Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and structure of pseudo-three dimensional hybrid iodobismuthate semiconductors

Adam Dennington, Mark Weller

Supplementary Information

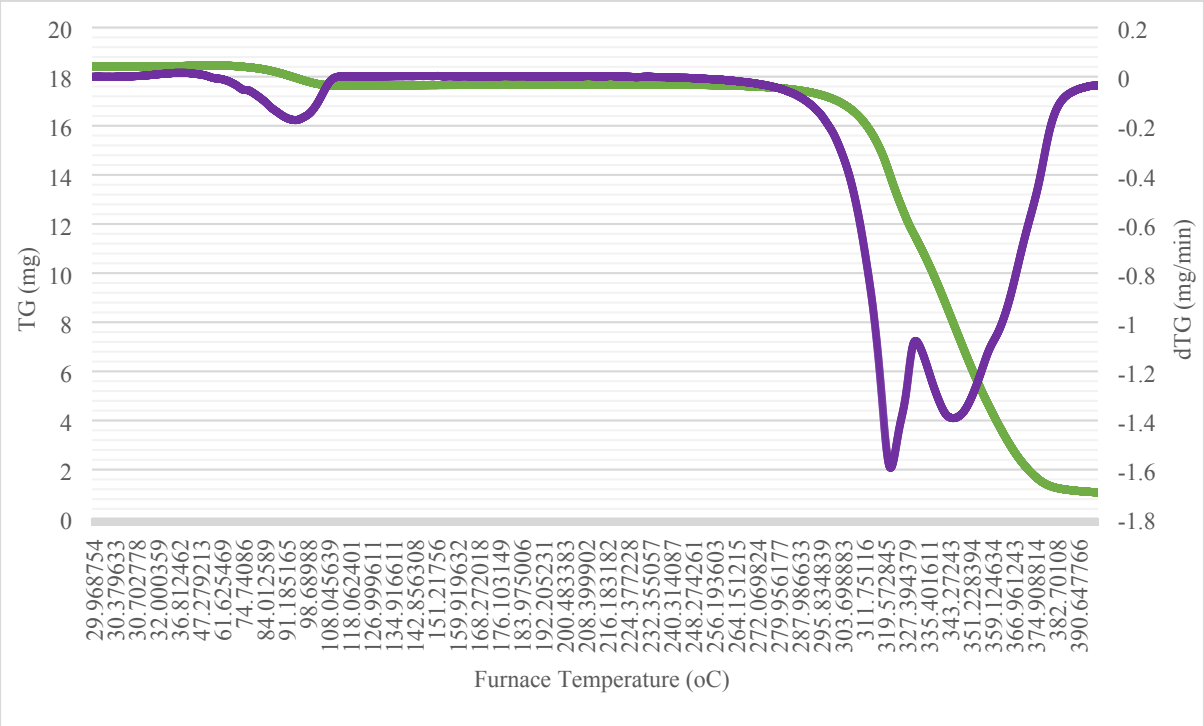

Figure S1. Thermogravimetric analysis of compound 1 (30-400°C)

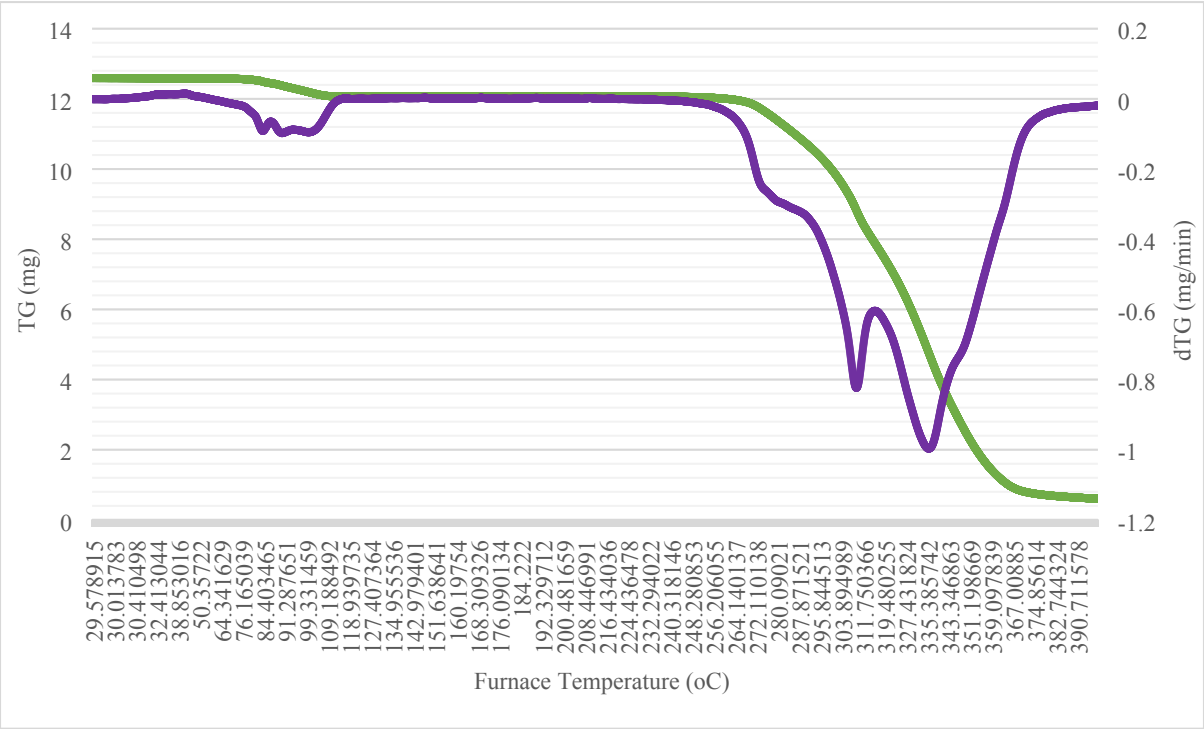

Figure S2. Thermogravimetric analysis of compound 2 (30-400°C)

Figure S3. Thermogravimetric analysis of compound 3 (30-400°C)

	Compound					
Parameters	1a (150K)	1b (RT)	2a (150K)	2b (RT)	3a (150K)	3b (RT)
Bi…Bi distances (Å)	4.457	4.508	4.512	4.569	4.588	4.625
	4.537	4.58	4.577	4.614	4.619	4.648
	7.351*	7.470*	7.543*	7.649*	7.729*	7.797*
Bi-I bonding interactions	2.891	2.892	2.899	2.905	2.923	2.921
	2.96	2.96	2.936	2.939	2.93	2.928
	3.058	3.065	3.045	3.061	3.056	3.064
	3.081	3.09	3.099	3.107	3.12	3.118
	3.215	3.277	3.216	3.237	3.24	3.252
	3.301	3.312	3.279	3.289	3.255	3.263
Intrachain I-I distances	4.416 (I2-I2)	4.478 (I2-I2)	4.345 (I2-I2)	4.337 (I2-I2)	4.397 (I2-I2)	4.304 (I2-I2)
	4.309 (I2-I3)	4.342 (I2-I3)	4.336 (I2-I3)	4.383 (I2-I3)	4.356 (I2-I3)	4.304 (I2-I3)
	4.325 (I2-I3)	4.377 (I2-I3)	4.416 (I2-I3)	4.448 (I2-I3)	4.492 (I2-I3)	4.378 (I2-I3)
	4.344 (I2-I3)	4.398 (I2-I3)	4.421 (I2-I3)	4.471 (I2-I3)	4.521 (I2-I3)	4.525 (I2-I3)
	4.225 (I2-I1)	4.214 (I2-I1)	4.162 (I2-I1)	4.179 (I2-I1)	4.192 (I2-I1)	4.131 (I2-I1)
	4.412 (I3-I1)	4.420 (I3-I1)	4.450 (I3-I1)	4.456 (I3-I1)	4.295 (I3-I1)	4.463 (I3-I1)
	4.554 (I3-I1)	4.348 (I3-I1)	4.494 (I3-I1)	4.483 (I3-I1)	4.351 (I3-I1)	4.499 (I3-I1)
	4.494 (I3-I3)	4.319 (I3-I3)	4.446 (I3-I3)	4.432 (I3-I3)	4.315 (I3-I3)	4.375 (I3-I3)
	4.344 (I2-I4)	4.522 (I2-I4)	4.311 (I2-I4)	4.324 (I2-I4)	4.464 (I2-I4)	4.307 (I2-I4)
	4.420 (I2-I4)	4.418 (I2-I4)	4.360 (I2-I4)	4.380 (I2-I4)	4.509 (I2-I4)	4.360 (I2-I4)
	4.250 (I1-I4)	4.263 (I1-I4)	4.284 (I1-I4)	4.295 (I1-I4)	4.343 (I1-I4)	4.338 (I1-I4)
	4.191 (I3-I4)	4.229 (I3-I4)	4.486 (I3-I4)	4.202 (I3-I4)	4.122 (I3-I4)	4.199 (I3-I4)
	4.237 (I4-I3)**	4.494 (I4-I3)**	4.316 (I4-I3)**	4.457 (I4-I3)**	4.718 (I4-I3)**	4.768 (I4-I3)**
	4.417 (I1-I2)**	4.335 (I1-I2)**	4.562 (I1-I2)**	4.634 (I1-I2)**	4.490 (I1-I2)**	4.557 (I1-I2)**
Interchain I-I interactions	3.761 (I2-I4)	4.338 (I2-I4)	3.765 (I2-I4)	3.811 (I2-I4)	4.015 (I2-I4)	3.817 (I2-I4)
	4.254 (I1-I3)	3.800 (I1-I3)	4.169 (I1-I3)	4.226 (I1-I3)	3.779 (I1-I3)	4.072 (I1-I3)
	4.396 (I1-I4)	4.436 (I1-I4)	4.324 (I1-I4)	4.357 (I1-I4)	4.210 (I1-I4)	4.244 (I1-I4)
Interchain Bi…Bi distances	8.488	8.53	8.393	8.446	8.299	8.34
	9.211	9.02	9.131	9.096	9.112	9.161
	9.914	9.202	9.782	9.168	9.146	9.167

Table S1. Interaction and bonding parameter analysis for compounds 1-3 (obtained from RT and 150K single-crystal data collections)

	Compound					
Parameters	1a (150K)	1b (RT)	2a (150K)	2b (RT)	3a (150K)	3b (RT)
I-Bi-I bond angles (o)	83.16	84.04	83.76	84.38	84.23	84.45
	85.22	85.75	87.84	87.01	86.48	85.88
	87.25	88.23	88.16	87.69	87.13	86.53
	89.15	88.49	88.34	88.26	87.18	87.26
	89.08	88.71	88.46	88.64	87.65	87.91
	89.45	89.14	88.5	88.86	88.08	88.22
	89.47	89.48	88.84	89.35	89.86	90.52
	90.55	90.41	89.52	89.6	91.45	91.73
	93.14	92.11	92.44	91.92	92.38	92.2
	93.16	93.5	94.33	94.46	93.22	93.36
	93.81	93.79	94.47	94.52	95.83	95.75
	95.93	95.77	94.98	94.92	96.46	96.25
Bi-I-Bi bond angles (o)	90.53	91.29	91.66	92.31	92.82	93.47
	90.55	91.51	92.16	92.99	93.52	94.12

Table S2. Bond angle analysis for compounds 1-3 (obtained from RT and 150K single-crystal data collections)

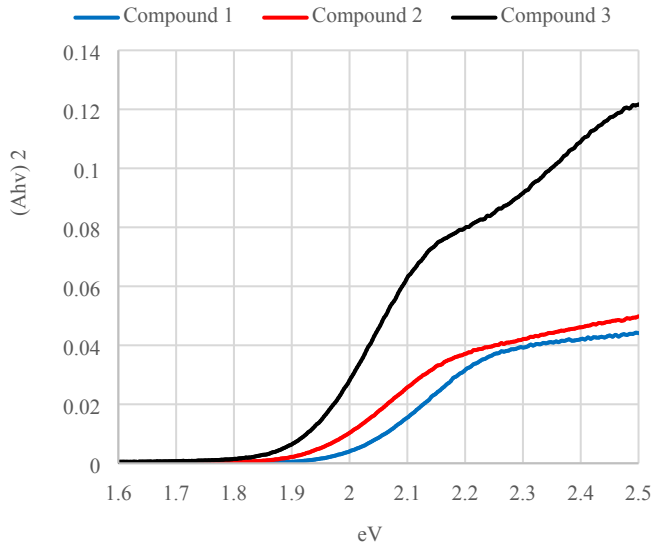

Figure S4. Tauc plot analysis of compounds 1-3

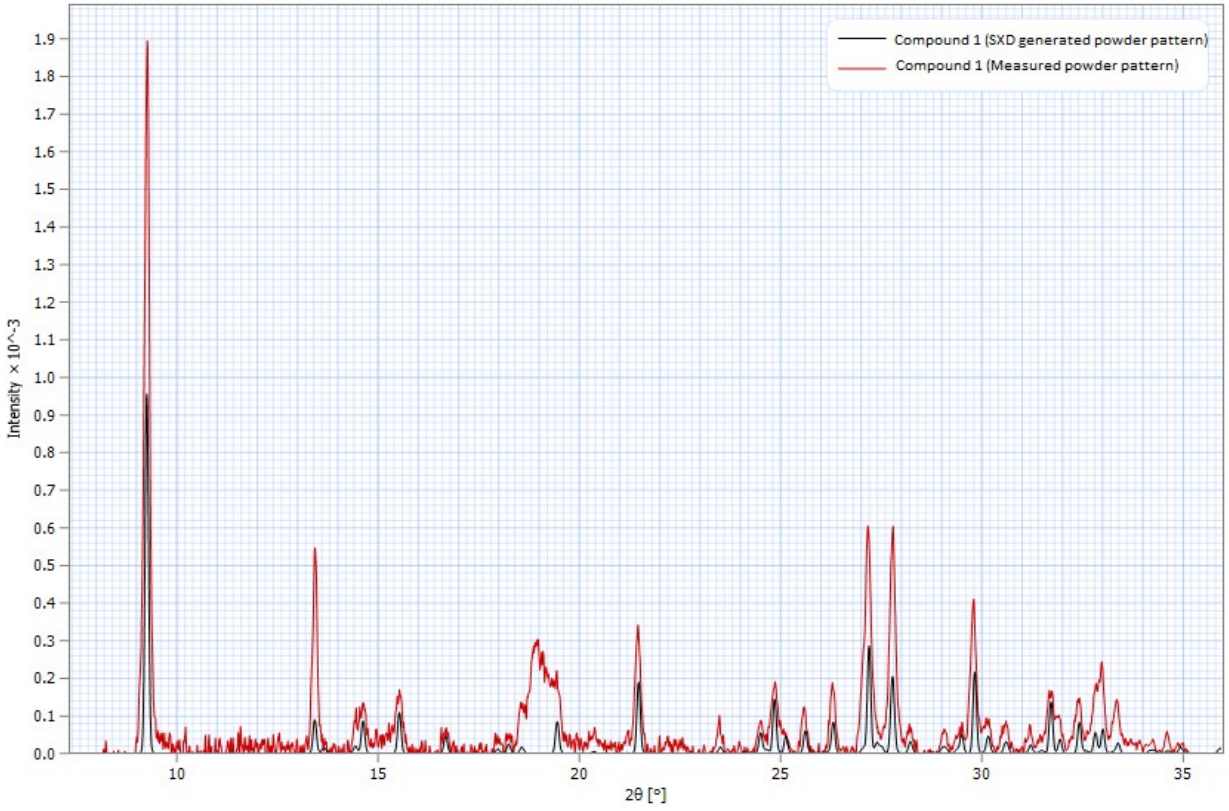

Figure S5. Compound 1 measured powder x-ray diffraction pattern compared to single-crystal data generated powder pattern. The broad feature at 2θ = 19° is from the sample holder.

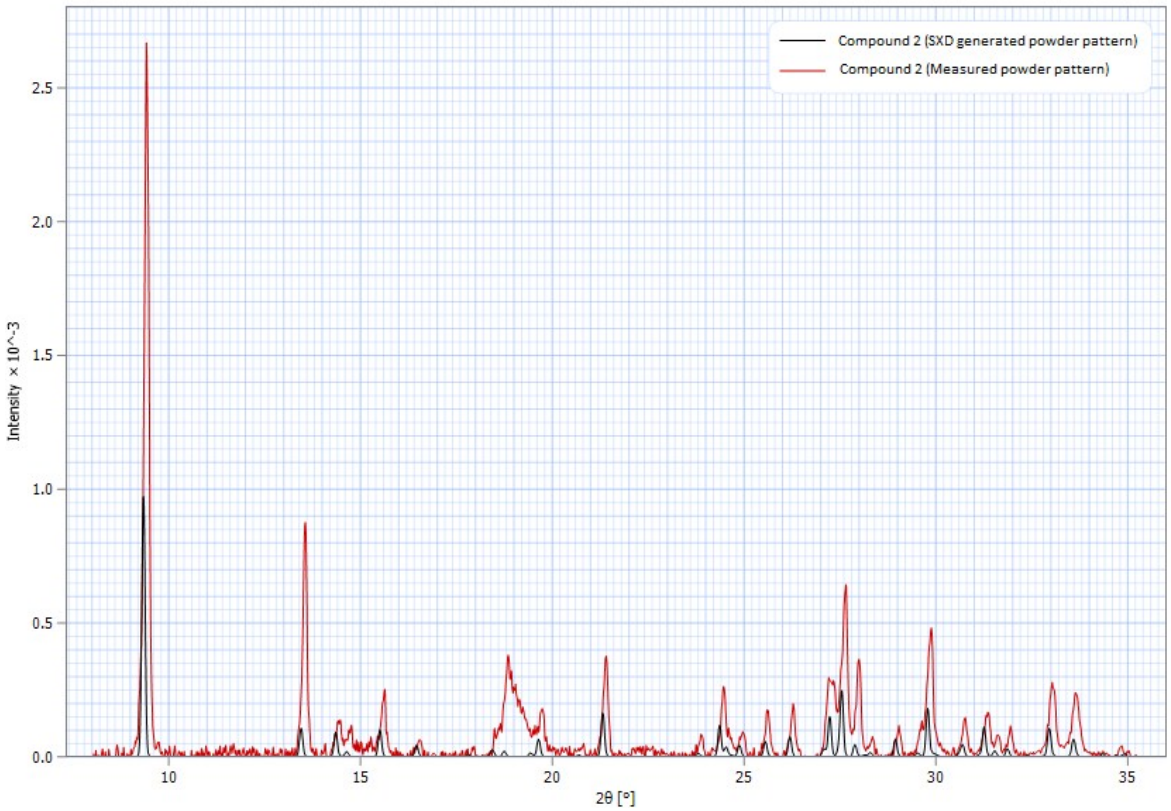

Figure S6. Compound 2 measured powder x-ray diffraction pattern compared to single-crystal data generated powder pattern. The broad feature at 2θ = 19° is from the sample holder.

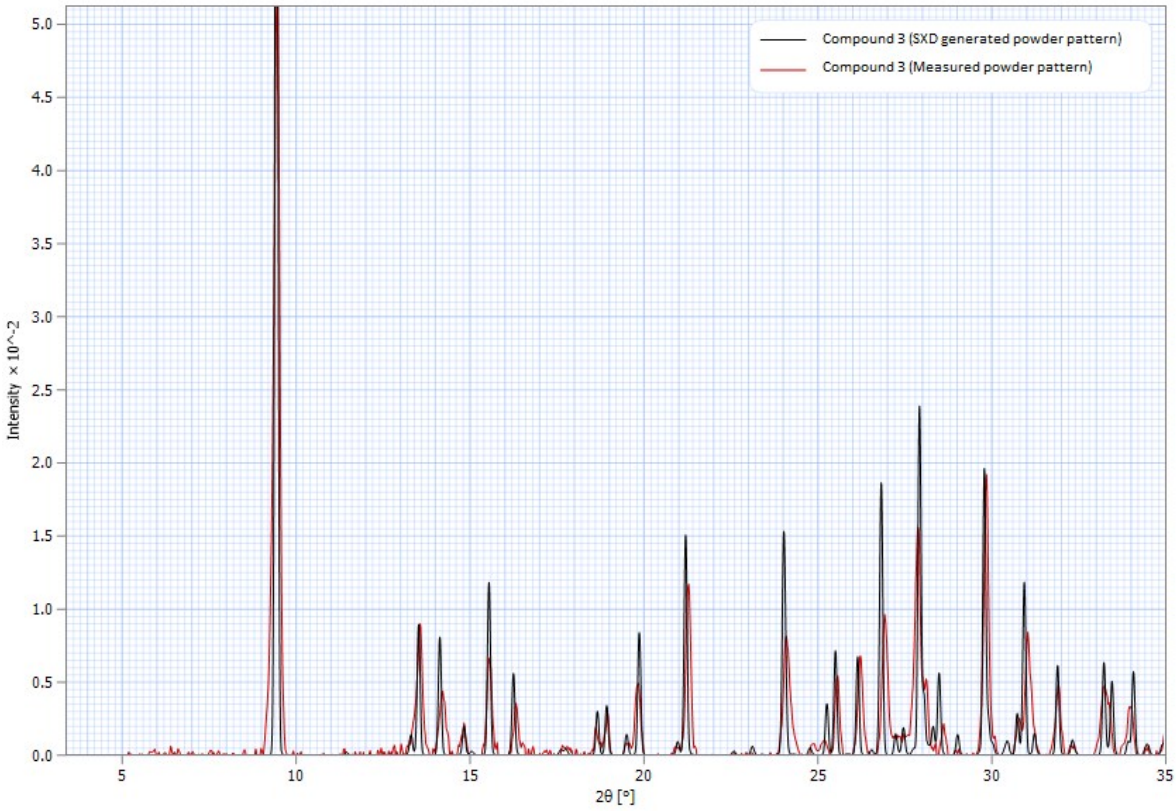

Figure S7. Compound 3 measured powder x-ray diffraction pattern compared to single-crystal data generated powder pattern