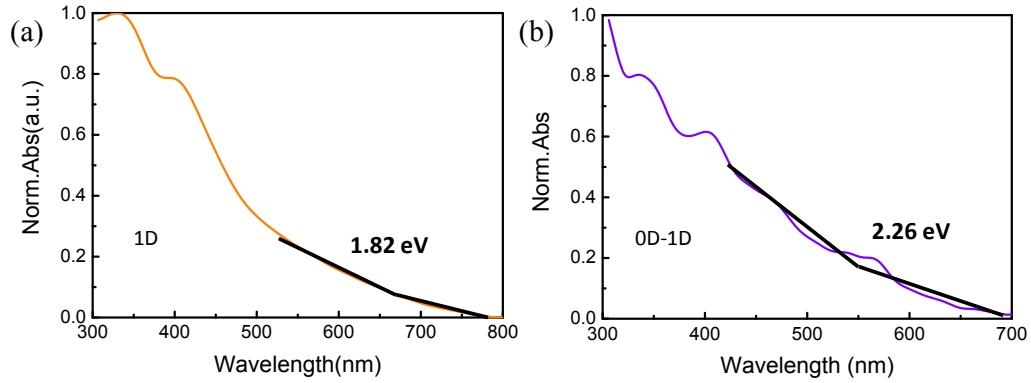

Fig. S4 UV-vis spectra of (a) 1D [Ni-Tpy_2]Pb_2I_6 and (b) 0D-1D hybrid [Ni-Tpy_2]$_2Pb_3I_{10}$ single crystals.

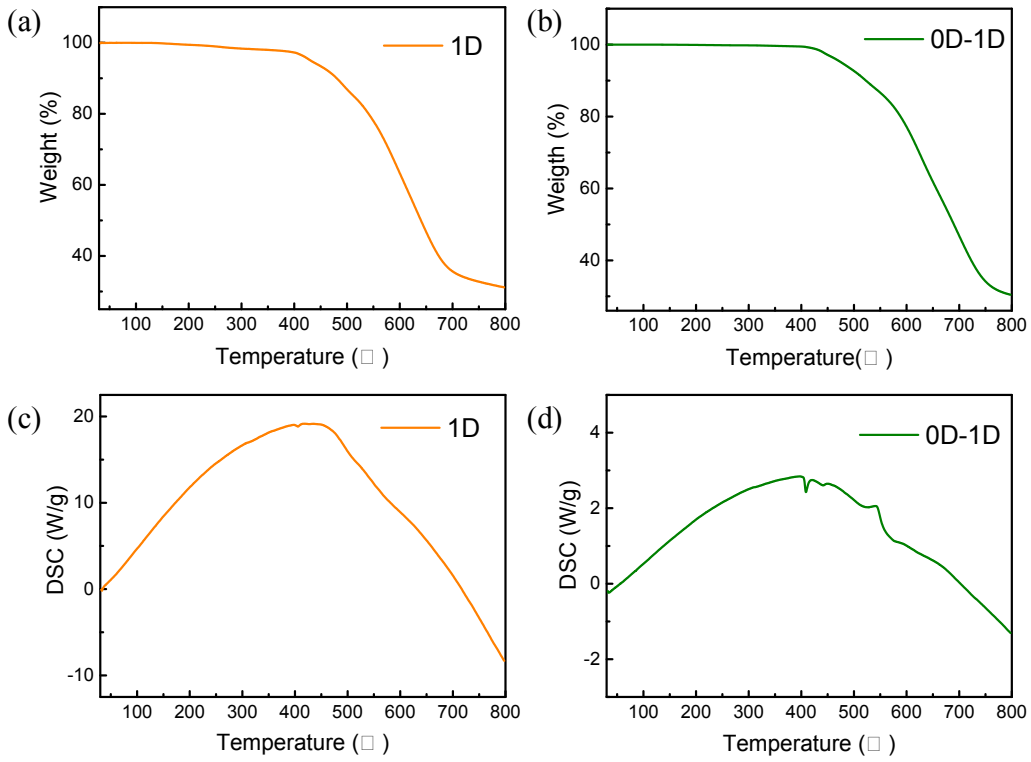

Fig. S5 TGA/DSC curves of the as-prepared (a) 1D [Ni-Tpy_2]Pb_2I_6 and (b) 0D-1D hybrid [Ni-Tpy_2]$_2Pb_3I_{10}$ single crystals. DSC curves of the as-prepared (c) 1D [Ni-Tpy_2]Pb_2I_6 and (d) 0D-1D hybrid [Ni-Tpy_2]$_2Pb_3I_{10}$ single crystals.

Table S1. Details of X-ray crystallographic parameters of Ni-Tpy$_2$ based perovskites.

Crystal type / Parameter	$[Ni\text{-}Tpy_2]_2Pb_3I_{10}$	$[Ni\text{-}Tpy_2]PbI_4$	$[Ni\text{-}Tpy_2]Pb_2I_6$	$Tpy_2Pb_3I_6$
CCDC NO.	1968999	1968998	1969000	1969001
Formula weight	2941.06g/mol	1240.03 g/mol	1701.02g/mol	1849.50 g/mol
Crystal system	orthorhombic	triclinic	cubic	monoclinic
Space group	P c a 21	P -1	I -4 3 d	P 1 21/c 1
Unit-cell dimensions	a = 22.3909 (6) Å b = 8.5089 (2) Å c = 39.5465 (9) Å α = 90° β = 90° γ = 90°	a = 9.1237(5) Å b = 13.4076 (7) Å c =14.8525 (8) Å α = 83.392°(4) β = 87.801°(5) γ = 74.413°(5)	a = 29.1712 (2) Å b = 29.1712 (2) Å c = 29.1712(2) Å α = 90° β = 90° γ = 90°	a =10.1531(3) Å b = 19.0353 (6) Å c = 30.5736(11) Å α = 90° β = 90.798°(3) γ = 90°
Volume	7534.5 (3) Å^3	1738.36 (17) Å^3	24823.5 (5) Å^3	5908.3 (3) Å^3
Z	4	2	24	6
ρ(calculated)	2.593 g/cm^3	2.369g/cm^3	2.731 g/cm^3	3.119 g/cm^3
Absorption coefficient	11.313	8.959	13.074	17.523
F(000)	5280	1132	18096	4848
Crystal size max/mid/min	0.2×0.2×0.1mm^3	0.2×0.2×0.1mm^3	0.2×0.2×0.1mm^3	0.2×0.2×0.1mm^3
Radiation	MoKα(λ=0.71073)	MoKα(λ=0.71073)	MoKα(λ=0.71073)	MoKα(λ=0.71073)
2θ range for data collection	5.958°to89.989°	5.986°to89.999°	5.243°to89.995°	5.465°to89.992°
Index ranges	-26≤h≤26, -8≤k≤10, -47≤l≤38	-10≤h≤10, -15≤k≤15, -15≤l≤17	-22≤h≤33, -22≤k≤22, -34≤l≤32	-12≤h≤11, -22≤k≤22, -36≤l≤36
Reflections collected	31947	10429	13778	30544
Independent reflections	11161[Rint=0.0474,Rsigna=0.0749]	5864 [Rint=0.0574, Rsigna=0.0938]	3185 [Rint=0.0176, Rsigna=0.0204]	10181[Rint=0.0338 ,Rsigna=0.0552]
Data/restraints/ parameters	11161/1/748	5864/0/379	3185/0/205	10181/0/610
Final R indexes [I>=2σ(I)]	R1=0.0749, wR2= 1.046	R1=0.0938, wR2=1.019	R1=0.0204, wR2=1.029	R1=0.0552, wR2= 1.031
Final R indexes [all data]	R1=0.0749, wR2=0.1140	R1=0.0984, wR2=0.1238	R1=0.0204, wR2=0.0283	R1=0.0552, wR2=0.0638
Goodness-of-fit on F^2	1.046	1.019	1.029	1.031

Largest difference map peak/hole	1.25/-1.37e Å^{-3}	2.69/-2.27e Å^{-3}	0.51/-0.53e Å^{-3}	1.50/-1.47e Å^{-3}

Table S2. Details of atoms occupation situation of $[Ni\text{-}Tpy_2]_2Pb_3I_{10}$.

Atom	x	y	z	Occ.	U	Site	Sym.
Pb01	0.7615	0.23746	0.29232	1	0.054	4a	1
Pb02	0.75971	0.73794	0.29146	1	0.053	4a	1
Pb00	0.31839	1.25627	0.54162	1	0.078	4a	1
I004	0.73897	0.49434	0.35357	1	0.056	4a	1
I005	0.66099	0.9879	0.31358	1	0.055	4a	1
I006	0.85932	0.4903	0.26965	1	0.054	4a	1
I007	0.78483	-0.00537	0.22998	1	0.057	4a	1
I008	0.84616	0.0008	0.33365	1	0.068	4a	1
I009	0.67441	0.4992	0.2506	1	0.068	4a	1
I00A	0.39369	1.291	0.47127	1	0.08	4a	1
I0B	0.37865	1.2052	0.61021	1	0.095	4a	1
I0C	0.25681	0.9517	0.53366	1	0.112	4a	1
Ni0D	0.52719	0.7074	0.65465	1	0.042	4a	1
Ni0E	0.55086	0.7876	0.4308	1	0.039	4a	1
I0F	0.2147	1.4639	0.55949	1	0.15	4a	1
N00G	0.5344	0.702	0.3821	1	0.036	4a	1
N00H	0.4383	0.755	0.6535	1	0.043	4a	1
N00I	0.5214	0.48	0.6748	1	0.063	4a	1
N00J	0.5879	0.577	0.4483	1	0.047	4a	1
N00K	0.5123	0.794	0.7029	1	0.039	4a	1
N00L	0.5036	0.646	0.605	1	0.06	4a	1
N00M	0.6133	0.652	0.6568	1	0.045	4a	1
N00N	0.4634	0.756	0.4333	1	0.04	4a	1
C00O	0.4144	0.807	0.6815	1	0.046	4a	1
N00P	0.6367	0.836	0.4271	1	0.06	4a	1
N00Q	0.5328	0.861	0.4806	1	0.046	4a	1
C00R	0.475	0.675	0.377	1	0.042	4a	1
N00S	0.5509	1.017	0.4106	1	0.06	4a	1
N00T	0.5711	0.913	0.6377	1	0.048	4a	1
C00U	0.6542	0.968	0.4136	1	0.076	4a	1
C00V	0.4746	0.869	0.4881	1	0.046	4a	1
C00W	0.5503	0.801	0.7277	1	0.058	4a	1
H00W	0.58986	0.77542	0.72325	1	0.069	4a	1
C00X	0.6752	0.722	0.4372	1	0.074	4a	1
C00Y	0.434	0.804	0.4614	1	0.054	4a	1
C00Z	0.5351	0.844	0.761	1	0.056	4a	1
H00Z	0.56366	0.85078	0.77805	1	0.066	4a	1
C010	0.5767	0.273	0.7008	1	0.075	4a	1

H010	0.61297	0.22562	0.70602	1	0.088	4a	1
C011	0.4731	0.409	0.6847	1	0.067	4a	1
H011	0.43702	0.45593	0.6788	1	0.083	4a	1
C012	0.6664	1.013	0.6212	1	0.08	4a	1
H012	0.70755	0.99956	0.61958	1	0.098	4a	1
C013	0.5446	1.047	0.6272	1	0.053	4a	1
H013	0.50335	1.05853	0.62875	1	0.063	4a	1
C014	0.589	0.322	0.4739	1	0.091	4a	1
H014	0.56699	0.23636	0.48163	1	0.111	4a	1
C015	0.64	1.145	0.6114	1	0.103	4a	1
H015	0.66319	1.22471	0.60227	1	0.123	4a	1
C016	0.5714	0.688	0.3565	1	0.051	4a	1
H016	0.6115	0.71115	0.36001	1	0.061	4a	1
C017	0.3417	0.726	0.4355	1	0.066	4a	1
H017	0.30049	0.71397	0.43642	1	0.079	4a	1
C018	0.4541	0.825	0.7099	1	0.049	4a	1
C019	0.6303	0.897	0.6337	1	0.057	4a	1
C01A	0.626	0.51	0.671	1	0.06	4a	1
C01B	0.4086	0.718	0.6263	1	0.07	4a	1
C01C	0.5758	0.416	0.6821	1	0.066	4a	1
C01D	0.4343	0.703	0.4061	1	0.045	4a	1
C01E	0.4961	0.978	0.541	1	0.089	4a	1
H01E	0.48391	1.01789	0.56185	1	0.107	4a	1
C01F	0.4455	0.66	0.5986	1	0.071	4a	1
C01G	0.604	1.071	0.4035	1	0.075	4a	1
C01H	0.7533	0.891	0.42	1	0.147	4a	1
H01H	0.79388	0.91138	0.41744	1	0.178	4a	1
C01I	0.3724	0.789	0.463	1	0.069	4a	1
H01I	0.35178	0.82155	0.48223	1	0.081	4a	1
C01J	0.5419	0.587	0.5823	1	0.094	4a	1
H01J	0.5821	0.57544	0.58766	1	0.111	4a	1
C01K	0.5552	0.968	0.5343	1	0.06	4a	1
H01K	0.58392	1.00129	0.54973	1	0.072	4a	1
C01L	0.525	0.206	0.7112	1	0.092	4a	1
H01L	0.52681	0.11483	0.72407	1	0.111	4a	1
C01M	0.5701	0.909	0.5043	1	0.055	4a	1
H01M	0.61064	0.90106	0.49959	1	0.066	4a	1
C01N	0.7264	0.568	0.6644	1	0.087	4a	1
H01N	0.76644	0.54131	0.6668	1	0.106	4a	1
C01O	0.4367	0.865	0.7413	1	0.066	4a	1
H01O	0.39665	0.88497	0.74566	1	0.08	4a	1
C01P	0.714	0.994	0.4104	1	0.123	4a	1
H01P	0.72731	1.08757	0.40101	1	0.148	4a	1

C01Q	0.4529	0.931	0.5178	1	0.071	4a	1
H01Q	0.41224	0.94148	0.522	1	0.083	4a	1
C01R	0.7141	0.713	0.6501	1	0.077	4a	1
H01R	0.74369	0.78234	0.64279	1	0.093	4a	1
C01S	0.608	1.215	0.385	1	0.113	4a	1
H01S	0.64487	1.25233	0.37853	1	0.136	4a	1
C01T	0.6539	0.746	0.6475	1	0.059	4a	1
C01U	0.6492	0.58	0.4498	1	0.06	4a	1
C01V	0.578	1.167	0.6143	1	0.081	4a	1
H01V	0.56092	1.26065	0.60759	1	0.097	4a	1
C01W	0.373	0.682	0.4064	1	0.065	4a	1
H01W	0.35333	0.63918	0.3878	1	0.078	4a	1
C01X	0.4955	0.611	0.3185	1	0.083	4a	1
H01X	0.48235	0.58268	0.29709	1	0.099	4a	1
C01Y	0.462	0.553	0.5427	1	0.123	4a	1
H01Y	0.44697	0.51992	0.52192	1	0.149	4a	1
C01Z	0.4778	0.876	0.7668	1	0.083	4a	1
H01Z	0.4656	0.9049	0.7884	1	0.098	4a	1
C020	0.7345	0.752	0.4339	1	0.103	4a	1
H020	0.76238	0.67796	0.44108	1	0.12	4a	1
C021	0.6839	0.459	0.6758	1	0.093	4a	1
H021	0.69374	0.36242	0.68548	1	0.111	4a	1
C022	0.3516	0.832	0.6821	1	0.078	4a	1
H022	0.33205	0.86786	0.70142	1	0.091	4a	1
C023	0.47	0.267	0.7035	1	0.097	4a	1
H023	0.43427	0.2207	0.70989	1	0.114	4a	1
C024	0.3222	0.802	0.6533	1	0.084	4a	1
H024	0.28146	0.82321	0.65303	1	0.099	4a	1
C025	0.646	0.324	0.4767	1	0.13	4a	1
H025	0.66613	0.23943	0.48654	1	0.156	4a	1
C026	0.5542	0.64	0.3251	1	0.064	4a	1
H026	0.5825	0.62801	0.3081	1	0.078	4a	1
C027	0.5603	0.453	0.4589	1	0.065	4a	1
H027	0.51896	0.4491	0.45652	1	0.077	4a	1
C028	0.3462	0.744	0.6246	1	0.093	4a	1
H028	0.32366	0.72234	0.6054	1	0.11	4a	1
C029	0.4555	0.625	0.3464	1	0.072	4a	1
H029	0.41539	0.60061	0.34344	1	0.085	4a	1
C02A	0.5023	1.097	0.4018	1	0.097	4a	1
H02A	0.46476	1.05837	0.40743	1	0.114	4a	1
C02B	0.6789	0.453	0.4647	1	0.113	4a	1
H02B	0.72026	0.45471	0.46667	1	0.137	4a	1
C17	0.52	0.542	0.5492	1	0.11	4a	1

H17	0.54588	0.50482	0.53276	1	0.132	4a	1
C19	0.4236	0.615	0.5674	1	0.1	4a	1
H19	0.38313	0.6254	0.56278	1	0.118	4a	1
C29	0.561	1.296	0.377	1	0.19	4a	1
H29	0.56405	1.39308	0.3664	1	0.23	4a	1
C45	0.507	1.233	0.3846	1	0.153	4a	1
H45	0.47291	1.28553	0.37789	1	0.187	4a	1

Table S3. Bond length of $[Ni\text{-}Tpy_2]_2Pb_3I_{10}$.

Atom	Atom	Length/ Å	Atom	Atom	Length/ Å
Pb01	I004	3.3014(19)	N00T	C013	1.35(3)
Pb01	I005	3.2061(19)	N00T	C019	1.34(3)
Pb01	I006	3.1986(19)	C00U	C01G	1.47(5)
Pb01	I007	3.259(2)	C00U	C01P	1.36(5)
Pb01	I008	3.212(2)	C00V	C00Y	1.50(3)
Pb01	I009	3.389(2)	C00V	C01Q	1.38(3)
Pb02	I004	3.247(2)	C00W	C00Z	1.41(3)
Pb02	I005	3.1898(19)	C00X	C01U	1.43(4)
Pb02	I006	3.1870(19)	C00X	C020	1.36(4)
Pb02	I007	3.316(2)	C00Y	C01I	1.39(3)
Pb02	I008	3.396(2)	C00Z	C01Z	1.33(4)
Pb02	I009	3.223(2)	C010	C01C	1.42(4)
Pb00	I00A	3.267(3)	C010	C01L	1.35(5)
Pb00	I0B	3.060(3)	C011	C023	1.42(4)
Pb00	I0C	2.952(3)	C012	C015	1.33(5)
Pb00	I0F	3.002(3)	C012	C019	1.37(4)
Ni0D	N00H	2.031(19)	C013	C01V	1.37(4)
Ni0D	N00I	2.09(2)	C014	C025	1.29(6)
Ni0D	N00K	2.07(2)	C014	C027	1.42(4)
Ni0D	N00L	2.10(2)	C015	C01V	1.39(5)
Ni0D	N00M	1.988(19)	C016	C026	1.36(3)
Ni0D	N00T	2.12(2)	C017	C01I	1.40(4)
Ni0E	N00G	2.093(19)	C017	C01W	1.40(4)
Ni0E	N00J	2.09(2)	C018	C01O	1.34(3)
Ni0E	N00N	1.977(18)	C019	C01T	1.49(4)
Ni0E	N00P	1.97(2)	C01A	C01C	1.45(4)
Ni0E	N00Q	2.107(19)	C01A	C021	1.38(4)
Ni0E	N00S	2.11(2)	C01B	C01F	1.46(4)
N00G	C00R	1.36(3)	C01B	C028	1.42(5)
N00G	C016	1.31(3)	C01D	C01W	1.38(3)
N00H	C00O	1.31(3)	C01E	C01K	1.35(4)
N00H	C01B	1.30(3)	C01E	C01Q	1.39(5)
N00I	C011	1.30(3)	C01F	C19	1.38(4)

N00I	C01C	1.37(3)	C01G	C01S	1.43(4)
N00J	C01U	1.37(3)	C01H	C01P	1.29(7)
N00J	C027	1.29(3)	C01H	C020	1.37(6)
N00K	C00W	1.30(3)	C01J	C17	1.45(5)
N00K	C018	1.36(3)	C01K	C01M	1.33(3)
N00L	C01F	1.33(3)	C01L	C023	1.37(5)
N00L	C01J	1.34(4)	C01N	C01R	1.39(4)
N00M	C01A	1.36(3)	C01N	C021	1.41(5)
N00M	C01T	1.27(3)	C01O	C01Z	1.37(4)
N00N	C00Y	1.35(3)	C01R	C01T	1.38(4)
N00N	C01D	1.34(3)	C01S	C29	1.29(7)
C00O	C018	1.44(3)	C01U	C02B	1.40(5)
C00O	C022	1.42(3)	C01X	C026	1.36(4)
N00P	C00U	1.31(4)	C01X	C029	1.42(4)
N00P	C00X	1.35(4)	C01Y	C17	1.32(5)
N00Q	C00V	1.34(3)	C01Y	C19	1.41(5)
N00Q	C01M	1.32(3)	C022	C024	1.34(4)
C00R	C01D	1.49(3)	C024	C028	1.35(5)
C00R	C029	1.35(3)	C025	C02B	1.40(6)
N00S	C01G	1.31(4)	C02A	C45	1.35(5)
N00S	C02A	1.33(4)	C29	C45	1.34(9)

Table S4. Bond Angles of $[Ni\text{-}Tpy_2]_2Pb_3I_{10}$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
I004	Pb01	I009	80.46(5)	C00U	N00P	C00X	123.(3)
I005	Pb01	I004	97.98(5)	C00X	N00P	Ni0E	117.(2)
I005	Pb01	I007	83.74(5)	C00V	N00Q	Ni0E	114.0(16)
I005	Pb01	I008	82.28(5)	C01M	N00Q	Ni0E	129.4(18)
I005	Pb01	I009	99.15(5)	C01M	N00Q	C00V	116.(2)
I006	Pb01	I004	82.24(5)	N00G	C00R	C01D	117.(2)
I006	Pb01	I005	178.45(6)	C029	C00R	N00G	120.(2)
I006	Pb01	I007	96.01(5)	C029	C00R	C01D	123.(2)
I006	Pb01	I008	99.22(5)	C01G	N00S	Ni0E	114.(2)
I006	Pb01	I009	79.37(5)	C01G	N00S	C02A	121.(3)
I007	Pb01	I004	177.88(6)	C02A	N00S	Ni0E	125.(2)
I007	Pb01	I009	98.08(5)	C013	N00T	Ni0D	126.3(18)
I008	Pb01	I004	97.57(5)	C019	N00T	Ni0D	114.1(17)
I008	Pb01	I007	83.86(5)	C019	N00T	C013	119.(2)
I008	Pb01	I009	177.69(6)	N00P	C00U	C01G	113.(3)
I004	Pb02	I007	177.67(6)	N00P	C00U	C01P	118.(4)
I004	Pb02	I008	97.49(6)	C01P	C00U	C01G	129.(4)
I005	Pb02	I004	96.84(5)	N00Q	C00V	C00Y	115.(2)
I005	Pb02	I007	83.07(5)	N00Q	C00V	C01Q	123.(3)

I005	Pb02	I008	79.69(5)	C01Q	C00V	C00Y	122.(3)
I005	Pb02	I009	98.46(5)	N00K	C00W	C00Z	124.(3)
I006	Pb02	I004	83.27(5)	N00P	C00X	C01U	116.(3)
I006	Pb02	I005	179.45(7)	N00P	C00X	C020	118.(4)
I006	Pb02	I007	96.79(5)	C020	C00X	C01U	126.(4)
I006	Pb02	I008	99.76(5)	N00N	C00Y	C00V	113.(2)
I006	Pb02	I009	82.09(5)	N00N	C00Y	C01I	120.(3)
I007	Pb02	I008	80.20(5)	C01I	C00Y	C00V	127.(3)
I009	Pb02	I004	83.81(5)	C01Z	C00Z	C00W	117.(3)
I009	Pb02	I007	98.51(6)	C01L	C010	C01C	120.(3)
I009	Pb02	I008	177.84(6)	N00I	C011	C023	126.(3)
I0B	Pb00	I00A	122.69(7)	C015	C012	C019	117.(4)
I0C	Pb00	I00A	103.27(7)	N00T	C013	C01V	120.(3)
I0C	Pb00	I0B	100.14(9)	C025	C014	C027	119.(4)
I0C	Pb00	I0F	100.4(1)	C012	C015	C01V	122.(4)
I0F	Pb00	I00A	123.12(9)	N00G	C016	C026	123.(3)
I0F	Pb00	I0B	102.47(9)	C01I	C017	C01W	120.(3)
Pb02	I004	Pb01	81.13(5)	N00K	C018	C00O	114.(2)
Pb02	I005	Pb01	83.30(5)	C01O	C018	N00K	121.(2)
Pb02	I006	Pb01	83.66(5)	C01O	C018	C00O	125.(2)
Pb01	I007	Pb02	80.55(5)	N00T	C019	C012	123.(3)
Pb01	I008	Pb02	80.01(5)	N00T	C019	C01T	113.(2)
Pb02	I009	Pb01	80.16(5)	C012	C019	C01T	123.(3)
N00H	Ni0D	N00I	97.5(8)	N00M	C01A	C01C	117.(2)
N00H	Ni0D	N00K	78.1(8)	N00M	C01A	C021	122.(3)
N00H	Ni0D	N00L	77.4(9)	C021	C01A	C01C	121.(3)
N00H	Ni0D	N00T	106.5(7)	N00H	C01B	C01F	114.(3)
N00I	Ni0D	N00L	96.3(8)	N00H	C01B	C028	120.(3)
N00I	Ni0D	N00T	155.8(9)	C028	C01B	C01F	125.(3)
N00K	Ni0D	N00I	88.2(8)	N00I	C01C	C010	118.(3)
N00K	Ni0D	N00L	155.4(9)	N00I	C01C	C01A	114.(3)
N00K	Ni0D	N00T	94.1(7)	C010	C01C	C01A	128.(3)
N00L	Ni0D	N00T	91.6(8)	N00N	C01D	C00R	112.(2)
N00M	Ni0D	N00H	177.4(8)	N00N	C01D	C01W	122.(2)
N00M	Ni0D	N00I	79.9(9)	C01W	C01D	C00R	126.(2)
N00M	Ni0D	N00K	101.6(8)	C01K	C01E	C01Q	122.(3)
N00M	Ni0D	N00L	103.0(9)	N00L	C01F	C01B	116.(2)
N00M	Ni0D	N00T	76.1(8)	N00L	C01F	C19	119.(4)
N00G	Ni0E	N00J	94.4(7)	C19	C01F	C01B	124.(3)
N00G	Ni0E	N00Q	158.6(8)	N00S	C01G	C00U	115.(3)
N00G	Ni0E	N00S	88.4(8)	N00S	C01G	C01S	117.(4)
N00J	Ni0E	N00Q	91.3(7)	C01S	C01G	C00U	127.(4)
N00J	Ni0E	N00S	156.6(10)	C01P	C01H	C020	119.(4)

N00N	Ni0E	N00G	79.9(8)	C00Y	C01I	C017	119.(3)
N00N	Ni0E	N00J	105.1(8)	N00L	C01J	C17	119.(4)
N00N	Ni0E	N00Q	78.6(8)	C01M	C01K	C01E	116.(3)
N00N	Ni0E	N00S	98.3(9)	C010	C01L	C023	123.(3)
N00P	Ni0E	N00G	100.1(8)	N00Q	C01M	C01K	126.(3)
N00P	Ni0E	N00J	79.4(10)	C01R	C01N	C021	126.(3)
N00P	Ni0E	N00N	175.5(10)	C018	C01O	C01Z	120.(3)
N00P	Ni0E	N00Q	101.2(8)	C01H	C01P	C00U	122.(5)
N00P	Ni0E	N00S	77.2(11)	C00V	C01Q	C01E	115.(3)
N00Q	Ni0E	N00S	94.5(8)	C01T	C01R	C01N	114.(3)
C00R	N00G	Ni0E	111.5(14)	C29	C01S	C01G	123.(5)
C016	N00G	Ni0E	129.1(16)	N00M	C01T	C019	113.(2)
C016	N00G	C00R	119.(2)	N00M	C01T	C01R	123.(3)
C00O	N00H	Ni0D	116.6(16)	C01R	C01T	C019	123.(3)
C01B	N00H	Ni0D	118.(2)	N00J	C01U	C00X	114.(3)
C01B	N00H	C00O	125.(3)	N00J	C01U	C02B	118.(3)
C011	N00I	Ni0D	127.(2)	C02B	C01U	C00X	127.(4)
C011	N00I	C01C	119.(3)	C013	C01V	C015	119.(3)
C01C	N00I	Ni0D	113.(2)	C01D	C01W	C017	118.(3)
C01U	N00J	Ni0E	113.0(19)	C026	C01X	C029	116.(3)
C027	N00J	Ni0E	128.1(18)	C17	C01Y	C19	119.(4)
C027	N00J	C01U	119.(3)	C00Z	C01Z	C01O	120.(3)
C00W	N00K	Ni0D	127.3(18)	C00X	C020	C01H	120.(4)
C00W	N00K	C018	118.(2)	C01A	C021	C01N	113.(4)
C018	N00K	Ni0D	114.3(15)	C024	C022	C00O	116.(3)
C01F	N00L	Ni0D	114.(2)	C01L	C023	C011	113.(4)
C01F	N00L	C01J	122.(3)	C022	C024	C028	126.(3)
C01J	N00L	Ni0D	124.(2)	C014	C025	C02B	120.(4)
C01A	N00M	Ni0D	115.5(18)	C016	C026	C01X	120.(3)
C01T	N00M	Ni0D	122.1(19)	N00J	C027	C014	124.(3)
C01T	N00M	C01A	122.(2)	C024	C028	C01B	114.(3)
C00Y	N00N	Ni0E	118.9(17)	C00R	C029	C01X	121.(3)
C01D	N00N	Ni0E	119.3(16)	N00S	C02A	C45	120.(4)
C01D	N00N	C00Y	122.(2)	C01U	C02B	C025	120.(4)
N00H	C00O	C018	116.(2)	C01Y	C17	C01J	119.(4)
N00H	C00O	C022	118.(2)	C01F	C19	C01Y	121.(4)
C022	C00O	C018	126.(3)	C01S	C29	C45	117.(4)
C00U	N00P	Ni0E	120.(2)	C29	C45	C02A	122.(6)

Table S5. Details of atoms occupation situation of [Ni-Tpy$_2$]PbI$_4$.

Atom	x	y	z	Occ.	U	Site	Sym.
Pb01	1.14568	0.2174	0.75974	1	0.081	2i	1
I02	0.89689	0.09027	0.82568	1	0.073	2i	1

I03	0.9828	0.42426	0.66	1	0.089	2i	1
I04	1.38171	0.13138	0.6198	1	0.098	2i	1
I05	1.32707	0.28521	0.89615	1	0.104	2i	1
Ni06	0.43458	0.69732	0.73333	1	0.035	2i	1
N007	0.317	0.7766	0.6162	1	0.039	2i	1
N008	0.4363	0.581	0.6607	1	0.035	2i	1
N009	0.2304	0.6963	0.8058	1	0.044	2i	1
N00A	0.4131	0.8149	0.807	1	0.043	2i	1
N00B	0.5605	0.5681	0.8178	1	0.038	2i	1
N00C	0.6286	0.7477	0.6936	1	0.044	2i	1
C00D	0.3488	0.6015	0.5876	1	0.037	2i	1
C00E	0.5765	0.4756	0.7855	1	0.039	2i	1
C00F	0.2932	0.7134	0.5567	1	0.038	2i	1
C00G	0.4955	0.4828	0.699	1	0.036	2i	1
C00H	0.6408	0.8305	0.7355	1	0.048	2i	1
C00I	0.5195	0.8678	0.8005	1	0.047	2i	1
C00J	0.4708	0.3999	0.6583	1	0.047	2i	1
H00J	0.5145	0.33149	0.68207	1	0.057	2i	1
C00K	0.2749	0.8796	0.5925	1	0.05	2i	1
H00K	0.29367	0.92304	0.63259	1	0.06	2i	1
C00L	0.2942	0.8396	0.8626	1	0.049	2i	1
C00M	0.3209	0.5206	0.5443	1	0.046	2i	1
H00M	0.26389	0.53404	0.49163	1	0.055	2i	1
C00N	0.1874	0.7742	0.8615	1	0.045	2i	1
C00O	0.2258	0.7538	0.474	1	0.051	2i	1
H00O	0.21153	0.70952	0.43332	1	0.061	2i	1
C00P	0.2051	0.9245	0.5115	1	0.063	2i	1
H00P	0.17614	0.9965	0.49775	1	0.075	2i	1
C00Q	0.382	0.4208	0.5837	1	0.053	2i	1
H00Q	0.3618	0.36566	0.55825	1	0.064	2i	1
C00R	0.144	0.633	0.7996	1	0.058	2i	1
H00R	0.17503	0.58043	0.76171	1	0.07	2i	1
C00T	0.6608	0.3836	0.8284	1	0.06	2i	1
H00T	0.67076	0.32132	0.80383	1	0.072	2i	1
C00U	0.009	0.6416	0.8472	1	0.076	2i	1
H00U	-0.04988	0.59569	0.84222	1	0.091	2i	1
C00V	0.1795	0.8608	0.4521	1	0.065	2i	1
H00V	0.13138	0.88889	0.39728	1	0.079	2i	1
C00W	0.6233	0.568	0.8971	1	0.062	2i	1
H00W	0.60751	0.63031	0.92247	1	0.074	2i	1
C00X	0.2783	0.9192	0.917	1	0.074	2i	1
H00X	0.19675	0.93548	0.95715	1	0.089	2i	1
C00Y	0.5075	0.9504	0.8504	1	0.068	2i	1

H00Y	0.57892	0.98891	0.84378	1	0.082	2i	1
C00Z	0.7115	0.4774	0.9426	1	0.075	2i	1
H00Z	0.75812	0.47949	0.99671	1	0.09	2i	1
C010	0.0529	0.7865	0.9104	1	0.067	2i	1
H010	0.02328	0.83898	0.94843	1	0.08	2i	1
C012	0.389	0.9741	0.9095	1	0.085	2i	1
H012	0.38188	1.02765	0.94545	1	0.103	2i	1
C013	-0.0358	0.7208	0.9025	1	0.085	2i	1
H013	-0.12716	0.7294	0.9345	1	0.102	2i	1
C014	0.8707	0.8299	0.652	1	0.082	2i	1
H014	0.9534	0.85731	0.63829	1	0.099	2i	1
C015	0.7633	0.8733	0.7135	1	0.07	2i	1
H015	0.77185	0.93077	0.74042	1	0.084	2i	1
C016	0.8575	0.7472	0.6108	1	0.074	2i	1
H016	0.92846	0.71799	0.56806	1	0.089	2i	1
C10	0.7355	0.7088	0.6348	1	0.058	2i	1
H10	0.727	0.65133	0.60801	1	0.07	2i	1
C11	0.73	0.3848	0.9077	1	0.079	2i	1
H11	0.78907	0.32329	0.93785	1	0.095	2i	1

Table S6. Bond length of [Ni-Tpy$_2$]PbI$_4$.

Atom	Atom	Length/ Å	Atom	Atom	Length/ Å
Pb01	I02	3.2468(11)	C00L	C00X	1.386(16)
Pb01	I03	3.0172(13)	C00M	H00M	0.93
Pb01	I04	3.0267(15)	C00M	C00Q	1.374(16)
Pb01	I05	3.0265(13)	C00N	C010	1.382(16)
Ni06	N007	2.101(8)	C00O	H00O	0.93
Ni06	N008	1.992(8)	C00O	C00V	1.385(16)
Ni06	N009	2.118(9)	C00P	H00P	0.93
Ni06	N00A	1.983(9)	C00P	C00V	1.364(17)
Ni06	N00B	2.106(8)	C00Q	H00Q	0.93
Ni06	N00C	2.100(9)	C00R	H00R	0.93
N007	C00F	1.354(12)	C00R	C00U	1.380(18)
N007	C00K	1.339(13)	C00T	H00T	0.93
N008	C00D	1.331(12)	C00T	C11	1.362(18)
N008	C00G	1.349(12)	C00U	H00U	0.93
N009	C00N	1.373(13)	C00U	C013	1.38(2)
N009	C00R	1.317(14)	C00V	H00V	0.93
N00A	C00I	1.343(13)	C00W	H00W	0.93
N00A	C00L	1.331(14)	C00W	C00Z	1.381(18)
N00B	C00E	1.350(12)	C00X	H00X	0.93
N00B	C00W	1.329(14)	C00X	C012	1.40(2)
N00C	C00H	1.365(13)	C00Y	H00Y	0.93

N00C	C10	1.323(14)	C00Y	C012	1.36(2)
C00D	C00F	1.472(14)	C00Z	H00Z	0.93
C00D	C00M	1.405(14)	C00Z	C11	1.367(19)
C00E	C00G	1.486(14)	C010	H010	0.93
C00E	C00T	1.366(15)	C010	C013	1.36(2)
C00F	C00O	1.381(15)	C012	H012	0.93
C00G	C00J	1.396(14)	C013	H013	0.93
C00H	C00I	1.462(16)	C014	H014	0.93
C00H	C015	1.400(16)	C014	C015	1.37(2)
C00I	C00Y	1.380(15)	C014	C016	1.36(2)
C00J	H00J	0.93	C015	H015	0.93
C00J	C00Q	1.356(16)	C016	H016	0.93
C00K	H00K	0.93	C016	C10	1.365(17)
C00K	C00P	1.378(16)	C10	H10	0.93
C00L	C00N	1.477(16)	C11	H11	0.93

Table S7. Bond Angles of [Ni-Tpy$_2$]PbI$_4$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
I03	Pb01	I02	108.69(3)	C00X	C00L	C00N	124.8(12)
I03	Pb01	I04	100.89(4)	C00D	C00M	H00M	121.6
I03	Pb01	I05	101.28(4)	C00Q	C00M	C00D	116.8(10)
I04	Pb01	I02	118.58(3)	C00Q	C00M	H00M	121.6
I05	Pb01	I02	120.88(3)	N009	C00N	C00L	114.6(9)
I05	Pb01	I04	103.47(4)	N009	C00N	C010	119.9(12)
N007	Ni06	N009	92.6(3)	C010	C00N	C00L	125.5(11)
N007	Ni06	N00B	156.5(3)	C00F	C00O	H00O	120.2
N008	Ni06	N007	77.9(3)	C00F	C00O	C00V	119.5(11)
N008	Ni06	N009	96.8(3)	C00V	C00O	H00O	120.2
N008	Ni06	N00B	78.7(3)	C00K	C00P	H00P	120.8
N008	Ni06	N00C	106.4(3)	C00V	C00P	C00K	118.4(11)
N00A	Ni06	N007	100.2(3)	C00V	C00P	H00P	120.8
N00A	Ni06	N008	174.9(4)	C00J	C00Q	C00M	122.2(10)
N00A	Ni06	N009	78.5(4)	C00J	C00Q	H00Q	118.9
N00A	Ni06	N00B	103.3(3)	C00M	C00Q	H00Q	118.9
N00A	Ni06	N00C	78.3(4)	N009	C00R	H00R	118.7
N00B	Ni06	N009	92.1(3)	N009	C00R	C00U	122.5(13)
N00C	Ni06	N007	91.9(3)	C00U	C00R	H00R	118.7
N00C	Ni06	N009	156.8(4)	C00E	C00T	H00T	120.6
N00C	Ni06	N00B	92.8(3)	C11	C00T	C00E	118.8(12)
C00F	N007	Ni06	114.1(7)	C11	C00T	H00T	120.6
C00K	N007	Ni06	127.4(7)	C00R	C00U	H00U	121.1
C00K	N007	C00F	118.3(9)	C00R	C00U	C013	117.8(14)
C00D	N008	Ni06	118.3(7)	C013	C00U	H00U	121.1

C00D	N008	C00G	121.9(8)	C00O	C00V	H00V	120.3
C00G	N008	Ni06	117.9(7)	C00P	C00V	C00O	119.4(12)
C00N	N009	Ni06	113.0(7)	C00P	C00V	H00V	120.3
C00R	N009	Ni06	127.0(8)	N00B	C00W	H00W	119.2
C00R	N009	C00N	119.9(10)	N00B	C00W	C00Z	121.5(12)
C00I	N00A	Ni06	119.5(8)	C00Z	C00W	H00W	119.2
C00L	N00A	Ni06	119.5(7)	C00L	C00X	H00X	121.2
C00L	N00A	C00I	121.0(9)	C00L	C00X	C012	117.6(14)
C00E	N00B	Ni06	114.2(7)	C012	C00X	H00X	121.2
C00W	N00B	Ni06	127.8(7)	C00I	C00Y	H00Y	120.7
C00W	N00B	C00E	118.0(9)	C012	C00Y	C00I	118.5(13)
C00H	N00C	Ni06	113.4(8)	C012	C00Y	H00Y	120.7
C10	N00C	Ni06	127.9(8)	C00W	C00Z	H00Z	120.2
C10	N00C	C00H	118.7(10)	C11	C00Z	C00W	119.7(13)
N008	C00D	C00F	113.8(8)	C11	C00Z	H00Z	120.2
N008	C00D	C00M	120.9(10)	C00N	C010	H010	120.3
C00M	C00D	C00F	125.3(10)	C013	C010	C00N	119.4(13)
N00B	C00E	C00G	114.2(9)	C013	C010	H010	120.3
N00B	C00E	C00T	122.8(11)	C00X	C012	H012	119.5
C00T	C00E	C00G	123.(1)	C00Y	C012	C00X	120.9(12)
N007	C00F	C00D	114.1(9)	C00Y	C012	H012	119.5
N007	C00F	C00O	121.(1)	C00U	C013	H013	119.8
C00O	C00F	C00D	124.8(10)	C010	C013	C00U	120.5(14)
N008	C00G	C00E	114.2(8)	C010	C013	H013	119.8
N008	C00G	C00J	119.1(10)	C015	C014	H014	119.7
C00J	C00G	C00E	126.6(10)	C016	C014	H014	119.7
N00C	C00H	C00I	115.4(9)	C016	C014	C015	120.6(12)
N00C	C00H	C015	119.2(12)	C00H	C015	H015	120.2
C015	C00H	C00I	125.4(11)	C014	C015	C00H	119.5(12)
N00A	C00I	C00H	113.4(9)	C014	C015	H015	120.2
N00A	C00I	C00Y	120.9(12)	C014	C016	H016	121.4
C00Y	C00I	C00H	125.7(12)	C014	C016	C10	117.2(14)
C00G	C00J	H00J	120.5	C10	C016	H016	121.4
C00Q	C00J	C00G	119.(1)	N00C	C10	C016	124.7(13)
C00Q	C00J	H00J	120.5	N00C	C10	H10	117.7
N007	C00K	H00K	118.4	C016	C10	H10	117.7
N007	C00K	C00P	123.3(11)	C00T	C11	C00Z	119.2(12)
C00P	C00K	H00K	118.4	C00T	C11	H11	120.4
N00A	C00L	C00N	114.3(9)	C00Z	C11	H11	120.4
N00A	C00L	C00X	121.0(12)				

Table S8. Details of atoms occupation situation of [Ni-Tpy$_2$]Pb$_2$I$_6$.

Atom	x	y	z	Occ.	U	Site	Sym.

Pb01	-0.09359	0.59359	0.40641	1	0.016	16c	.3.
Pb02	-0.01211	0.51211	0.48789	1	0.016	16c	.3.
Pb03	0.06996	0.43004	0.56996	1	0.015	16c	.3.
I004	-0.12689	0.58244	0.29994	1	0.018	48e	1
I005	0.09548	0.52209	0.51756	1	0.019	48e	1
I006	-0.11325	0.4943	0.44895	1	0.027	48e	1
Ni07	0.125	0.5	0.25	1	0.013	12b	-4..
Ni08	0.25	0.625	0.5	1	0.015	12a	-4..
N009	0.0572	0.5	0.25	1	0.012	24d	2..
N00A	0.2126	0.61128	0.55979	1	0.017	48e	1
N00B	0.11078	0.56784	0.26818	1	0.016	48e	1
N00C	0.25	0.5576	0.5	1	0.013	24d	2..
C00D	0.1848	0.5507	0.6071	1	0.028	48e	1
H00D	0.18097	0.51941	0.61215	1	0.034	48e	1
C00E	0.1411	0.6013	0.277	1	0.021	48e	1
H00E	0.17217	0.59453	0.27516	1	0.025	48e	1
C00F	0.0661	0.5783	0.2707	1	0.014	48e	1
C00G	0.0352	0.5388	0.26	1	0.015	48e	1
C00H	-0.0125	0.5397	0.2604	1	0.019	48e	1
H00H	-0.02818	0.56652	0.26757	1	0.022	48e	1
C00I	0.2079	0.5662	0.5682	1	0.018	48e	1
C00J	0.0823	0.655	0.2912	1	0.029	48e	1
H00J	0.07249	0.68438	0.2987	1	0.034	48e	1
C00K	0.173	0.628	0.6294	1	0.038	48e	1
H00K	0.16201	0.64978	0.64994	1	0.045	48e	1
C00L	-0.0358	0.5	0.25	1	0.021	24d	2..
H00L	-0.06768	0.5	0.25	1	0.025	36	
C00M	0.2283	0.5352	0.5334	1	0.016	48e	1
C00N	0.25	0.4642	0.5	1	0.026	24d	2..
H00N	0.25	0.43229	0.5	1	0.031	36	
C00O	0.1282	0.6456	0.2887	1	0.028	48e	1
H00O	0.15001	0.66814	0.29459	1	0.033	48e	1
C00P	0.1952	0.6412	0.5895	1	0.027	48e	1
H00P	0.19795	0.6723	0.58333	1	0.033	48e	1
C00Q	0.0509	0.6213	0.2826	1	0.024	48e	1
H00Q	0.01968	0.62731	0.28491	1	0.029	48e	1
C00R	0.227	0.4879	0.5337	1	0.023	48e	1
H00R	0.21075	0.47231	0.55633	1	0.028	48e	1
C00S	0.1676	0.5822	0.638	1	0.037	48e	1
H00S	0.15259	0.57243	0.66434	1	0.045	48e	1

Table S9. Bond length of [Ni-Tpy$_2$]Pb$_2$I$_6$.

Atom	Atom	Length/ Å	Atom	Atom	Length/ Å

Pb01	I004	3.2705(5)	Ni08	N00A	2.096(5)
Pb01	I004	3.2705(5)	Ni08	N00C	1.966(7)
Pb01	I004	3.2705(5)	Ni08	N00C	1.965(7)
Pb01	I006	3.2029(5)	N009	C00G	1.332(7)
Pb01	I006	3.2029(5)	N009	C00G	1.332(7)
Pb01	I006	3.2029(5)	N00A	C00I	1.346(8)
Pb02	I005	3.2687(6)	N00A	C00P	1.330(8)
Pb02	I005	3.2687(6)	N00B	C00E	1.342(8)
Pb02	I005	3.2687(6)	N00B	C00F	1.340(8)
Pb02	I006	3.2039(5)	N00C	C00M	1.332(7)
Pb02	I006	3.2039(5)	N00C	C00M	1.332(7)
Pb02	I006	3.2039(5)	C00D	C00I	1.395(9)
Pb03	I004	3.2940(5)	C00D	C00S	1.383(10)
Pb03	I004	3.2940(5)	C00E	C00O	1.388(9)
Pb03	I004	3.2940(5)	C00F	C00G	1.495(9)
Pb03	I005	3.1783(5)	C00F	C00Q	1.376(9)
Pb03	I005	3.1782(5)	C00G	C00H	1.392(8)
Pb03	I005	3.1782(5)	C00H	C00L	1.378(8)
Ni07	N009	1.977(7)	C00I	C00M	1.483(9)
Ni07	N009	1.977(7)	C00J	C00O	1.368(9)
Ni07	N00B	2.090(5)	C00J	C00Q	1.368(9)
Ni07	N00B	2.090(5)	C00K	C00P	1.387(10)
Ni07	N00B	2.090(5)	C00K	C00S	1.367(10)
Ni07	N00B	2.090(5)	C00M	C00R	1.382(8)
Ni08	N00A	2.096(5)	C00N	C00R	1.378(8)
Ni08	N00A	2.096(5)	C00N	C00R	1.378(8)
Ni08	N00A	2.096(5)			

Table S10. Bond Angles of [Ni-Tpy$_2$]Pb$_2$I$_6$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
I004	Pb01	I004	80.908(15)	N00B	Ni07	N00B	92.26(6)
I004	Pb01	I004	80.906(15)	N00B	Ni07	N00B	92.26(6)
I004	Pb01	I004	80.908(15)	N00B	Ni07	N00B	92.26(6)
I006	Pb01	I004	102.993(12)	N00B	Ni07	N00B	157.1(3)
I006	Pb01	I004	172.620(13)	N00B	Ni07	N00B	157.1(3)
I006	Pb01	I004	102.993(12)	N00B	Ni07	N00B	92.26(6)
I006	Pb01	I004	93.440(11)	N00A	Ni08	N00A	92.09(5)
I006	Pb01	I004	172.621(13)	N00A	Ni08	N00A	92.09(5)
I006	Pb01	I004	93.441(11)	N00A	Ni08	N00A	92.09(6)
I006	Pb01	I004	172.620(13)	N00A	Ni08	N00A	92.09(6)
I006	Pb01	I004	93.442(11)	N00A	Ni08	N00A	158.0(3)
I006	Pb01	I004	102.991(12)	N00A	Ni08	N00A	158.0(3)
I006	Pb01	I006	83.159(15)	N00C	Ni08	N00A	101.01(15)

I006	Pb01	I006	83.160(15)	N00C	Ni08	N00A	78.99(14)
I006	Pb01	I006	83.158(15)	N00C	Ni08	N00A	78.99(15)
I005	Pb02	I005	81.655(15)	N00C	Ni08	N00A	78.99(14)
I005	Pb02	I005	81.653(15)	N00C	Ni08	N00A	101.01(15)
I005	Pb02	I005	81.655(15)	N00C	Ni08	N00A	78.99(15)
I006	Pb02	I005	102.443(13)	N00C	Ni08	N00A	101.01(14)
I006	Pb02	I005	172.991(13)	N00C	Ni08	N00A	101.01(15)
I006	Pb02	I005	172.991(13)	N00C	Ni08	N00C	180
I006	Pb02	I005	93.242(12)	C00G	N009	Ni07	118.8(4)
I006	Pb02	I005	102.444(13)	C00G	N009	Ni07	118.8(4)
I006	Pb02	I005	93.241(12)	C00G	N009	C00G	122.5(8)
I006	Pb02	I005	172.990(13)	C00I	N00A	Ni08	113.0(5)
I006	Pb02	I005	93.243(11)	C00P	N00A	Ni08	128.0(5)
I006	Pb02	I005	102.445(13)	C00P	N00A	C00I	118.9(6)
I006	Pb02	I006	83.126(16)	C00E	N00B	Ni07	127.4(5)
I006	Pb02	I006	83.127(16)	C00F	N00B	Ni07	114.9(4)
I006	Pb02	I006	83.128(16)	C00F	N00B	C00E	117.7(6)
I004	Pb03	I004	80.208(15)	C00M	N00C	Ni08	119.4(4)
I004	Pb03	I004	80.208(15)	C00M	N00C	Ni08	119.4(4)
I004	Pb03	I004	80.208(15)	C00M	N00C	C00M	121.3(8)
I005	Pb03	I004	96.308(11)	C00S	C00D	C00I	119.3(7)
I005	Pb03	I004	176.502(16)	N00B	C00E	C00O	123.1(7)
I005	Pb03	I004	176.502(16)	N00B	C00F	C00G	113.5(6)
I005	Pb03	I004	98.954(11)	N00B	C00F	C00Q	122.3(6)
I005	Pb03	I004	98.955(11)	C00Q	C00F	C00G	124.2(6)
I005	Pb03	I004	96.309(11)	N009	C00G	C00F	114.2(6)
I005	Pb03	I004	98.954(11)	N009	C00G	C00H	120.0(7)
I005	Pb03	I004	176.503(16)	C00H	C00G	C00F	125.8(6)
I005	Pb03	I004	96.308(11)	C00L	C00H	C00G	118.3(7)
I005	Pb03	I005	84.503(16)	N00A	C00I	C00D	120.9(7)
I005	Pb03	I005	84.503(16)	N00A	C00I	C00M	115.4(6)
I005	Pb03	I005	84.504(16)	C00D	C00I	C00M	123.6(6)
Pb01	I004	Pb03	83.416(13)	C00O	C00J	C00Q	120.2(7)
Pb03	I005	Pb02	80.049(14)	C00S	C00K	C00P	118.5(8)
Pb01	I006	Pb02	79.971(13)	C00H	C00L	C00H	120.8(9)
N009	Ni07	N009	180	N00C	C00M	C00I	113.1(6)
N009	Ni07	N00B	101.45(15)	N00C	C00M	C00R	120.6(7)
N009	Ni07	N00B	101.45(15)	C00R	C00M	C00I	126.2(6)
N009	Ni07	N00B	78.55(15)	C00R	C00N	C00R	119.7(9)
N009	Ni07	N00B	101.45(15)	C00J	C00O	C00E	117.6(7)
N009	Ni07	N00B	78.55(15)	N00A	C00P	C00K	122.9(7)
N009	Ni07	N00B	101.45(15)	C00J	C00Q	C00F	119.1(7)
N009	Ni07	N00B	78.55(15)	C00N	C00R	C00M	118.9(7)

N009	Ni07	N00B	78.55(15)	C00K	C00S	C00D	119.3(8)

Table S11. Details of atoms occupation situation of $Tpy_2Pb_3I_6$.

Atom	x	y	z	Occ.	U	Site	Sym.
Pb01	0.71548	0.58007	0.63588	1	0.034	4e	1
Pb02	-0.07476	0.39803	0.66777	1	0.034	4e	1
Pb03	0.31522	0.49479	0.65102	1	0.036	4e	1
Pb04	1	1	0.5	1	0.038	2c	-1
Pb05	1.40319	1.03625	0.55585	1	0.042	4e	1
I006	0.19521	0.3379	0.63816	1	0.037	4e	1
I007	-0.39772	0.41818	0.68102	1	0.044	4e	1
I008	0.7248	0.99114	0.55376	1	0.045	4e	1
I009	1.13669	1.1037	0.57332	1	0.047	4e	1
I00A	0.04651	0.56455	0.6174	1	0.053	4e	1
I00B	0.15691	0.4853	0.74414	1	0.05	4e	1
I00C	0.45706	0.64667	0.6695	1	0.053	4e	1
I00D	0.44904	0.50534	0.56263	1	0.062	4e	1
I00E	0.85933	1.12407	0.44886	1	0.059	4e	1
N00F	0.751	0.6456	0.5651	1	0.035	4e	1
N00G	0.7873	0.6142	0.7133	1	0.038	4e	1
N00H	0.787	0.7052	0.6447	1	0.032	4e	1
N00I	1.4323	0.9729	0.627	1	0.047	4e	1
N00J	-0.1405	0.3651	0.5897	1	0.047	4e	1
N00K	-0.1376	0.2719	0.6565	1	0.042	4e	1
C00L	0.7507	0.6118	0.5269	1	0.044	4e	1
H00L	0.72288	0.56522	0.52636	1	0.053	4e	1
N00M	1.4744	1.1116	0.619	1	0.042	4e	1
N00N	-0.1101	0.3281	0.738	1	0.045	4e	1
C00O	0.796	0.6828	0.7231	1	0.036	4e	1
C00P	0.7994	0.8186	0.614	1	0.044	4e	1
H00P	0.80633	0.84704	0.58936	1	0.053	4e	1
C00Q	0.7948	0.8046	0.6912	1	0.048	4e	1
H00Q	0.79602	0.82418	0.71912	1	0.057	4e	1
C00R	0.8007	0.5685	0.7454	1	0.047	4e	1
H00R	0.79692	0.52097	0.7385	1	0.056	4e	1
C00S	0.7911	0.733	0.6858	1	0.034	4e	1
C00T	0.7967	0.8466	0.655	1	0.057	4e	1
H00T	0.79621	0.89516	0.65842	1	0.069	4e	1
C00U	-0.1493	0.2964	0.5796	1	0.045	4e	1
C00V	1.4834	1.0831	0.6597	1	0.049	4e	1

C00W	0.7914	0.7465	0.6103	1	0.034	4e	1
C00X	0.7914	0.7125	0.5662	1	0.034	4e	1
C00Y	0.8137	0.7055	0.7659	1	0.049	4e	1
H00Y	0.81643	0.75324	0.77245	1	0.058	4e	1
C00Z	-0.1472	0.2202	0.7731	1	0.075	4e	1
H00Z	-0.16003	0.17195	0.77122	1	0.09	4e	1
C11	-0.1517	0.2458	0.616	1	0.046	4e	1
C12	1.4723	1.0078	0.6635	1	0.044	4e	1
C13	0.8294	0.7108	0.49	1	0.05	4e	1
H13	0.85559	0.73305	0.46452	1	0.06	4e	1
C15	-0.1326	0.2584	0.7356	1	0.041	4e	1
C17	-0.1239	0.3221	0.8153	1	0.063	4e	1
H17	-0.12244	0.34527	0.84207	1	0.075	4e	1
C18	0.7889	0.6419	0.4888	1	0.049	4e	1
H18	0.78771	0.61663	0.46277	1	0.059	4e	1
C19	0.8202	0.5872	0.7889	1	0.048	4e	1
H19	0.82816	0.55341	0.81071	1	0.058	4e	1
N10	1.4756	1.1601	0.5356	1	0.058	4e	1
C4AA	-0.143	0.2281	0.6913	1	0.051	4e	1
C0AA	0.8271	0.6566	0.7981	1	0.052	4e	1
H0AA	0.84124	0.67103	0.82685	1	0.062	4e	1
C14	1.5056	1.1271	0.6959	1	0.066	4e	1
H14	1.51343	1.10778	0.72381	1	0.079	4e	1
C16	0.831	0.7465	0.5289	1	0.05	4e	1
H16	0.85841	0.79305	0.53011	1	0.06	4e	1
C1AA	1.454	0.865	0.665	1	0.073	4e	1
H1AA	1.44649	0.81634	0.66486	1	0.087	4e	1
C2AA	1.5079	1.2264	0.65	1	0.071	4e	1
H2AA	1.51456	1.27476	0.6463	1	0.085	4e	1
C3AA	-0.1066	0.3581	0.7771	1	0.054	4e	1
H3AA	-0.09157	0.40623	0.77867	1	0.066	4e	1
C20	-0.1581	0.1553	0.6853	1	0.068	4e	1
H20	-0.15637	0.12485	0.70909	1	0.081	4e	1
C7AA	1.4894	1.182	0.6137	1	0.056	4e	1
C5AA	1.4239	0.9033	0.6287	1	0.065	4e	1
H5AA	1.39597	0.87951	0.60369	1	0.078	4e	1
C6AA	1.5023	0.9695	0.7011	1	0.073	4e	1
H6AA	1.52777	0.9929	0.72653	1	0.087	4e	1
C8AA	1.4906	1.2076	0.5679	1	0.055	4e	1
C3BA	-0.1563	0.2767	0.5357	1	0.071	4e	1
H3BA	-0.16055	0.22929	0.52845	1	0.085	4e	1
C1BA	-0.1434	0.2516	0.8131	1	0.075	4e	1
H1BA	-0.15383	0.22524	0.83845	1	0.09	4e	1

C0BA	1.5186	1.2982	0.5168	1	0.088	4e	1
H0BA	1.53388	1.34517	0.51024	1	0.106	4e	1
C2BA	-0.1727	0.1746	0.6088	1	0.064	4e	1
H2BA	-0.18471	0.15745	0.58056	1	0.076	4e	1
C9AA	1.4847	1.181	0.4949	1	0.074	4e	1
H9AA	1.47528	1.14832	0.47244	1	0.089	4e	1
C8BA	-0.1516	0.3947	0.5138	1	0.08	4e	1
H8BA	-0.15557	0.42943	0.49241	1	0.096	4e	1
C4BA	1.5072	1.2788	0.5584	1	0.078	4e	1
H4BA	1.51029	1.31204	0.58066	1	0.094	4e	1
C5BA	1.5157	1.1979	0.6905	1	0.086	4e	1
H5BA	1.52808	1.22681	0.71469	1	0.103	4e	1
C9BA	-0.157	0.3263	0.5031	1	0.084	4e	1
H9BA	-0.16128	0.31267	0.47386	1	0.1	4e	1
C7BA	-0.1398	0.4116	0.5576	1	0.072	4e	1
H7BA	-0.1309	0.45881	0.56495	1	0.086	4e	1
C6BA	1.4948	0.8994	0.7011	1	0.09	4e	1
H6BA	1.51795	0.87433	0.72611	1	0.108	4e	1
C1CA	-0.1755	0.1303	0.6437	1	0.081	4e	1
H1CA	-0.1894	0.0825	0.63924	1	0.097	4e	1
C0CA	1.5084	1.2514	0.4843	1	0.089	4e	1
H0CA	1.51686	1.26529	0.45536	1	0.107	4e	1

Table S12. Bond length of $Tpy_2Pb_3I_6$.

Atom	Atom	Length/ Å	Atom	Atom	Length/ Å
Pb01	I00A	3.4287(7)	C00W	C00X	1.497(13)
Pb01	I00C	3.1021(7)	C00X	C16	1.375(13)
Pb01	N00F	2.528(8)	C00Y	H00Y	0.93
Pb01	N00G	2.550(7)	C00Y	C0AA	1.361(14)
Pb01	N00H	2.504(7)	C00Z	H00Z	0.93
Pb02	I006	3.1163(7)	C00Z	C15	1.367(14)
Pb02	I007	3.3318(7)	C00Z	C1BA	1.361(17)
Pb02	N00J	2.548(8)	C11	C2BA	1.388(14)
Pb02	N00K	2.507(8)	C12	C6AA	1.391(15)
Pb02	N00N	2.556(8)	C13	H13	0.93
Pb03	I006	3.2473(7)	C13	C18	1.375(14)
Pb03	I007	3.3745(6)	C13	C16	1.369(14)
Pb03	I00A	3.1914(7)	C15	C4AA	1.476(15)
Pb03	I00B	3.2937(8)	C17	H17	0.93
Pb03	I00C	3.2754(7)	C17	C3AA	1.367(14)
Pb03	I00D	3.0483(8)	C17	C1BA	1.358(17)
Pb04	I008	3.2657(7)	C18	H18	0.93
Pb04	I008	3.2658(6)	C19	H19	0.93

Pb04	I009	3.2804(6)	C19	C0AA	1.353(14)
Pb04	I009	3.2805(6)	N10	C8AA	1.347(14)
Pb04	I00E	3.1623(7)	N10	C9AA	1.312(14)
Pb04	I00E	3.1623(7)	C4AA	C20	1.406(15)
Pb05	I008	3.3778(7)	C0AA	H0AA	0.93
Pb05	I009	3.0489(7)	C14	H14	0.93
Pb05	N00I	2.500(8)	C14	C5BA	1.363(18)
Pb05	N00M	2.503(8)	C16	H16	0.93
Pb05	N10	2.549(9)	C1AA	H1AA	0.93
N00F	C00L	1.333(12)	C1AA	C5AA	1.359(15)
N00F	C00X	1.337(11)	C1AA	C6BA	1.342(18)
N00G	C00O	1.342(11)	C2AA	H2AA	0.93
N00G	C00R	1.316(12)	C2AA	C7AA	1.407(15)
N00H	C00S	1.363(11)	C2AA	C5BA	1.351(18)
N00H	C00W	1.312(11)	C3AA	H3AA	0.93
N00I	C12	1.357(12)	C20	H20	0.93
N00I	C5AA	1.328(14)	C20	C1CA	1.366(17)
N00J	C00U	1.346(12)	C7AA	C8AA	1.482(16)
N00J	C7BA	1.323(14)	C5AA	H5AA	0.93
N00K	C11	1.340(12)	C6AA	H6AA	0.93
N00K	C4AA	1.353(13)	C6AA	C6BA	1.336(19)
C00L	H00L	0.93	C8AA	C4BA	1.397(15)
C00L	C18	1.360(13)	C3BA	H3BA	0.93
N00M	C00V	1.361(13)	C3BA	C9BA	1.375(18)
N00M	C7AA	1.358(13)	C1BA	H1BA	0.93
N00N	C15	1.348(12)	C0BA	H0BA	0.93
N00N	C3AA	1.325(13)	C0BA	C4BA	1.329(19)
C00O	C00S	1.489(13)	C0BA	C0CA	1.338(19)
C00O	C00Y	1.388(12)	C2BA	H2BA	0.93
C00P	H00P	0.93	C2BA	C1CA	1.361(17)
C00P	C00T	1.365(14)	C9AA	H9AA	0.93
C00P	C00W	1.379(12)	C9AA	C0CA	1.398(18)
C00Q	H00Q	0.93	C8BA	H8BA	0.93
C00Q	C00S	1.375(12)	C8BA	C9BA	1.343(19)
C00Q	C00T	1.366(14)	C8BA	C7BA	1.381(16)
C00R	H00R	0.93	C4BA	H4BA	0.93
C00R	C19	1.388(13)	C5BA	H5BA	0.93
C00T	H00T	0.93	C9BA	H9BA	0.93
C00U	C11	1.471(15)	C7BA	H7BA	0.93
C00U	C3BA	1.395(14)	C6BA	H6BA	0.93
C00V	C12	1.443(14)	C1CA	H1CA	0.93
C00V	C14	1.404(14)	C0CA	H0CA	0.93

Table S13. Bond Angles of $Tpy_2Pb_3I_6$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
I00C	Pb01	I00A	157.73(2)	N00M	C00V	C12	117.8(9)
N00F	Pb01	I00A	75.51(15)	N00M	C00V	C14	119.5(11)
N00F	Pb01	I00C	102.31(16)	C14	C00V	C12	122.7(12)
N00F	Pb01	N00G	128.8(2)	N00H	C00W	C00P	122.3(9)
N00G	Pb01	I00A	84.63(16)	N00H	C00W	C00X	117.6(8)
N00G	Pb01	I00C	79.68(16)	C00P	C00W	C00X	120.1(9)
N00H	Pb01	I00A	79.41(15)	N00F	C00X	C00W	115.4(8)
N00H	Pb01	I00C	79.69(16)	N00F	C00X	C16	121.4(9)
N00H	Pb01	N00F	65.0(3)	C16	C00X	C00W	123.2(9)
N00H	Pb01	N00G	65.1(3)	C00O	C00Y	H00Y	120.7
I006	Pb02	I007	161.57(2)	C0AA	C00Y	C00O	118.6(10)
N00J	Pb02	I006	81.81(17)	C0AA	C00Y	H00Y	120.7
N00J	Pb02	I007	84.08(18)	C15	C00Z	H00Z	119.4
N00J	Pb02	N00N	128.4(3)	C1BA	C00Z	H00Z	119.4
N00K	Pb02	I006	80.29(16)	C1BA	C00Z	C15	121.2(13)
N00K	Pb02	I007	82.99(15)	N00K	C11	C00U	116.9(9)
N00K	Pb02	N00J	64.7(3)	N00K	C11	C2BA	121.5(12)
N00K	Pb02	N00N	65.1(3)	C2BA	C11	C00U	121.6(11)
N00N	Pb02	I006	100.79(17)	N00I	C12	C00V	116.3(10)
N00N	Pb02	I007	78.91(16)	N00I	C12	C6AA	118.9(11)
I006	Pb03	I007	87.517(17)	C6AA	C12	C00V	124.8(11)
I006	Pb03	I00B	82.382(19)	C18	C13	H13	120.1
I006	Pb03	I00C	174.851(19)	C16	C13	H13	120.1
I00A	Pb03	I006	91.490(19)	C16	C13	C18	119.8(10)
I00A	Pb03	I007	176.93(2)	N00N	C15	C00Z	119.9(12)
I00A	Pb03	I00B	82.87(2)	N00N	C15	C4AA	116.4(9)
I00A	Pb03	I00C	93.45(2)	C00Z	C15	C4AA	123.7(11)
I00B	Pb03	I007	99.870(19)	C3AA	C17	H17	120.9
I00C	Pb03	I007	87.625(17)	C1BA	C17	H17	120.9
I00C	Pb03	I00B	96.78(2)	C1BA	C17	C3AA	118.3(12)
I00D	Pb03	I006	97.14(2)	C00L	C18	C13	117.9(10)
I00D	Pb03	I007	82.85(2)	C00L	C18	H18	121.1
I00D	Pb03	I00A	94.39(2)	C13	C18	H18	121.1
I00D	Pb03	I00B	177.21(2)	C00R	C19	H19	121.4
I00D	Pb03	I00C	83.94(2)	C0AA	C19	C00R	117.2(10)

I008	Pb04	I008	180	C0AA	C19	H19	121.4
I008	Pb04	I009	87.483(17)	C8AA	N10	Pb05	118.2(8)
I008	Pb04	I009	92.517(17)	C9AA	N10	Pb05	122.4(9)
I008	Pb04	I009	87.484(17)	C9AA	N10	C8AA	119.0(11)
I008	Pb04	I009	92.516(17)	N00K	C4AA	C15	118.6(9)
I009	Pb04	I009	180.000(18)	N00K	C4AA	C20	120.7(12)
I00E	Pb04	I008	95.523(19)	C20	C4AA	C15	120.7(11)
I00E	Pb04	I008	84.477(19)	C00Y	C0AA	H0AA	119.6
I00E	Pb04	I008	95.525(19)	C19	C0AA	C00Y	120.9(10)
I00E	Pb04	I008	84.475(19)	C19	C0AA	H0AA	119.6
I00E	Pb04	I009	85.850(18)	C00V	C14	H14	119.9
I00E	Pb04	I009	85.851(18)	C5BA	C14	C00V	120.3(13)
I00E	Pb04	I009	94.150(18)	C5BA	C14	H14	119.9
I00E	Pb04	I009	94.150(18)	C00X	C16	H16	120.5
I00E	Pb04	I00E	180.00(2)	C13	C16	C00X	119.(1)
I009	Pb05	I008	166.14(2)	C13	C16	H16	120.5
N00I	Pb05	I008	77.95(18)	C5AA	C1AA	H1AA	120.9
N00I	Pb05	I009	98.35(19)	C6BA	C1AA	H1AA	120.9
N00I	Pb05	N00M	65.0(3)	C6BA	C1AA	C5AA	118.2(14)
N00I	Pb05	N10	128.8(3)	C7AA	C2AA	H2AA	120.4
N00M	Pb05	I008	83.76(15)	C5BA	C2AA	H2AA	120.4
N00M	Pb05	I009	82.60(15)	C5BA	C2AA	C7AA	119.1(13)
N00M	Pb05	N10	64.9(3)	N00N	C3AA	C17	123.5(12)
N10	Pb05	I008	87.05(18)	N00N	C3AA	H3AA	118.2
N10	Pb05	I009	84.98(19)	C17	C3AA	H3AA	118.2
Pb02	I006	Pb03	87.542(17)	C4AA	C20	H20	120.8
Pb02	I007	Pb03	149.82(2)	C1CA	C20	C4AA	118.5(13)
Pb04	I008	Pb05	146.15(2)	C1CA	C20	H20	120.8
Pb05	I009	Pb04	89.709(18)	N00M	C7AA	C2AA	120.9(12)
Pb03	I00A	Pb01	144.92(3)	N00M	C7AA	C8AA	116.(1)
Pb01	I00C	Pb03	87.365(18)	C2AA	C7AA	C8AA	123.1(12)
C00L	N00F	Pb01	120.8(6)	N00I	C5AA	C1AA	123.6(12)
C00L	N00F	C00X	118.6(8)	N00I	C5AA	H5AA	118.2
C00X	N00F	Pb01	119.8(6)	C1AA	C5AA	H5AA	118.2
C00O	N00G	Pb01	118.2(6)	C12	C6AA	H6AA	119.6
C00R	N00G	Pb01	123.3(7)	C6BA	C6AA	C12	120.7(13)
C00R	N00G	C00O	118.0(8)	C6BA	C6AA	H6AA	119.6
C00S	N00H	Pb01	118.2(6)	N10	C8AA	C7AA	118.1(10)
C00W	N00H	Pb01	119.7(6)	N10	C8AA	C4BA	120.6(13)
C00W	N00H	C00S	120.3(8)	C4BA	C8AA	C7AA	121.3(13)
C12	N00I	Pb05	120.7(7)	C00U	C3BA	H3BA	119.5
C5AA	N00I	Pb05	120.6(7)	C9BA	C3BA	C00U	121.0(13)

C5AA	N00I	C12	118.3(10)	C9BA	C3BA	H3BA	119.5
C00U	N00J	Pb02	117.9(7)	C00Z	C1BA	H1BA	120.7
C7BA	N00J	Pb02	121.8(8)	C17	C1BA	C00Z	118.6(12)
C7BA	N00J	C00U	118.9(10)	C17	C1BA	H1BA	120.7
C11	N00K	Pb02	120.4(7)	C4BA	C0BA	H0BA	119.4
C11	N00K	C4AA	119.5(9)	C4BA	C0BA	C0CA	121.2(15)
C4AA	N00K	Pb02	119.6(7)	C0CA	C0BA	H0BA	119.4
N00F	C00L	H00L	118.3	C11	C2BA	H2BA	120.5
N00F	C00L	C18	123.3(10)	C1CA	C2BA	C11	119.1(12)
C18	C00L	H00L	118.3	C1CA	C2BA	H2BA	120.5
C00V	N00M	Pb05	119.5(6)	N10	C9AA	H9AA	119.2
C7AA	N00M	Pb05	120.4(8)	N10	C9AA	C0CA	121.6(15)
C7AA	N00M	C00V	119.7(9)	C0CA	C9AA	H9AA	119.2
C15	N00N	Pb02	119.5(7)	C9BA	C8BA	H8BA	121.1
C3AA	N00N	Pb02	122.1(7)	C9BA	C8BA	C7BA	117.7(14)
C3AA	N00N	C15	118.4(9)	C7BA	C8BA	H8BA	121.1
N00G	C00O	C00S	116.8(8)	C8AA	C4BA	H4BA	120.6
N00G	C00O	C00Y	121.5(9)	C0BA	C4BA	C8AA	118.8(15)
C00Y	C00O	C00S	121.7(9)	C0BA	C4BA	H4BA	120.6
C00T	C00P	H00P	121.3	C14	C5BA	H5BA	119.8
C00T	C00P	C00W	117.4(10)	C2AA	C5BA	C14	120.4(13)
C00W	C00P	H00P	121.3	C2AA	C5BA	H5BA	119.8
C00S	C00Q	H00Q	120.6	C3BA	C9BA	H9BA	120.4
C00T	C00Q	H00Q	120.6	C8BA	C9BA	C3BA	119.3(13)
C00T	C00Q	C00S	118.9(10)	C8BA	C9BA	H9BA	120.4
N00G	C00R	H00R	118.1	N00J	C7BA	C8BA	124.2(13)
N00G	C00R	C19	123.9(10)	N00J	C7BA	H7BA	117.9
C19	C00R	H00R	118.1	C8BA	C7BA	H7BA	117.9
N00H	C00S	C00O	117.3(8)	C1AA	C6BA	H6BA	119.9
N00H	C00S	C00Q	119.8(9)	C6AA	C6BA	C1AA	120.3(14)
C00Q	C00S	C00O	122.9(9)	C6AA	C6BA	H6BA	119.9
C00P	C00T	C00Q	121.2(10)	C20	C1CA	H1CA	119.7
C00P	C00T	H00T	119.4	C2BA	C1CA	C20	120.6(12)
C00Q	C00T	H00T	119.4	C2BA	C1CA	H1CA	119.7
N00J	C00U	C11	117.8(9)	C0BA	C0CA	C9AA	118.6(16)
N00J	C00U	C3BA	118.9(11)	C0BA	C0CA	H0CA	120.7
C3BA	C00U	C11	123.4(11)	C9AA	C0CA	H0CA	120.7

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