

Supplementary Information

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1 BPGA Global Minimum Structures

Coordinates for the putative global minimum structures from the BPGA searches.

10

Ir 1.637573 0.454113999999 2.408292999999
Ir -0.211537000002 -0.249426000001 -2.504007
Ir -0.539307000002 -0.450706000001 1.627213
Ir 1.481993 -0.913646000001 0.337482999998
Ir 1.100313 1.018134 -0.948427000002
Ir 0.178372999998 -2.217536 -1.188387
Ir 1.261933 2.435183999999 1.095493
Ir -1.805287 -1.763946 0.073672999998
Ir -2.191697000001 0.206463999999 -1.240907
Ir -0.912357000002 1.481363999999 0.339572999998

11

Ir -1.62681727272 0.795521818181 0.127981818182
Ir -0.483207272726 -0.183128181819 2.02769181818
Ir 2.50166272727 0.113261818181 0.470521818182
Ir -0.422227272726 -0.612688181819 -1.36830818182
Ir 0.118772727274 2.51283181819 0.0550518181818
Ir 0.765952727274 -1.57343818181 0.605701818182
Ir 1.22426272727 1.50308181818 1.94916181819
Ir -1.31810727273 -2.59842818182 -0.252568181818
Ir -2.61122727273 -1.21929818181 1.21856181818
Ir 1.36558272728 1.10279181819 -1.40750818181
Ir 0.485352727274 0.159491818181 -3.42628818181

12

Ir 1.167575 0.954565833336 -0.762094999998
Ir -1.167945 -0.954004166664 0.761185000002
Ir 1.868365 1.81921583333 1.375585
Ir 0.424885000003 -2.12750416667 -1.992105
Ir -1.863325 -1.82360416667 -1.373175
Ir -0.479244999997 -0.104894166664 2.904965
Ir -1.114145 1.26304583333 -0.144404999998
Ir 0.473325000003 0.109135833336 -2.906765
Ir -1.812905 0.415495833336 -2.286825
Ir 1.114605 -1.26300416667 0.144635000002
Ir -0.419974999997 2.13209583333 1.99050500001
Ir 1.80878500001 -0.420544166664 2.288495

13

Ir 1.07438538462 0.237976153846 -3.48596538462
Ir -1.63251461538 0.491226153846 -0.171325384615
Ir -0.761994615385 2.75252615385 -0.581655384615
Ir -0.395794615385 0.412146153846 1.86734461538
Ir 0.459655384615 2.62103615385 1.49439461538
Ir 0.204685384615 -0.538983846154 -1.36462538462
Ir 0.586515384615 -2.75415384615 1.17633461538
Ir 1.12649538462 1.81280615385 -1.73822538462
Ir -1.26963461538 -1.77181384615 2.33840461538
Ir 1.45007538462 -0.558733846154 0.708934615385
Ir -0.674964615385 -2.69802384615 -0.858985384615
Ir 2.35591538462 1.69187615385 0.324644615385
Ir -2.52282461538 -1.69788384615 0.290724615385

14

Ir -2.86693 -1.68567 -0.08702
Ir -0.78737 -1.39707 -1.26735
Ir 1.31419 -1.20363 -2.48997
Ir -1.66284 -2.13679 1.93369
Ir 0.41927 -1.84960 0.75997
Ir 2.53586 -1.65626 -0.43824
Ir -2.88481 0.64791 0.44095
Ir -0.82548 0.97761 -0.72301
Ir -1.67915 0.19319 2.46647
Ir 0.38785 0.52269 1.31831
Ir 1.40406 1.13685 -2.00253
Ir 2.60859 0.68924 0.01847
Ir 0.41698 3.10684 -0.97659
Ir 1.61977 2.65470 1.04685

15

Ir	0.62151	0.27718	1.12295
Ir	-2.06912	2.41582	1.80879
Ir	2.07866	2.93329	-0.60255
Ir	-0.62003	0.73038	-0.90134
Ir	1.44549	1.02162	-2.12223
Ir	2.70388	0.55599	-0.06723
Ir	0.00069	2.67932	0.59336
Ir	-0.61603	-1.66413	-1.41859
Ir	-2.70409	0.49711	0.30220
Ir	1.45491	-1.35078	-2.65398
Ir	0.60623	-2.11159	0.57084
Ir	-1.43914	0.03825	2.35989
Ir	2.70782	-1.81184	-0.61540
Ir	-2.71252	-1.87745	-0.20864
Ir	-1.45826	-2.33318	1.83191

16

Ir	-1.63981	-2.38681	2.06888
Ir	-2.92475	-2.03035	0.06940
Ir	0.42489	-2.34421	0.75384
Ir	-1.59239	0.01002	2.45366
Ir	-0.86542	-1.98244	-1.25255
Ir	2.50633	-2.10089	-0.52171
Ir	-2.86666	0.36329	0.47079
Ir	0.45377	0.01643	1.16180
Ir	1.19785	-1.73350	-2.55451
Ir	-0.83279	0.37898	-0.84439
Ir	0.23173	2.36015	1.71550
Ir	2.47622	0.31241	-0.08674
Ir	-1.04143	2.71856	-0.26665
Ir	2.28439	2.68802	0.46252
Ir	1.18767	0.67659	-2.09353
Ir	1.00040	3.05375	-1.53631

17

Ir	-2.87163	-2.07654	-0.11103
Ir	-1.63813	-2.63038	1.89916
Ir	-2.72917	0.26559	0.45488
Ir	-1.53718	-0.29856	2.46292
Ir	-0.75644	-2.03431	-1.33974
Ir	-3.00866	2.56468	-0.10258
Ir	0.57504	-0.17880	1.21029

Ir	-0.63203	2.70679	-0.18276
Ir	0.45488	-2.53488	0.66512
Ir	-0.62274	0.33023	-0.80452
Ir	0.61682	2.20721	1.80842
Ir	1.33603	-1.82906	-2.58111
Ir	2.56995	-2.35534	-0.54565
Ir	1.47080	0.54417	-2.01341
Ir	1.43608	2.91647	-1.41391
Ir	2.65583	0.02362	-0.00067
Ir	2.68056	2.37911	0.59459

18

Ir	1.54268	0.47696	-2.20228
Ir	1.57894	2.84214	-1.65034
Ir	1.43626	-1.89575	-2.77788
Ir	-0.51209	2.65016	-0.43840
Ir	2.72335	-0.03425	-0.19801
Ir	2.78627	2.31979	0.39875
Ir	2.64125	-2.41730	-0.74085
Ir	-2.64372	2.42054	0.72648
Ir	-0.58945	0.25755	-1.00395
Ir	-0.66434	-2.14478	-1.56560
Ir	0.59051	-0.25514	1.00031
Ir	0.66685	2.13856	1.56651
Ir	0.51709	-2.65278	0.43007
Ir	-1.44147	1.90508	2.76686
Ir	-2.72650	0.03566	0.20407
Ir	-2.78325	-2.33246	-0.38022
Ir	-1.54732	-0.46773	2.20437
Ir	-1.57506	-2.84626	1.66011

19

Ir	-2.33471	2.52687	1.06742
Ir	-2.49730	0.09031	1.10445
Ir	-2.64304	-2.34847	1.16546
Ir	-2.36971	2.47692	-1.36091
Ir	0.06662	2.42644	1.04348
Ir	-2.56364	0.05891	-1.27270
Ir	-2.72046	-2.37874	-1.26744
Ir	1.42457	1.19105	2.87913
Ir	-0.05300	-0.06800	1.07110
Ir	-0.20473	-2.51238	1.06185
Ir	0.05094	2.39310	-1.37739
Ir	2.59369	2.27984	0.93490

Ir	-0.11920	-0.07868	-1.36060
Ir	2.43662	-0.25859	0.99214
Ir	-0.28393	-2.52727	-1.31917
Ir	2.22592	-2.65236	0.97930
Ir	2.51276	2.24745	-1.46775
Ir	2.35009	-0.22509	-1.42259
Ir	2.12851	-2.64131	-1.45066

20

Ir	1.46608	2.62017	-2.25432
Ir	1.41917	0.21329	-2.59718
Ir	-0.64416	2.54942	-0.99966
Ir	1.31323	-2.17469	-3.02726
Ir	-2.75521	2.40436	0.23861
Ir	2.73296	2.27885	-0.21683
Ir	-0.71115	0.08190	-1.36040
Ir	2.66712	-0.14340	-0.59098
Ir	-0.76611	-2.33717	-1.75866
Ir	0.60017	2.29544	1.02075
Ir	2.56913	-2.55382	-0.97208
Ir	-2.80442	-0.05902	-0.06236
Ir	0.55813	-0.33576	0.68432
Ir	-2.85392	-2.44497	-0.51930
Ir	0.47185	-2.70182	0.23923
Ir	-1.53420	-0.46796	1.96869
Ir	-1.48050	2.17320	2.27370
Ir	1.69846	0.76018	2.58783
Ir	-1.58993	-2.83853	1.51611
Ir	-0.35670	0.68034	3.82978

2 Additional Minima

Coordinates for the additional minima discussed for Ir₁₁, Ir₁₃, Ir₁₆ and Ir₁₉.

2.1 Ir₁₁

11

Ir	-1.62681727272	0.795521818181	0.127981818182
Ir	-0.483207272726	-0.183128181819	2.02769181818
Ir	2.50166272727	0.113261818181	0.470521818182
Ir	-0.422227272726	-0.612688181819	-1.36830818182

Ir 0.118772727274 2.51283181819 0.0550518181818
 Ir 0.765952727274 -1.57343818181 0.605701818182
 Ir 1.22426272727 1.50308181818 1.94916181819
 Ir -1.31810727273 -2.59842818182 -0.252568181818
 Ir -2.61122727273 -1.21929818181 1.21856181818
 Ir 1.36558272728 1.10279181819 -1.40750818181
 Ir 0.485352727274 0.159491818181 -3.42628818181

2.2 Ir_{13}

13

Ir -1.43513384615 0.00261307692308 -1.20249923077
 Ir 0.968546153846 0.188623076923 1.18399076923
 Ir -1.53801384615 2.40398307692 -1.28477923077
 Ir 1.05231615385 -2.36867692308 -1.05393923077
 Ir 1.01874615385 -2.22971692308 1.31788076923
 Ir 0.861896153846 2.59173307692 1.10953076923
 Ir -1.46185384615 0.0902730769231 1.18830076923
 Ir -1.36834384615 -2.43805692308 -1.11004923077
 Ir -1.41851384615 -2.33506692308 1.31630076923
 Ir 0.994686153846 0.130873076923 -1.19286923077
 Ir -1.53758384615 2.49063307692 1.10436076923
 Ir 0.863506153846 2.50833307692 -1.28740923077
 Ir 2.99974615385 -1.03554692308 -0.0888192307692

13

Ir 2.59041769231 3.40788384615 -0.000899230769231
 Ir 0.990767692308 -0.276006153846 -1.18728923077
 Ir 0.976927692308 2.13827384615 -1.23821923077
 Ir -1.40754230769 -0.284866153846 -1.18768923077
 Ir -1.43009230769 2.12548384615 -1.22820923077
 Ir 0.987737692308 -0.279676153846 1.19424076923
 Ir -1.42256230769 -2.69382615385 1.18275076923
 Ir 0.980517692308 2.13693384615 1.24043076923
 Ir -1.41689230769 -2.68639615385 -1.20113923077
 Ir -1.40888230769 -0.290646153846 1.18712076923
 Ir 0.990177692308 -2.71270615385 1.19057076923
 Ir -1.42529230769 2.12151384615 1.24234076923
 Ir 0.994717692308 -2.70596615385 -1.19400923077

13

Ir -0.252229230769 1.23383923077 -1.16329692308

Ir -0.419929230769 -1.19241076923 1.16013307692
 Ir -2.66641923077 1.39927923077 -1.19175692308
 Ir 2.15598076923 1.07674923077 1.26583307692
 Ir 1.99957076923 -1.36088076923 1.25347307692
 Ir -2.83516923077 -1.03468076923 1.15792307692
 Ir -0.400849230769 -1.13967076923 -1.21988692308
 Ir 2.17457076923 1.12636923077 -1.18365692308
 Ir 2.02090076923 -1.30375076923 -1.28129692308
 Ir -0.271089230769 1.18097923077 1.21166307692
 Ir -2.81678923077 -0.981060769231 -1.25006692308
 Ir -2.68620923077 1.34592923077 1.20991307692
 Ir 3.99766076923 -0.350690769231 0.0310230769231

2.3 Ir_{16}

16

Ir -0.212085 2.765120625 0.96028375
 Ir 2.491335 2.322730625 -1.06658625
 Ir -2.692155 0.884300625 0.77671375
 Ir -0.036315 0.168460625 -1.23773625
 Ir 2.325595 -0.108559375 -0.90081625
 Ir -2.789195 -1.685409375 -1.45533625
 Ir 2.173155 2.511680625 1.30885375
 Ir -0.355545 0.357840625 1.14356375
 Ir 2.006485 0.080860625 1.48203375
 Ir 0.103245 2.578810625 -1.39563625
 Ir -3.105105 -1.499269375 0.92048375
 Ir -2.375715 0.699500625 -1.57924625
 Ir -0.426435 -2.195289375 -1.10480625
 Ir 1.657365 -2.340699375 1.64339375
 Ir 1.978825 -2.532969375 -0.77448625
 Ir -0.743455 -2.007109375 1.27932375

16

Ir -0.0434575 2.08376875 1.150988125
 Ir 0.0077825 -0.39618125 -1.206871875
 Ir 2.3853425 2.15784875 1.173038125
 Ir -2.4697375 2.01739875 -1.244651875
 Ir -2.4639275 -0.41819125 -1.184891875
 Ir 2.4790825 -0.31814125 -1.178471875
 Ir 0.0038025 -0.35475125 1.218698125
 Ir -2.4724575 2.06038875 1.167338125

Ir -2.4651875 -0.37697125 1.193658125
Ir -0.0396775 2.04306875 -1.224771875
Ir 2.4731225 -0.27710125 1.199138125
Ir 2.3903225 2.11516875 -1.238171875
Ir -1.2451775 -2.63000125 -1.150051875
Ir 1.3515925 -2.53816125 1.238108125
Ir 1.3564325 -2.57632125 -1.147151875
Ir -1.2478575 -2.59182125 1.234068125

16

Ir -1.236828125 -1.183874375 1.196524375
Ir -1.221638125 1.180935625 -1.212665625
Ir -3.687348125 -1.183174375 1.189214375
Ir 1.238411875 -1.205924375 -1.175415625
Ir 1.238911875 1.191695625 -1.192255625
Ir -3.681338125 1.182565625 -1.238075625
Ir -1.236158125 1.193855625 1.182154375
Ir 1.222741875 -1.187794375 1.203134375
Ir 1.223811875 1.208235625 1.186614375
Ir -1.222998125 -1.196704375 -1.200445625
Ir -3.693038125 1.192355625 1.180294375
Ir -3.677988125 -1.192724375 -1.225035625
Ir 3.689591875 -1.216804375 -1.151115625
Ir 3.678591875 1.219495625 1.204734375
Ir 3.686941875 1.196965625 -1.171435625
Ir 3.678331875 -1.199104375 1.223774375

2.4 Ir_{19}

19

Ir -2.51978736842 -2.46162578947 -1.10508315789
Ir -2.65240736842 -0.0266757894737 -1.07378315789
Ir -2.75706736842 2.40280421053 -1.07964315789
Ir -2.54320736842 -2.47439578947 1.32214684211
Ir -0.0705573684211 -2.35886578947 -1.07310315789
Ir -2.66135736842 -0.0412357894737 1.30844684211
Ir -2.76656736842 2.38909421053 1.35359684211
Ir 3.69226263158 -1.15167578947 -2.46587315789
Ir -0.193457368421 0.0989142105263 -1.07505315789
Ir -0.332507368421 2.55507421053 -1.04108315789
Ir -0.114557368421 -2.37158578947 1.31286684211
Ir 2.34552263158 -2.43250578947 -1.01060315789

Ir -0.204507368421 0.0682642105263 1.31501684211
Ir 2.32069263158 0.246464210526 -1.09121315789
Ir -0.335897368421 2.51861421053 1.33942684211
Ir 2.10217263158 2.63167421053 -1.02562315789
Ir 2.32534263158 -2.33866578947 1.38937684211
Ir 2.26672263158 0.160954210526 1.31217684211
Ir 2.09916263158 2.58537421053 1.38800684211