

Supplementary Information

Synthesis, characterization, and thermoelectric properties of superconducting (BEDT-TTF)₂I₃ nanoparticles

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XRD assignments for (BEDT-TTF)₂I₃ nanoparticles (*obs*: NPs; *calc*: single crystal)

No.	h	k	l	2θ (calc) [°]	2θ (obs) [°]	2θ (diff) [°]	d-sp. (calc) [Å]	d-sp. (obs) [Å]	d-sp. (diff) [Å]
1	0	0	1	5,8513	5,8213	0,0301	15,091980	15,169830	-0,077853
2	0	1	-1	11,3259	11,3853	-0,0594	7,806358	7,765741	0,040617
3	0	0	2	11,7180	11,7494	-0,0314	7,545990	7,525892	0,020098
4	0	1	1	12,5513	12,5543	-0,0030	7,046807	7,045113	0,001695
5	0	1	-2	14,7361	14,6488	0,0873	6,006573	6,042185	-0,035612
6	1	0	-1	14,7804	14,8307	-0,0503	5,988656	5,968466	0,020190
7	1	-1	-1	15,4098	15,4426	-0,0328	5,745470	5,733345	0,012125
8	1	-1	1	15,9053	15,9372	-0,0319	5,567558	5,556479	0,011079
9	1	0	1	16,2291	16,0900	0,1391	5,457213	5,504070	-0,046856
10	1	0	-2	17,3196	17,4260	-0,1064	5,115986	5,084981	0,031005
11	0	0	3	17,6157	17,6386	-0,0230	5,030660	5,024158	0,006502
12	1	-1	-2	18,2706	18,3282	-0,0576	4,851781	4,836667	0,015114
13	1	-1	2	19,1054	19,1526	-0,0472	4,641621	4,630288	0,011332
14	0	1	-3	19,3921	19,3004	0,0917	4,573648	4,595175	-0,021526
15	1	0	2	19,7558	19,5888	0,1670	4,490262	4,528158	-0,037896
16	1	1	-1	20,4759	20,3190	0,1569	4,333936	4,367038	-0,0331
17	1	1	0	20,5382	20,6920	-0,1537	4,320920	4,289160	0,031760
18	0	2	0	20,9173	20,9526	-0,0354	4,243474	4,236389	0,007085
19	1	-2	1	21,5140	21,4234	0,0905	4,127107	4,144343	-0,017236
20	0	1	3	21,5658	21,6926	-0,1267	4,117298	4,093532	0,023767
21	1	1	-2	22,0617	21,9721	0,0896	4,025872	4,042087	-0,016215
22	1	-1	-3	22,3764	22,3805	-0,0041	3,969944	3,969234	0,000710
23	0	2	1	22,4126	22,5451	-0,1326	3,963627	3,940617	0,023010
24	0	2	-2	22,7643	22,8339	-0,0696	3,903179	3,891441	0,011738
25	1	-1	3	23,4079	23,4552	-0,0473	3,797291	3,789747	0,007544
26	0	0	4	23,5608	23,5924	-0,0316	3,772995	3,768020	0,004975
27	1	-2	2	23,6886	23,7030	-0,0144	3,752927	3,750682	0,00224
28	1	-2	-2	24,2778	24,3906	-0,1128	3,663161	3,646474	0,016688
29	1	1	-3	24,9983	24,8418	0,1565	3,559196	3,581256	-0,022060
30	1	1	2	25,2555	25,2418	0,0137	3,523533	3,525409	-0,001876
31	0	2	2	25,2564	25,3571	-0,1007	3,523404	3,509642	0,013762

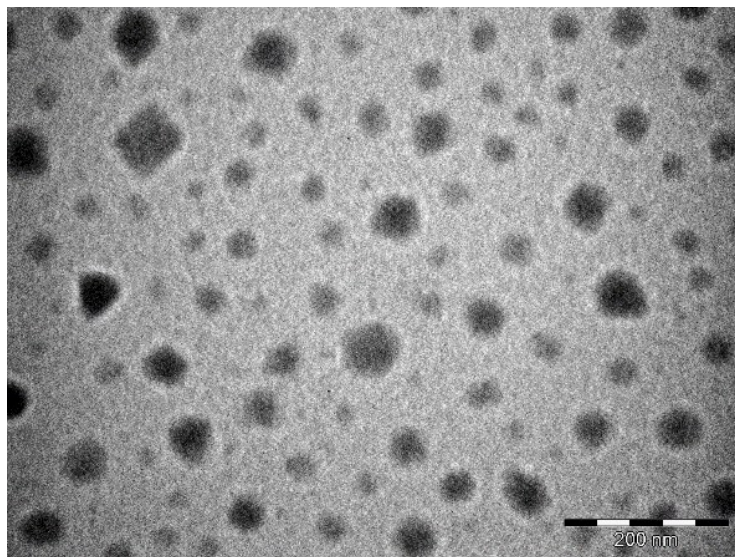
32	1	0	-4	25,9868	25,9381	0,0487	3,426006	3,432329	-0,006323
33	2	-1	0	27,1085	27,0989	0,0096	3,286734	3,287882	-0,001148
34	1	-1	-4	27,2023	27,2130	-0,0107	3,275618	3,274354	0,001263
35	1	-2	-3	27,8141	27,9397	-0,1257	3,204942	3,190811	0,01413
36	1	-1	4	28,3503	28,3637	-0,0135	3,145533	3,144069	0,00146
37	2	-1	-2	28,5504	28,4600	0,0904	3,123936	3,133652	-0,0097
38	2	0	0	28,9591	28,9566	0,0025	3,080776	3,081031	-0,000255
39	2	-2	0	29,2644	29,2473	0,0171	3,049318	3,051063	-0,001745
40	0	0	5	29,5710	29,5393	0,0318	3,018396	3,021568	-0,0031
41	0	2	-4	29,7232	29,7103	0,0130	3,003286	3,004569	-0,001283
42	1	2	-2	30,0087	30,0272	-0,0185	2,975365	2,973573	0,001793
43	0	1	-5	30,1938	30,1755	0,0183	2,957546	2,959298	-0,001753
44	1	2	1	30,8883	30,8574	0,0310	2,892609	2,895440	-0,002831
45	2	-1	-3	31,0306	30,9737	0,0569	2,879671	2,884827	-0,005156
46	1	0	-5	31,1980	31,1919	0,0061	2,864598	2,865143	-0,000545
47	1	-3	2	31,3929	31,4015	-0,0086	2,847257	2,846500	0,00075
48	2	-2	2	32,1279	32,2301	-0,1023	2,783779	2,775180	0,00859
49	2	0	2	32,7956	32,7562	0,0394	2,728606	2,731799	-0,003192
50	0	3	1	32,8735	32,9087	-0,0352	2,722325	2,719493	0,002832
51	1	1	-5	33,4736	33,5212	-0,0476	2,674873	2,671185	0,003688
52	1	-3	3	33,8168	33,7832	0,0336	2,648511	2,651067	-0,002557
53	2	1	-1	33,8400	33,8668	-0,0267	2,646744	2,644717	0,002027
54	2	-1	3	33,9409	33,9780	-0,0371	2,639108	2,636311	0,002798
55	0	2	-5	34,3138	34,3514	-0,0376	2,611279	2,608508	0,002771
56	2	1	-2	34,5193	34,5338	-0,0145	2,596202	2,595147	0,001056
57	2	-3	-1	35,2580	35,2291	0,0289	2,543480	2,545498	-0,002018
58	2	1	1	35,6439	35,4770	0,1669	2,516821	2,528280	-0,011459
59	1	-3	-3	35,7790	35,7567	0,0223	2,507632	2,509142	-0,00151
60	2	0	3	36,1186	36,1584	-0,0397	2,484824	2,482184	0,002640
61	2	-3	2	36,8160	36,8882	-0,0721	2,439340	2,434735	0,004605
62	0	3	-4	37,3542	37,3256	0,0286	2,405425	2,407200	-0,001775
63	1	-1	-6	38,0449	38,0841	-0,0392	2,363326	2,360980	0,002345
64	0	3	3	38,2870	38,1809	0,1061	2,348936	2,355219	-0,006283
65	0	2	5	38,5817	38,6586	-0,0769	2,331671	2,327209	0,004463
66	1	3	-1	38,9420	38,9858	-0,0438	2,310922	2,308428	0,002494
67	0	2	-6	39,3692	39,3729	-0,0037	2,286824	2,286618	0,000206
68	1	3	-2	39,4511	39,4603	-0,0092	2,282268	2,281755	0,000512
69	1	0	6	40,4566	40,5123	-0,0558	2,227833	2,224895	0,002938
70	3	-1	-1	41,2017	41,2246	-0,0229	2,189248	2,188083	0,001165
71	2	2	-1	41,2599	41,3289	-0,0690	2,186292	2,182802	0,003490
72	3	-2	0	41,6054	41,5900	0,0155	2,168932	2,169703	-0,000771
73	0	0	7	41,8667	41,8465	0,0203	2,155997	2,156994	-0,000997
74	0	1	-7	41,9517	41,9804	-0,0287	2,151826	2,150420	0,001406
75	2	-3	-4	42,3729	42,3412	0,0317	2,131405	2,132929	-0,001524
76	0	4	0	42,5754	42,6126	-0,0373	2,121737	2,119968	0,001769
77	2	-4	1	42,7052	42,7116	-0,0064	2,115589	2,115286	0,00030
78	2	-4	-1	43,0571	43,0035	0,0536	2,099107	2,101601	-0,002494
79	2	0	-6	43,2853	43,2787	0,0066	2,088571	2,088873	-0,000302
80	3	0	-1	43,6474	43,5620	0,0854	2,072077	2,075942	-0,003864
81	1	-3	-5	43,8298	43,8231	0,0066	2,063880	2,064175	-0,0002
82	0	1	7	44,5418	44,5822	-0,0403	2,032523	2,030779	0,001744
83	1	-4	4	45,0125	45,0223	-0,0098	2,012359	2,011945	0,000414
84	1	-1	7	45,2010	45,1959	0,0050	2,004405	2,004617	-0,000212
85	2	2	2	45,3683	45,3512	0,0171	1,997398	1,998111	-0,000713
86	1	2	5	45,4195	45,4748	-0,0552	1,995266	1,992971	0,002295
87	1	-3	6	45,5797	45,5862	-0,0065	1,988628	1,988360	0,000268
88	2	-4	3	45,7851	45,8107	-0,0256	1,980182	1,979136	0,001046

89	1	3	3	45,8900	45,9384	-0,0484	1,975899	1,973931	0,00196
90	1	0	7	46,3869	46,4323	-0,0454	1,955885	1,954078	0,00180
91	1	-2	7	46,6457	46,6557	-0,0100	1,945632	1,945240	0,000393
92	2	-4	-3	46,7792	46,8089	-0,0297	1,940391	1,939230	0,00116
93	3	0	2	47,3470	47,3220	0,0250	1,918437	1,919391	-0,0009
94	3	-3	-3	47,4331	47,4386	-0,0055	1,915156	1,914947	0,00020
95	2	-2	6	47,8712	47,8499	0,0213	1,898645	1,899440	-0,000795
96	0	1	-8	48,1050	48,0438	0,0612	1,889962	1,892228	-0,002266
97	2	2	3	48,2937	48,3433	-0,0496	1,883018	1,881202	0,00181
98	1	-3	-6	48,6367	48,6851	-0,0484	1,870537	1,868792	0,00174
99	3	1	-2	48,8088	48,9039	-0,0951	1,864344	1,860939	0,00340
100	0	4	-5	49,4301	49,3928	0,0373	1,842354	1,843657	-0,0013
101	1	-1	-8	49,9111	49,9053	0,0057	1,825722	1,825918	-0,000196
102	2	3	-1	50,2154	50,1914	0,0240	1,815369	1,816181	-0,00081
103	2	1	-7	50,6298	50,6421	-0,0123	1,801478	1,801068	0,00041
104	1	-5	-1	51,4576	51,4191	0,0386	1,774424	1,775664	-0,001241
105	2	2	4	51,8547	51,8540	0,0007	1,761766	1,761790	-0,000023
106	3	-1	-6	52,4346	52,4082	0,0264	1,743637	1,744453	-0,000816
107	0	4	-6	52,9931	53,0158	-0,0227	1,726570	1,725885	0,000686
108	1	-5	-2	53,1458	53,1778	-0,0321	1,721970	1,721007	0,00096
109	2	-1	-8	53,6254	53,6209	0,0045	1,707695	1,707828	-0,00013
110	2	1	6	54,1657	54,1804	-0,0147	1,691929	1,691504	0,000425
111	0	0	9	54,6920	54,6401	0,0519	1,676887	1,678356	-0,001469
112	1	0	-9	54,7513	54,7883	-0,0370	1,675210	1,674165	0,001045
113	0	3	-8	55,1552	55,1688	-0,0136	1,663894	1,663515	0,000379
114	4	-2	-1	55,6350	55,6388	-0,0038	1,650676	1,650571	0,000105
115	2	-4	6	55,7402	55,7600	-0,0197	1,647808	1,647271	0,000537
116	1	-4	-6	56,7663	56,7528	0,0135	1,620436	1,620789	-0,00035
117	2	3	3	56,9998	57,0050	-0,0052	1,614351	1,614215	0,000136
118	4	-2	-3	57,2505	57,2660	-0,0155	1,607875	1,607477	0,000398
119	3	-5	-1	57,4484	57,4285	0,0200	1,602805	1,603315	-0,000510
120	4	-1	-3	57,7428	57,7583	-0,0154	1,595332	1,594942	0,000390
121	4	-1	1	57,9822	57,9113	0,0709	1,589314	1,591091	-0,001777
122	1	4	-6	58,1553	58,1343	0,0210	1,584995	1,585517	-0,000523
123	1	3	6	58,3106	58,2962	0,0143	1,581145	1,581499	-0,000354
124	2	-5	-4	58,6158	58,6260	-0,0103	1,573636	1,573385	0,000251
125	1	0	9	58,9156	58,9223	-0,0067	1,566341	1,566180	0,00016
126	2	0	-9	59,0851	59,0768	0,0083	1,562252	1,562451	-0,000199
127	1	-3	-8	59,4406	59,4386	0,0020	1,553753	1,553801	-0,000048
128	4	0	-2	59,5985	59,6069	-0,0084	1,550015	1,549816	0,000198
129	4	0	0	60,0090	60,0511	-0,0421	1,540388	1,539409	0,000979
130	2	2	6	60,5879	60,5716	0,0163	1,527049	1,527420	-0,000371
131	4	-2	3	60,8951	60,9048	-0,0097	1,520078	1,519861	0,000218
132	1	5	0	61,4641	61,4653	-0,0012	1,507365	1,507338	0,000027
133	4	0	-4	61,9288			1,497164		
134	3	0	6	61,9476	61,9439	0,0037	1,496754	1,496835	-0,000081
135	2	-4	-7	62,0927	62,0709	0,0218	1,493605	1,494077	-0,000472
136	1	-6	-1	62,9045	62,8926	0,0119	1,476269	1,476519	-0,000250
137	1	3	7	63,4123	63,3664	0,0459	1,465664	1,466615	-0,000951
138	3	3	-1	63,9275	63,9194	0,0081	1,455089	1,455254	-0,000165
139	3	-3	7	64,3401	64,3191	0,0210	1,446750	1,447172	-0,000421
140	4	1	-2	64,4883	64,4891	-0,0008	1,443783	1,443767	0,000016
141	1	-3	-9	65,3799	65,3680	0,0119	1,426235	1,426466	-0,000231
142	0	6	-2	65,6332	65,6169	0,0163	1,421343	1,421657	-0,000314
143	1	-5	-6	66,2762	66,2709	0,0053	1,409104	1,409203	-0,000099
144	3	-4	-7	66,5021	66,5046	-0,0025	1,404863	1,404817	0,000046

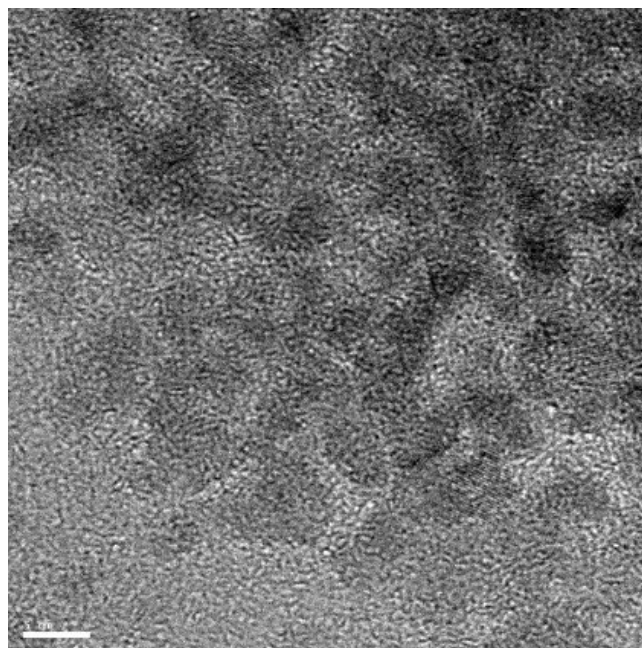
145	4	-5	-2	67,1331	67,1227	0,0104	1,393184	1,393375	-0,000191
146	4	-2	5	67,3649	67,3609	0,0041	1,388953	1,389027	-0,000074
147	3	3	2	68,0650	68,0648	0,0002	1,376362	1,376365	-0,000003
148	4	-5	-3	68,5927	68,6200	-0,0274	1,367056	1,366577	0,000479

Electron micrographs for the compressed (BEDT-TTF)₂I₃ powder used for thermoelectric characterizations

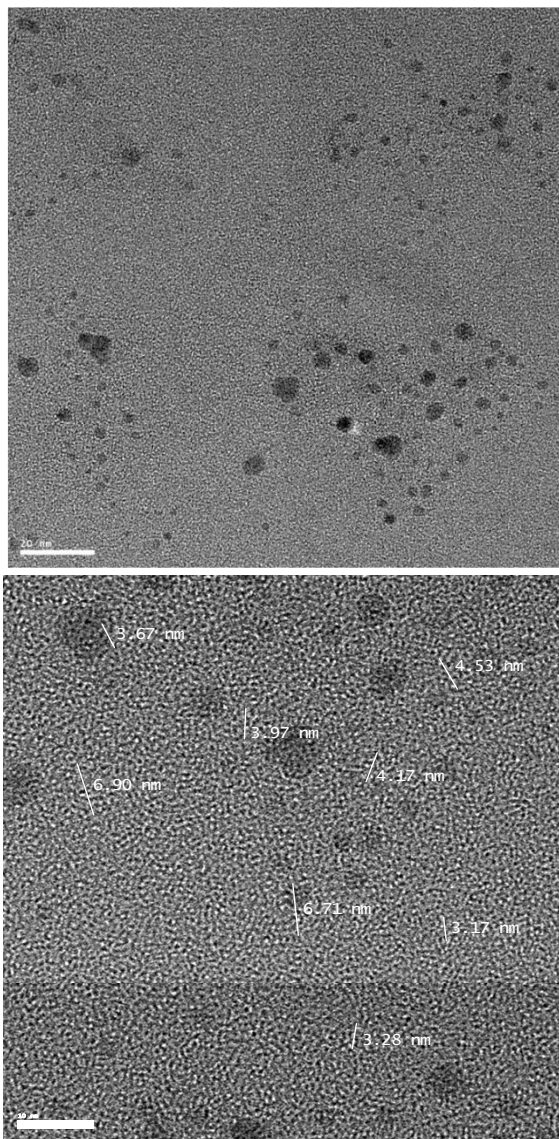
Aggregates (sizes in the 20-70 nm range) have been observed at low magnification (figure below, bar = 200 nm).



At higher magnification (figure below, bar = 5 nm), it has been evidenced that aggregates are made of small individual particles.



Moreover, as observed for the uncompressed sample, small isolated particles (2-10 nm) are clearly present on the grid (figures below):



Top: bar = 20 nm; bottom: bar = 10 nm

On individual nanoparticles, crystal planes can be observed (images below, bar = 5 nm for each image).

