

Supplementary Material:

Electronic Transport Properties of Sandwich-Type Phthalocyanine $\text{Th}(\text{Pc})_2$

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Supplementary Figures:

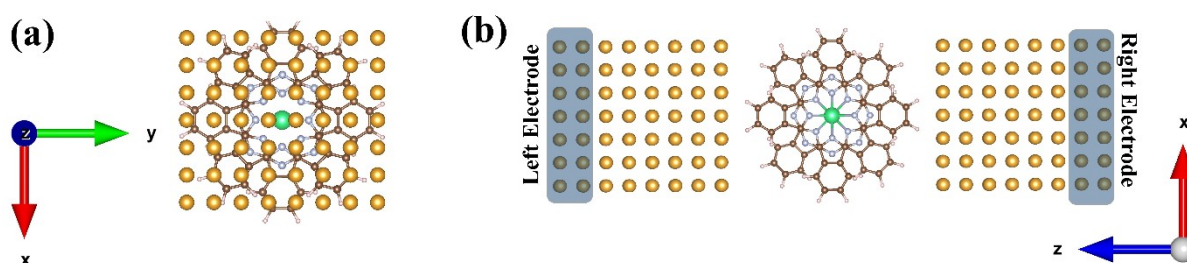


Figure S1. (a) Top View of $\text{Th}(\text{Pc})_2\text{-TB}$; (b) Top view of $\text{Th}(\text{Pc})_2\text{-LR}$.

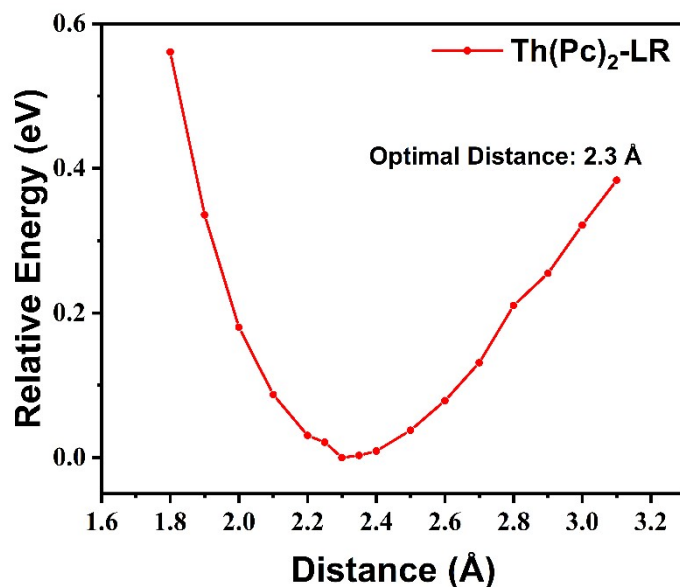


Figure S2. Energy scan of the $\text{Th}(\text{Pc})_2\text{-LR}$ optimal distance between $\text{Th}(\text{Pc})_2$ and the Au buffer layer. The dashed lines show the optimal distance point of $\text{Th}(\text{Pc})_2\text{-LR}$.

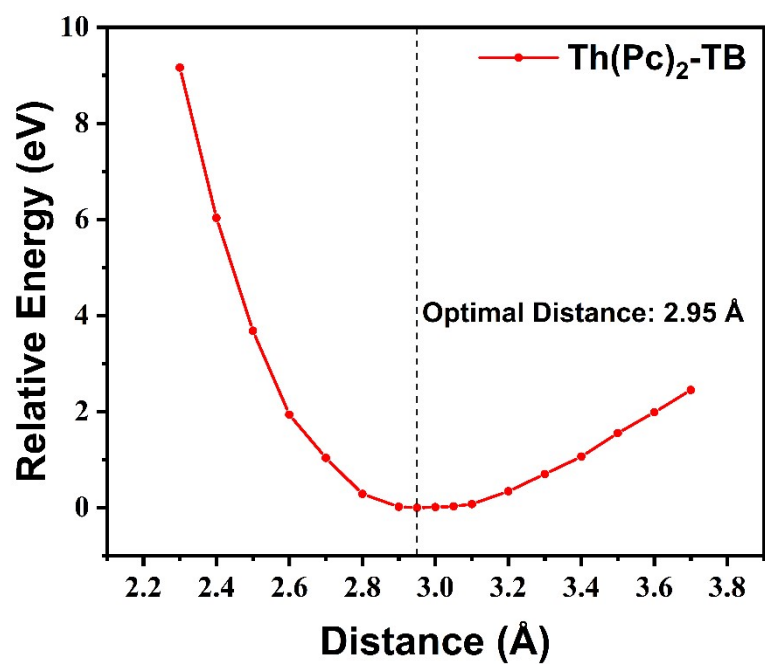


Figure S3. Energy scan of the Th(Pc)₂-TB optimal distance between Th(Pc)₂ and the Au buffer layer. The dashed lines show the optimal distance point of Th(Pc)₂-TB.

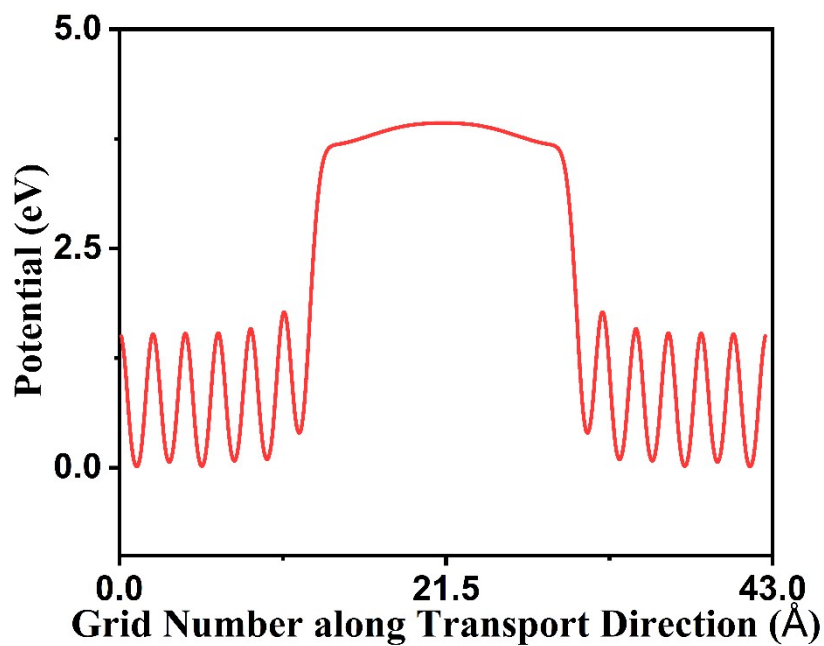


Figure S4. Calculated equilibrium potential distribution function of Th(Pc)₂-LR.

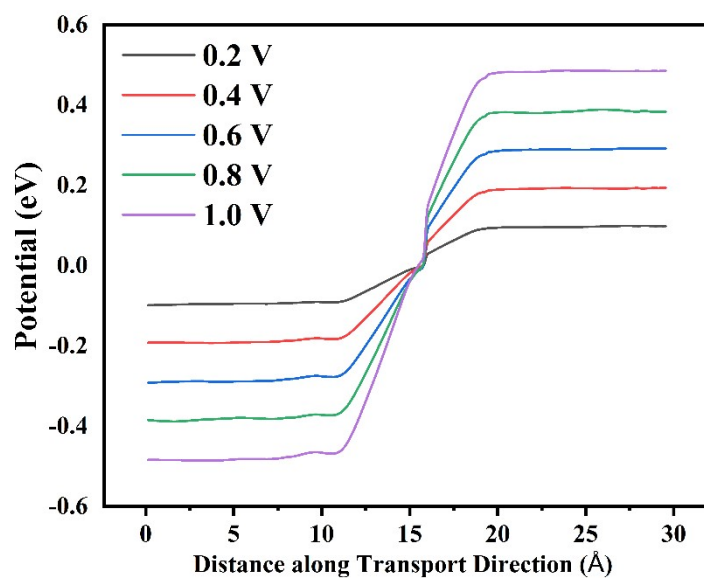


Figure S5. Voltage drop plot of Th(Pc)₂-TB from 0.2 to 1.0V.

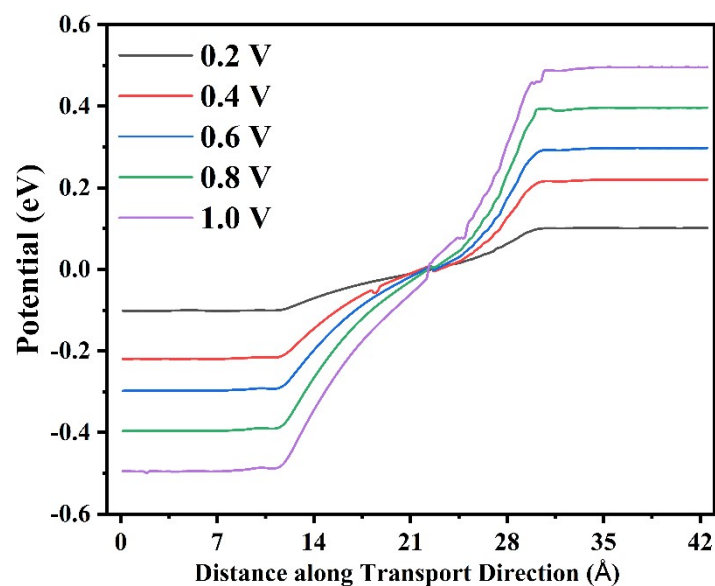


Figure S6. Voltage drop plot of Th(Pc)₂-LR from 0.2 to 1.0V.

Supplementary Tables

Table S1. The orbital compositions of Th(Pc)₂ by Hirshfeld method.

Orbital	C atom <i>p</i> orbital	N atom <i>p</i> orbital	Th atom
HOMO-39	70.047%	12.248%	1.746%
HOMO-38	74.102%	7.238%	0.253%
HOMO-37	74.097%	7.243%	0.251%

HOMO-36	61.530%	34.367%	2.027%
HOMO-35	61.532%	34.366%	2.026%
HOMO-34	23.785%	65.715%	9.646%
HOMO-33	56.863%	40.544%	1.407%
HOMO-32	56.865%	40.542%	1.407%
HOMO-31	26.936%	63.027%	9.350%
HOMO-30	26.937%	63.027%	9.350%
HOMO-29	48.359%	41.692%	7.821%
HOMO-28	48.350%	41.702%	7.822%
HOMO-27	28.659%	69.191%	0.775%
HOMO-26	32.973%	62.158%	3.626%
HOMO-25	92.254%	3.314%	0.202%
HOMO-24	28.697%	69.134%	0.734%
HOMO-23	28.698%	69.133%	0.734%
HOMO-22	29.002%	67.785%	1.973%
HOMO-21	29.002%	67.785%	1.973%
HOMO-20	93.557%	2.042%	0.075%
HOMO-19	45.048%	46.417%	6.795%
HOMO-18	39.307%	57.732%	0.510%
HOMO-17	39.445%	57.602%	0.511%
HOMO-16	84.763%	9.589%	0.197%
HOMO-15	84.764%	9.589%	0.197%
HOMO-14	47.515%	49.625%	1.415%
HOMO-13	73.960%	21.266%	0.154%
HOMO-12	73.843%	21.395%	0.154%
HOMO-11	89.133%	5.927%	0.379%
HOMO-10	89.133%	5.927%	0.379%
HOMO-9	72.535%	22.169%	1.635%
HOMO-8	72.535%	22.169%	1.635%
HOMO-7	57.958%	36.583%	3.281%
HOMO-6	75.907%	19.878%	1.221%
HOMO-5	75.908%	19.878%	1.221%
HOMO-4	73.517%	22.489%	1.125%
HOMO-3	73.517%	22.491%	1.123%
HOMO-2	61.636%	35.412%	0.870%
HOMO-1	86.547%	9.811%	0.649%
HOMO	87.366%	10.002%	0.357%
LUMO	66.081%	30.860%	1.318%
LUMO+1	66.081%	30.859%	1.318%
LUMO+2	69.177%	27.268%	1.771%
LUMO+3	69.177%	27.268%	1.771%
LUMO+4	74.685%	19.272%	1.761%
LUMO+5	74.658%	19.260%	1.807%
LUMO+6	71.608%	18.205%	5.136%
LUMO+7	71.545%	18.196%	5.184%
LUMO+8	76.298%	8.041%	7.049%
LUMO+9	82.059%	7.098%	1.991%
LUMO+10	82.059%	7.098%	1.991%
LUMO+11	77.815%	6.651%	7.376%

LUMO+12	80.281%	7.764%	3.902%
LUMO+13	80.280%	7.765%	3.903%
LUMO+14	16.694%	13.247%	69.038%
LUMO+15	16.668%	13.246%	69.070%
LUMO+16	12.616%	8.413%	78.155%
LUMO+17	12.612%	8.413%	78.159%
LUMO+18	88.626%	2.758%	0.244%
LUMO+19	49.492%	5.913%	40.203%
LUMO+20	49.499%	5.913%	40.196%
LUMO+21	81.599%	4.710%	5.878%
LUMO+22	81.603%	4.711%	5.874%
LUMO+23	43.470%	20.267%	30.413%
LUMO+24	88.766%	2.738%	0.110%
LUMO+25	13.008%	6.907%	79.027%
LUMO+26	46.954%	8.223%	40.065%
LUMO+27	46.960%	8.223%	40.058%
LUMO+28	66.069%	14.296%	14.923%
LUMO+29	66.023%	14.298%	14.962%
LUMO+30	37.944%	15.038%	29.104%

Table S2. The coordinates of the ground state in Th(Pc)₂ between different functionals and basis sets.

Level	Nun	A	x (Å)	y (Å)	z (Å)
M06-2x/ def-TZVP			1.767741	-0.911833	1.469411
			0.911835	1.767741	1.469416
			-1.76774	0.911833	1.469412
			-0.911834	-1.76774	1.469413
			1.023153	-3.202912	1.615376
			3.202913	1.023153	1.615373
			-1.023153	3.202911	1.61538
			-3.202913	-1.023153	1.615371
			1.952295	-2.259978	1.594968
			2.25998	1.952295	1.594969
			-1.952295	2.259978	1.59497
			0.280487	2.973119	1.59485
			-2.97312	0.280487	1.594841
			-0.280487	-2.973119	1.594846
			2.97312	-0.280487	1.594842
			-2.259979	-1.952295	1.594966
			3.378291	-2.529463	1.739447
			2.529464	3.37829	1.739453
			-3.378291	2.529463	1.739446
			1.285864	4.019551	1.73911
			-4.019553	1.285863	1.739096
			-1.285863	-4.019551	1.739108
			4.019553	-1.285863	1.739098
			-2.529463	-3.37829	1.739453
			4.097542	-3.712059	1.848561
			3.71206	4.097541	1.848565

-4.097542	3.712059	1.848559
1.185759	5.400063	1.847569
-5.400065	1.185758	1.847546
-1.185758	-5.400063	1.847569
5.400066	-1.185759	1.847549
-3.712059	-4.097541	1.848569
5.476865	-3.613237	1.948076
3.613238	5.476863	1.948087
-5.476865	3.613237	1.948071
2.366681	6.119613	1.947543
-6.119616	2.36668	1.947518
-2.366679	-6.119613	1.947545
6.119616	-2.36668	1.947523
-3.613236	-5.476864	1.948091
3.589445	-4.667702	1.843855
4.667703	3.589444	1.843848
-3.589445	4.667701	1.843852
0.217488	5.883696	1.84213
-5.883698	0.217487	1.842103
-0.217486	-5.883696	1.84213
5.883698	-0.217487	1.842106
-4.667702	-3.589444	1.843856
6.073777	-4.513096	2.027164
4.513097	6.073775	2.027173
-6.073777	4.513096	2.027157
2.331061	7.198872	2.026365
-7.198875	2.33106	2.026333
-2.331059	-7.198872	2.026368
7.198875	-2.33106	2.02634
-4.513095	-6.073775	2.027181
0.604863	-1.894466	-1.468531
1.894467	0.604863	-1.468532
-0.604864	1.894466	-1.468533
-1.894467	-0.604863	-1.468529
-1.541637	-2.987897	-1.615337
2.987898	-1.541637	-1.615331
1.541636	2.987896	-1.615342
-2.987899	1.541637	-1.615329
-0.217974	-2.978166	-1.594565
2.978167	-0.217974	-1.59456
0.217973	2.978166	-1.594569
2.300683	1.903402	-1.594852
-1.903404	2.300684	-1.594847
-2.300684	-1.903403	-1.594848
1.903403	-2.300684	-1.594847
-2.978168	0.217974	-1.594557
0.599306	-4.177244	-1.739494
4.177246	0.599306	-1.739481
-0.599307	4.177243	-1.739496

3.751447	1.932277	-1.739962
-1.932278	3.751447	-1.739964
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1.932277	-3.751447	-1.739965
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5.522026	0.271397	-1.848004
-0.271396	5.522023	-1.848032
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-4.656835	-2.979087	-1.849526
2.979087	-4.656834	-1.849529
-5.522027	-0.271396	-1.848005
1.316524	-6.427484	-1.947847
6.427486	1.316527	-1.947818
-1.316525	6.427483	-1.947846
6.000565	2.652609	-1.948642
-2.652609	6.000565	-1.948656
-6.000566	-2.652608	-1.948647
2.652607	-6.000565	-1.948661
-6.427487	-1.316526	-1.947823
-0.763645	-5.83853	-1.841834
5.838534	-0.763643	-1.841801
0.763643	5.838529	-1.841839
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-4.005845	4.314432	-1.845025
-4.314431	-4.005844	-1.845037
4.005844	-4.314431	-1.845032
-5.838534	0.763643	-1.841802
1.102318	-7.48593	-2.026084
7.485933	1.102322	-2.026046
-1.102319	7.48593	-2.026084
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3.440778	-6.738693	-2.027637
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1.988149	-0.010911	-1.468072
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-2.371031	2.397269	-1.592176
2.397238	2.371065	-1.592179
2.371063	-2.397262	-1.592182
-2.781147	-1.099869	-1.576659
-1.099868	2.781141	-1.576753

2.781136	1.099896	-1.576654
1.130369	2.768885	-1.576750
2.768891	-1.130373	-1.576653
-1.130381	-2.768888	-1.576750
-2.768879	1.130399	-1.576648
1.099875	-2.781146	-1.576754
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4.167190	-0.724196	-1.684498
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5.350356	-1.454899	-1.750803
-1.454938	-5.350313	-1.751368
-5.350312	1.454962	-1.750822
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-0.667174	6.548320	-1.810646
6.548407	0.667217	-1.809439
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6.540697	-0.739062	-1.809430
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2.481149	-5.358381	-1.742441
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-1.413502	-1.398062	1.474429
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1.398065	-1.413497	1.474437
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2.757272	1.158645	1.581281
1.158630	-2.757296	1.581247
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-2.472662	-3.432009	1.685920
-3.431987	2.472660	1.686023
2.472629	3.432013	1.685982
-2.434795	3.458951	1.685996
3.458929	2.434826	1.686015
2.434821	-3.458955	1.685915
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-4.781916	2.807606	1.746518
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4.812457	2.754924	1.746496
2.754948	-4.812495	1.746278
-4.812504	-2.754882	1.746342
4.781967	-2.807580	1.746327
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-5.102795	4.159270	1.799635
4.159225	5.102835	1.799570
-4.102931	5.148198	1.799608
5.148165	4.102984	1.799599
4.103017	-5.148193	1.799320
-5.148239	-4.102937	1.799367
5.102866	-4.159244	1.799343
-2.034880	-5.543752	1.735938
-5.543703	2.034837	1.736207
2.034801	5.543724	1.736084
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5.565710	1.973833	1.736181
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-5.565742	-1.973775	1.736016
5.543742	-2.034796	1.736003
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4.462054	6.144523	1.839197
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4.394400	-6.193146	1.838871
-6.193196	-4.394300	1.838943
6.144560	-4.462070	1.838912
0.000004	-0.000043	0.003777

B3LYP/def-TZVP

2.001937	0.053020	1.486655
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-2.001967	-0.053077	1.486612
0.053034	-2.001981	1.486585
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-2.445687	2.319375	1.685278
-2.319423	-2.445703	1.685190
2.811508	-1.045488	1.650824
1.045451	2.811485	1.650888
-2.811542	1.045425	1.650806
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-2.752231	-1.192922	1.650699
1.192885	-2.752236	1.650717
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0.592790	4.183562	1.833456
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-6.508246	-0.874808	2.110393
0.874743	-6.508241	2.110574
6.508202	0.874728	2.110559
-0.528894	-6.545413	2.110770
5.400178	-2.361778	1.973819
2.361720	5.400142	1.974091
-5.400218	2.361702	1.973797

-2.644439	5.267578	1.973338
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2.644399	-5.267653	1.973188
5.267612	2.644382	1.973219
-2.361761	-5.400218	1.973834
7.499030	-1.031935	2.214552
1.031877	7.498976	2.214924
-7.499075	1.031850	2.214437
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1.427573	-7.433930	2.214235
7.433899	1.427548	2.214199
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1.377972	1.453249	-1.488922
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-1.377942	-1.453193	-1.489004
0.089573	-3.369458	-1.686714
3.369449	0.089586	-1.686538
-0.089539	3.369522	-1.686585
-3.369414	-0.089522	-1.686612
1.249079	-2.727313	-1.652361
2.727340	1.249101	-1.652222
-1.249045	2.727375	-1.652282
1.102426	2.789832	-1.652178
-2.789764	1.102450	-1.652197
-1.102392	-2.789769	-1.652309
2.789798	-1.102388	-1.652181
-2.727307	-1.249038	-1.652327
2.539592	-3.377410	-1.833424
3.377459	2.539602	-1.833260
-2.539555	3.377479	-1.833345
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-2.356502	-3.507546	-1.833365
3.507597	-2.356481	-1.833222
-3.377421	-2.539532	-1.833434
2.902385	-4.711500	-1.976568
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-2.902345	4.711575	-1.976445
2.647773	4.859137	-1.976090
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-2.647731	-4.859061	-1.976346
4.859129	-2.647679	-1.976106
-4.711526	-2.902290	-1.976532
4.255462	-5.002259	-2.107140
5.002358	4.255432	-2.106911
-4.255419	5.002339	-2.107032
3.983433	5.221530	-2.106781

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5.221548	-3.983322	-2.106889
-5.002313	-4.255350	-2.107199
2.149625	-5.488734	-1.972110
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-2.149585	5.488809	-1.971941
1.854698	5.595187	-1.971344
-5.595118	1.854660	-1.971308
-1.854657	-5.595111	-1.971612
5.595158	-1.854585	-1.971267
-5.488740	-2.149509	-1.971969
4.574363	-6.032360	-2.209407
6.032470	4.574319	-2.209108
-4.574318	6.032444	-2.209265
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-6.267143	4.247004	-2.208919
-4.247001	-6.267077	-2.209226
6.267187	-4.246920	-2.208958
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2.391422	2.393980	-1.646805
2.394009	-2.391406	-1.646831
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2.787905	1.123391	-1.619348
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2.789111	-1.120382	-1.619359
-1.120387	-2.789105	-1.619506
-2.789115	1.120396	-1.619398
1.123403	-2.787895	-1.619487
-4.180556	-0.707801	-1.745373
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4.180542	0.707806	-1.745294
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4.181302	-0.703297	-1.745303
-0.703306	-4.181280	-1.745673
-4.181306	0.703324	-1.745368
0.707825	-4.180518	-1.745659
-5.370624	-1.430547	-1.822379
-1.430529	5.370568	-1.822884
5.370580	1.430568	-1.822275

1.424815	5.372065	-1.822861
5.372121	-1.424775	-1.822295
-1.424769	-5.372110	-1.822926
-5.372133	1.424812	-1.822370
1.430584	-5.370558	-1.822893
-6.562324	-0.708099	-1.889189
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6.563049	-0.701059	-1.889087
-0.701042	-6.563021	-1.889929
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0.708156	-6.562255	-1.889913
-5.356758	-2.515662	-1.810882
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5.356704	2.515673	-1.810770
2.509935	5.359333	-1.811356
5.359415	-2.509897	-1.810802
-2.509898	-5.359401	-1.811441
-5.359411	2.509937	-1.810862
2.515693	-5.356668	-1.811384
-7.509475	-1.238529	-1.938249
-1.238506	7.509389	-1.939102
7.509433	1.238574	-1.938123
1.230549	7.510686	-1.939081
7.510765	-1.230474	-1.938139
-1.230462	-7.510727	-1.939147
-7.510780	1.230533	-1.938239
1.238601	-7.509386	-1.939118
-1.412716	-1.414235	1.488708
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1.412716	1.414232	1.488655
1.414236	-1.412713	1.488674
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-3.383896	-0.001804	1.648003
-0.001799	3.383893	1.647856
3.383873	0.001819	1.647935
-1.177041	-2.765835	1.620915
-2.765814	1.177049	1.620969
1.177043	2.765822	1.620868
-1.179993	2.764567	1.620889
2.764546	1.179995	1.620919
1.180010	-2.764558	1.620892
-2.764555	-1.180002	1.620979
2.765819	-1.177029	1.620931
-2.455746	-3.456748	1.745629
-3.456726	2.455758	1.745654
2.455754	3.456727	1.745560
-2.459431	3.454114	1.745598

3.454093	2.459438	1.745592
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5.136835	4.145318	1.885636
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-5.564717	-2.015143	1.809257
5.566856	-2.009154	1.809166
-4.434586	-6.186143	1.933174
-6.186104	4.434609	1.933224
4.434592	6.186099	1.933077
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6.181384	4.441134	1.933129
4.441225	-6.181354	1.933113
-6.181398	-4.441176	1.933243
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2.770243	-1.162482	1.737284
1.162482	2.770243	1.737293

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1.078143	-2.804144	1.737281
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4.143603	-0.768901	2.039423
0.768901	4.143598	2.039455
4.164958	0.643194	2.039453
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-4.143603	0.768901	2.039423
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5.291930	-1.507901	2.333578
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5.335099	1.347119	2.333669
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-5.335099	-1.347119	2.333668
1.347120	-5.335089	2.333719
-5.291930	1.507901	2.333578
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6.465419	-0.802499	2.608386
0.802499	6.465405	2.608458
6.486725	0.606545	2.608430
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-6.465420	0.802499	2.608385
-2.598529	-5.263477	2.341202
5.263487	-2.598529	2.341151
2.598529	5.263477	2.341203
5.339652	2.438108	2.341283
-2.438108	5.339641	2.341336
-5.339651	-2.438108	2.341282
2.438108	-5.339641	2.341333
-5.263488	2.598529	2.341150
-1.349167	-7.383976	2.831158
7.383995	-1.349167	2.831073
1.349167	7.383976	2.831161
7.421411	1.125178	2.831141
-1.125178	7.421392	2.831229
-7.421411	-1.125178	2.831139
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1.443134	1.400436	-1.503457
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1.137210	-2.780817	-1.737931
2.780816	1.137210	-1.737932
2.745421	-1.220202	-1.737915
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-1.137210	2.780817	-1.737931
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2.386806	-3.473558	-2.039511
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3.400315	-2.490026	-2.039557
2.490026	3.400315	-2.039556
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-2.386806	3.473558	-2.039511
-4.808236	-2.676547	-2.332720
2.676547	-4.808236	-2.332721
4.808236	2.676547	-2.332722
4.725678	-2.819701	-2.332843
2.819702	4.725678	-2.332841
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-5.139213	-4.005323	-2.606553
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-5.016616	4.157826	-2.606612
-4.157827	-5.016616	-2.606609
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1.885331	-5.559400	-2.340223
5.559400	1.885330	-2.340223
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-2.051390	-5.500255	-2.340386
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4.268565	-6.175402	-2.828436
6.175403	4.268564	-2.828436
6.044430	-4.452060	-2.828516
4.452061	6.044430	-2.828513

	-6.044430	4.452060	-2.828514
	-4.452061	-6.044430	-2.828510
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	-1.996825	0.000847	-1.486534
	0.000847	1.996837	-1.486528
	1.996816	-0.000849	-1.486547
	2.403478	-2.405528	-1.655294
	-2.405528	-2.403508	-1.655319
	-2.403509	2.405556	-1.655347
	2.405543	2.403491	-1.655322
	1.124261	-2.796118	-1.623208
	-2.796130	-1.124277	-1.623176
	-1.124265	2.796141	-1.623230
	-2.795183	1.126645	-1.623186
	1.126643	2.795175	-1.623223
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	-1.126632	-2.795171	-1.623216
	2.796126	1.124264	-1.623176
	0.707256	-4.191030	-1.757418
	-4.191060	-0.707274	-1.757312
	-0.707251	4.191057	-1.757468
	-4.190466	0.710816	-1.757320
	0.710827	4.190445	-1.757461
	4.190441	-0.710825	-1.757271
	-0.710802	-4.190436	-1.757425
	4.191053	0.707246	-1.757278
	1.431779	-5.386392	-1.842157
	-5.386456	-1.431790	-1.841940
	-1.431750	5.386453	-1.842239
	-5.385264	1.436326	-1.841957
	1.436363	5.385207	-1.842225
	5.385204	-1.436360	-1.841870
	-1.436319	-5.385198	-1.842172
	5.386452	1.431742	-1.841886
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	-6.582686	-0.704384	-1.915309
	-0.704320	6.582661	-1.915746
	-6.582099	0.709910	-1.915318
	0.709977	6.582046	-1.915739
	6.582052	-0.709976	-1.915212
	-0.709911	-6.582024	-1.915656
	6.582668	0.704312	-1.915221
	2.525535	-5.373304	-1.830325
	-5.373361	-2.525553	-1.830108
	-2.525517	5.373385	-1.830414
	-5.371260	2.530082	-1.830136

2.530115	5.371187	-1.830389
5.371179	-2.530106	-1.830040
-2.530068	-5.371201	-1.830350
5.373380	2.525504	-1.830068
1.238087	-7.537169	-1.970056
-7.537246	-1.238100	-1.969622
-1.238017	7.537227	-1.970175
-7.536213	1.244423	-1.969636
1.244501	7.536149	-1.970162
7.536157	-1.244500	-1.969506
-1.244417	-7.536134	-1.970069
7.537237	1.238009	-1.969520
1.411398	-1.412634	1.489099
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1.412603	1.411438	1.489096
3.400566	-0.001453	1.656441
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0.001451	3.400645	1.656443
2.772263	-1.182247	1.624773
-1.182233	-2.772308	1.624757
-2.772285	1.182253	1.624789
-2.773279	-1.179902	1.624786
-1.179889	2.773323	1.624773
2.773275	1.179887	1.624775
1.179880	-2.773304	1.624755
1.182247	2.772313	1.624772
3.463799	-2.463593	1.757451
-2.463583	-3.463833	1.757463
-3.463828	2.463598	1.757510
-3.465901	-2.460665	1.757485
-2.460657	3.465934	1.757498
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2.460648	-3.465909	1.757437
2.463609	3.463827	1.757473
4.821476	-2.796657	1.839995
-2.796656	-4.821512	1.840007
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-4.823865	-2.792603	1.840056
-2.792606	4.823901	1.840066
4.823878	2.792538	1.840030
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2.796723	4.821502	1.840026
5.153064	-4.156959	1.911220
-4.156957	-5.153098	1.911270
-5.153103	4.156986	1.911352
-5.156588	-4.152631	1.911296
-4.152634	5.156621	1.911339

5.156641	4.152553	1.911278
4.152600	-5.156586	1.911206
4.157038	5.153048	1.911275
5.585640	-2.014021	1.828083
-2.014022	-5.585678	1.828067
-5.585686	2.014036	1.828174
-5.587377	-2.009321	1.828150
-2.009327	5.587418	1.828133
5.587366	2.009240	1.828107
2.009305	-5.587372	1.828038
2.014106	5.585695	1.828103
6.205498	-4.454614	1.963784
-4.454614	-6.205533	1.963832
-6.205542	4.454637	1.963940
-6.209274	-4.449400	1.963877
-4.449406	6.209308	1.963917
6.209333	4.449299	1.963848
4.449374	-6.209269	1.963759
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-1.987063	-0.001580	1.478463
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2.375058	-2.371258	1.669393
2.371265	2.375062	1.669362
-2.375054	2.371271	1.669367
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1.110274	2.767408	1.635903
-2.767400	1.110281	1.635872
-1.114693	2.765629	1.635901
-2.765622	-1.114689	1.635885
1.114696	-2.765621	1.635942
2.765623	1.114702	1.635861
-1.110274	-2.767400	1.635949
4.147922	-0.697253	1.817168
0.697262	4.147909	1.817337
-4.147921	0.697269	1.817159
-0.703889	4.146790	1.817330
-4.146802	-0.703883	1.817160
0.703892	-4.146785	1.817337
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