

Supporting Information for

Aromaticity of biphenylene networks

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Table 1. The Cartesian coordinates of the optimized molecular structures of nBp-nanoribbons with armchair edges (n=2-10) at the B3LYP/6-31G(d,p) level of theory

2Bp_H				2Bp_F_Br			
6	-1.521510000	3.114443000	0.000000000	6	1.524779251	0.679261333	0.000000000
6	1.521510000	3.114443000	0.000000000	6	0.837463502	1.882511884	0.000000000
6	0.740239000	1.918288000	0.000000000	6	-0.640242649	1.958830319	0.000000000
6	-0.740239000	1.918288000	0.000000000	6	-1.457427073	0.839617228	0.000000000
6	-1.493252000	0.757482000	0.000000000	6	-1.524779251	-0.679261333	0.000000000
6	-2.912732000	0.753376000	0.000000000	6	-0.837463502	-1.882511884	0.000000000
6	-2.909858000	3.109763000	0.000000000	6	0.640242649	-1.958830319	0.000000000
6	2.909858000	3.109763000	0.000000000	6	1.457427073	-0.839617228	0.000000000
6	1.493252000	0.757482000	0.000000000	6	2.943696644	0.599568764	0.000000000
6	3.658637000	1.905828000	0.000000000	6	2.877285278	-0.889129699	0.000000000
6	2.912732000	0.753376000	0.000000000	6	3.754128991	1.702382122	0.000000000
6	-3.658637000	1.905828000	0.000000000	6	3.062265960	2.936767268	0.000000000
1	-4.744308000	1.919295000	0.000000000	6	1.685131831	3.034061308	0.000000000
6	-0.740239000	-1.918288000	0.000000000	1	1.270201671	4.029365015	0.000000000
6	-1.493252000	-0.757482000	0.000000000	9	3.780931236	4.069460469	0.000000000
6	-3.658637000	-1.905828000	0.000000000	35	5.638667905	1.644711678	0.000000000
6	-2.909858000	-3.109763000	0.000000000	6	3.564635668	-2.072967450	0.000000000
6	-1.521510000	-3.114443000	0.000000000	6	2.784147545	-3.248413593	0.000000000
6	0.740239000	-1.918288000	0.000000000	6	1.404569265	-3.170594775	0.000000000
6	1.521510000	-3.114443000	0.000000000	9	0.760995421	-4.360396682	0.000000000
6	1.493252000	-0.757482000	0.000000000	1	3.246683027	-4.227798399	0.000000000
6	2.909858000	-3.109763000	0.000000000	35	5.453807530	-2.183759573	0.000000000
6	2.912732000	-0.753376000	0.000000000	6	-1.404569265	3.170594775	0.000000000
6	3.658637000	-1.905828000	0.000000000	6	-2.784147545	3.248413593	0.000000000
6	-2.912732000	-0.753376000	0.000000000	6	-3.564635668	2.072967450	0.000000000
1	-4.744308000	-1.919295000	0.000000000	6	-2.877285278	0.889129699	0.000000000
1	-3.435798000	-4.060728000	0.000000000	6	-2.943696644	-0.599568764	0.000000000
1	-1.019368000	-4.076141000	0.000000000	6	-3.754128991	-1.702382122	0.000000000
1	1.019368000	-4.076141000	0.000000000	6	-3.062265960	-2.936767268	0.000000000
1	3.435798000	-4.060728000	0.000000000	6	-1.685131831	-3.034061308	0.000000000
1	-1.019368000	4.076141000	0.000000000	1	-3.246683027	4.227798399	0.000000000
1	1.019368000	4.076141000	0.000000000	9	-0.760995421	4.360396682	0.000000000
1	-3.435798000	4.060728000	0.000000000	35	-5.453807530	2.183759573	0.000000000
1	3.435798000	4.060728000	0.000000000	35	-5.638667905	-1.644711678	0.000000000
1	4.744308000	1.919295000	0.000000000	9	-3.780931236	-4.069460469	0.000000000
1	4.744308000	-1.919295000	0.000000000	1	-1.270201671	-4.029365015	0.000000000
3Bp_H				3Bp_F_Br			
6	-5.118243000	3.110157000	0.000000000	6	5.939308289	1.726768788	0.000000000
6	-5.870318000	1.907729000	0.000000000	6	5.214336694	2.941878069	0.000000000
6	-3.730155000	3.112345000	0.000000000	6	3.835077126	3.003307263	0.000000000
6	-5.126652000	0.753791000	0.000000000	6	3.015798972	1.829941213	0.000000000
6	-2.951146000	1.914135000	0.000000000	6	3.737073924	0.648407325	0.000000000
6	-3.707140000	0.756318000	0.000000000	6	5.157384762	0.603876677	0.000000000
6	-5.870318000	-1.907729000	0.000000000	35	7.824642945	1.718078296	0.000000000
6	-5.118243000	-3.110157000	0.000000000	9	5.903036160	4.093454479	0.000000000
6	-5.126652000	-0.753791000	0.000000000	1	3.396060032	3.987773553	0.000000000
6	-3.730155000	-3.112345000	0.000000000	6	5.125610668	-0.885963271	0.000000000
6	-3.707140000	-0.756318000	0.000000000	6	3.704838746	-0.866629440	0.000000000
6	-2.951146000	-1.914135000	0.000000000	6	2.908104078	-1.998184972	0.000000000
1	-5.642390000	-4.062128000	0.000000000	6	5.836549403	-2.055028378	0.000000000
1	-3.226705000	-4.073189000	0.000000000	6	5.078518197	-3.245499532	0.000000000
6	0.692652000	3.105337000	0.000000000	6	3.697742529	-3.195688445	0.000000000

6	3.730155000	3.112345000	0.000000000	35	7.727581033	-2.126507954	0.000000000
6	2.951146000	1.914135000	0.000000000	1	5.559872880	-4.215840476	0.000000000
6	1.472587000	1.911834000	0.000000000	9	3.082157916	-4.400211671	0.000000000
6	0.707848000	0.757547000	0.000000000	6	1.537514107	1.869535634	0.000000000
6	-0.707848000	0.757547000	0.000000000	6	0.723664139	0.742955599	0.000000000
6	-0.692652000	3.105337000	0.000000000	6	0.693409191	-0.772589439	0.000000000
6	5.118243000	3.110157000	0.000000000	6	1.430509803	-1.950030861	0.000000000
6	3.707140000	0.756318000	0.000000000	6	0.620809376	-3.118988567	0.000000000
6	5.870318000	1.907729000	0.000000000	6	-0.756091571	-3.061418485	0.000000000
6	5.126652000	0.753791000	0.000000000	6	-1.537514107	-1.869535634	0.000000000
6	-1.472587000	1.911834000	0.000000000	6	-0.723664139	-0.742955599	0.000000000
6	1.472587000	-1.911834000	0.000000000	6	-0.693409191	0.772589439	0.000000000
6	0.707848000	-0.757547000	0.000000000	6	0.756091571	3.061418485	0.000000000
6	-1.472587000	-1.911834000	0.000000000	6	-0.620809376	3.118988567	0.000000000
6	-0.692652000	-3.105337000	0.000000000	6	-1.430509803	1.950030861	0.000000000
6	0.692652000	-3.105337000	0.000000000	9	1.375705736	4.266339829	0.000000000
6	2.951146000	-1.914135000	0.000000000	1	-1.057777874	4.104134258	0.000000000
6	3.730155000	-3.112345000	0.000000000	1	1.057777874	-4.104134258	0.000000000
6	3.707140000	-0.756318000	0.000000000	9	-1.375705736	-4.266339829	0.000000000
6	5.118243000	-3.110157000	0.000000000	6	-3.015798972	-1.829941213	0.000000000
6	5.126652000	-0.753791000	0.000000000	6	-3.737073924	-0.648407325	0.000000000
6	5.870318000	-1.907729000	0.000000000	6	-2.908104078	1.998184972	0.000000000
6	-0.707848000	-0.757547000	0.000000000	6	-3.704838746	0.866629440	0.000000000
1	6.955974000	1.924073000	0.000000000	6	-5.125610668	0.885963271	0.000000000
1	-1.192402000	-4.068083000	0.000000000	6	-5.157384762	-0.603876677	0.000000000
1	1.192402000	-4.068083000	0.000000000	6	-5.939308289	-1.726768788	0.000000000
1	3.226705000	-4.073189000	0.000000000	6	-5.214336694	-2.941878069	0.000000000
1	5.642390000	-4.062128000	0.000000000	6	-3.835077126	-3.003307263	0.000000000
1	6.955974000	-1.924073000	0.000000000	1	-3.396060032	-3.987773553	0.000000000
1	-5.642390000	4.062128000	0.000000000	9	-5.903036160	-4.093454479	0.000000000
1	-6.955974000	1.924073000	0.000000000	35	-7.824642945	-1.718078296	0.000000000
1	-3.226705000	4.073189000	0.000000000	6	-3.697742529	3.195688445	0.000000000
1	-6.955974000	-1.924073000	0.000000000	6	-5.078518197	3.245499532	0.000000000
1	1.192402000	4.068083000	0.000000000	6	-5.836549403	2.055028378	0.000000000
1	3.226705000	4.073189000	0.000000000	35	-7.727581033	2.126507954	0.000000000
1	-1.192402000	4.068083000	0.000000000	1	-5.559872880	4.215840476	0.000000000
1	5.642390000	4.062128000	0.000000000	9	-3.082157916	4.400211671	0.000000000
4Bp_H				4Bp_F_Br			
6	-5.941524000	3.112688000	0.000000000	6	8.147165053	1.744226979	0.000000000
6	-2.902639000	3.104884000	0.000000000	6	7.410331961	2.952404629	0.000000000
6	-3.684244000	1.911904000	0.000000000	6	6.030445669	3.000251490	0.000000000
6	-5.162622000	1.914251000	0.000000000	6	5.223035759	1.818999210	0.000000000
6	-5.918354000	0.756375000	0.000000000	6	5.955659886	0.644361989	0.000000000
6	-7.337763000	0.753587000	0.000000000	6	7.376341749	0.613640744	0.000000000
6	-7.329501000	3.110286000	0.000000000	35	10.032523056	1.753058686	0.000000000
6	-1.517444000	3.103700000	0.000000000	6	3.744797075	1.843657096	0.000000000
6	-2.920616000	0.757436000	0.000000000	6	2.943900878	0.708688894	0.000000000
6	-0.738382000	1.908363000	0.000000000	6	2.928859457	-0.806701450	0.000000000
6	-1.505340000	0.756349000	0.000000000	6	1.526776856	0.722407350	0.000000000
6	-8.081426000	1.907442000	0.000000000	6	1.511729995	-0.789245024	0.000000000
1	-9.167057000	1.923925000	0.000000000	6	3.675109696	-1.977415666	0.000000000
6	-5.162622000	-1.914251000	0.000000000	6	5.152873556	-2.011189633	0.000000000
6	-5.918354000	-0.756375000	0.000000000	6	5.938289960	-0.871431580	0.000000000
6	-8.081426000	-1.907442000	0.000000000	6	7.359099037	-0.876671875	0.000000000
6	-7.329501000	-3.110286000	0.000000000	6	8.081310710	-2.038944286	0.000000000
6	-5.941524000	-3.112688000	0.000000000	6	7.335216214	-3.236875191	0.000000000
6	-3.684244000	-1.911904000	0.000000000	6	5.953895905	-3.200770083	0.000000000
6	-2.902639000	-3.104884000	0.000000000	9	5.349323254	-4.411117993	0.000000000
6	-2.920616000	-0.757436000	0.000000000	1	7.826285611	-4.202297204	0.000000000
6	-1.517444000	-3.103700000	0.000000000	35	9.972957613	-2.092481804	0.000000000
6	-1.505340000	-0.756349000	0.000000000	9	8.087572020	4.110759008	0.000000000
6	-0.738382000	-1.908363000	0.000000000	1	5.580878044	3.980157858	0.000000000
6	-7.337763000	-0.753587000	0.000000000	6	2.948188776	3.025584689	0.000000000
1	-9.167057000	-1.923925000	0.000000000	6	1.570490611	3.066246398	0.000000000
1	-7.854066000	-4.061990000	0.000000000	6	0.773012804	1.887277056	0.000000000
1	-5.437818000	-4.073399000	0.000000000	6	0.704197306	-1.918063864	0.000000000
1	-3.401489000	-4.068107000	0.000000000	6	1.495788873	-3.105300913	0.000000000
1	-1.016836000	-4.065985000	0.000000000	6	2.873298233	-3.152131438	0.000000000
6	2.902639000	3.104884000	0.000000000	1	3.317392621	-4.134160445	0.000000000
6	5.941524000	3.112688000	0.000000000	9	0.888509161	-4.316923314	0.000000000
6	5.162622000	1.914251000	0.000000000	6	-0.704197306	1.918063864	0.000000000
6	3.684244000	1.911904000	0.000000000	6	-1.511729995	0.789245024	0.000000000
6	2.920616000	0.757436000	0.000000000	6	-1.526776856	-0.722407350	0.000000000
6	1.505340000	0.756349000	0.000000000	6	-0.773012804	-1.887277056	0.000000000

6	1.517444000	3.103700000	0.000000000	6	-1.570490611	-3.066246398	0.000000000
6	7.329501000	3.110286000	0.000000000	6	-2.948188776	-3.025584689	0.000000000
6	5.918354000	0.756375000	0.000000000	6	-3.744797075	-1.843657096	0.000000000
6	8.081426000	1.907442000	0.000000000	6	-2.943900878	-0.708688894	0.000000000
6	7.337763000	0.753587000	0.000000000	6	-2.928859457	0.806701450	0.000000000
6	0.738382000	1.908363000	0.000000000	6	-1.495788873	3.105300913	0.000000000
6	3.684244000	-1.911904000	0.000000000	6	-2.873298233	3.152131438	0.000000000
6	2.920616000	-0.757436000	0.000000000	6	-3.675109696	1.977415666	0.000000000
6	0.738382000	-1.908363000	0.000000000	6	-5.152873556	2.011189633	0.000000000
6	1.517444000	-3.103700000	0.000000000	6	-5.938289960	0.871431580	0.000000000
6	2.902639000	-3.104884000	0.000000000	6	-5.955659886	-0.644361989	0.000000000
6	5.162622000	-1.914251000	0.000000000	6	-5.223035759	-1.818999210	0.000000000
6	5.941524000	-3.112688000	0.000000000	6	-7.359099037	0.876671875	0.000000000
6	5.918354000	-0.756375000	0.000000000	6	-7.376341749	-0.613640744	0.000000000
6	7.329501000	-3.110286000	0.000000000	6	-8.147165053	-1.744226979	0.000000000
6	7.337763000	-0.753587000	0.000000000	6	-7.410331961	-2.952404629	0.000000000
6	8.081426000	-1.907442000	0.000000000	6	-6.030445669	-3.000251490	0.000000000
6	1.505340000	-0.756349000	0.000000000	1	-5.580878044	-3.980157858	0.000000000
1	9.167057000	1.923925000	0.000000000	9	-8.087572020	-4.110759008	0.000000000
1	1.016836000	-4.065985000	0.000000000	35	-10.032523056	-1.753058686	0.000000000
1	3.401489000	-4.068107000	0.000000000	9	-3.554026800	-4.238007510	0.000000000
1	5.437818000	-4.073399000	0.000000000	1	-1.122894069	-4.046283723	0.000000000
1	7.854066000	-4.061990000	0.000000000	1	-3.317392621	4.134160445	0.000000000
1	9.167057000	-1.923925000	0.000000000	9	-0.888509161	4.316923314	0.000000000
1	-5.437818000	4.073399000	0.000000000	1	1.122894069	4.046283723	0.000000000
1	-3.401489000	4.068107000	0.000000000	9	3.554026800	4.238007510	0.000000000
1	-7.854066000	4.061990000	0.000000000	6	-5.953895905	3.200770083	0.000000000
1	-1.016836000	4.065985000	0.000000000	6	-7.335216214	3.236875191	0.000000000
1	3.401489000	4.068107000	0.000000000	6	-8.081310710	2.038944286	0.000000000
1	5.437818000	4.073399000	0.000000000	35	-9.972957613	2.092481804	0.000000000
1	1.016836000	4.065985000	0.000000000	1	-7.826285611	4.202297204	0.000000000
1	7.854066000	4.061990000	0.000000000	9	-5.349323254	4.411117993	0.000000000
5Bp_H				5Bp_F_Br			
6	-8.152808000	3.112808000	0.000000000	6	-10.362825248	-1.757254965	0.000000000
6	-5.895348000	1.912663000	0.000000000	6	-9.619999519	-2.961545835	0.000000000
6	-7.373680000	1.914884000	0.000000000	6	-8.239932155	-3.002545488	0.000000000
6	-8.129191000	0.756535000	0.000000000	6	-7.438432551	-1.817103172	0.000000000
6	-9.548543000	0.753633000	0.000000000	6	-8.177151880	-0.646124311	0.000000000
6	-9.540987000	3.110193000	0.000000000	6	-9.597887381	-0.622663440	0.000000000
6	-3.728575000	3.104211000	0.000000000	6	-5.959943881	-1.834229528	0.000000000
6	-5.131711000	0.757665000	0.000000000	6	-5.165245744	-0.694791010	0.000000000
6	-2.949715000	1.909506000	0.000000000	6	-5.157064838	-3.012048217	0.000000000
6	-3.716283000	0.756714000	0.000000000	6	-3.779234887	-3.045768662	0.000000000
6	-10.292442000	1.907576000	0.000000000	6	-2.988323313	-1.862497643	0.000000000
1	-11.378107000	1.923255000	0.000000000	6	-3.748189815	-0.701323656	0.000000000
6	-7.373680000	-1.914884000	0.000000000	6	-5.158054730	0.820744489	0.000000000
6	-8.129191000	-0.756535000	0.000000000	6	-8.167581092	0.869661008	0.000000000
6	-10.292442000	-1.907576000	0.000000000	6	-7.388359097	2.013599962	0.000000000
6	-9.540987000	-3.110193000	0.000000000	6	-5.910432071	1.987660394	0.000000000
6	-8.152808000	-3.112808000	0.000000000	6	-3.740956187	0.810629448	0.000000000
6	-5.895348000	-1.912663000	0.000000000	6	-9.588441758	0.867601879	0.000000000
6	-5.113834000	-3.105279000	0.000000000	6	-10.316822339	2.025946788	0.000000000
6	-5.131711000	-0.757665000	0.000000000	6	-9.577095133	3.227938726	0.000000000
6	-3.728575000	-3.104211000	0.000000000	6	-8.195712664	3.198916030	0.000000000
6	-3.716283000	-0.756714000	0.000000000	6	-5.115029275	3.166994730	0.000000000
6	-2.949715000	-1.909506000	0.000000000	6	-3.737376475	3.127154805	0.000000000
6	-9.548543000	-0.753633000	0.000000000	6	-2.939909175	1.944212677	0.000000000
1	-11.378107000	-1.923255000	0.000000000	6	-1.511237178	-1.885148554	0.000000000
1	-10.065369000	-4.061963000	0.000000000	6	-0.711908844	-0.751446685	0.000000000
1	-7.649514000	-4.073731000	0.000000000	6	0.705072922	-0.759643722	0.000000000
1	-5.612681000	-4.068455000	0.000000000	6	1.462813858	-1.921025828	0.000000000
1	-3.228006000	-4.066457000	0.000000000	6	0.668078528	-3.102444007	0.000000000
6	0.692609000	3.103488000	0.000000000	6	-0.709746982	-3.065920808	0.000000000
6	1.473344000	1.909548000	0.000000000	9	-1.308609978	-4.281725317	0.000000000
6	0.707644000	0.756635000	0.000000000	1	1.118287615	-4.081389313	0.000000000
6	-0.707644000	0.756635000	0.000000000	1	-3.325819258	-4.023232344	0.000000000
6	-0.692609000	3.103488000	0.000000000	9	-5.756305410	-4.227501005	0.000000000
6	-1.473344000	1.909548000	0.000000000	1	-7.785590620	-3.980083977	0.000000000
6	1.473344000	-1.909548000	0.000000000	9	-10.291771350	-4.123142026	0.000000000
6	0.707644000	-0.756635000	0.000000000	35	-12.248230358	-1.776727623	0.000000000
6	-1.473344000	-1.909548000	0.000000000	35	-12.208862824	2.068782262	0.000000000
6	-0.692609000	-3.103488000	0.000000000	1	-10.073268601	4.190779573	0.000000000
6	0.692609000	-3.103488000	0.000000000	9	-7.597459531	4.412169823	0.000000000
6	-0.707644000	-0.756635000	0.000000000	1	-5.564391968	4.146616384	0.000000000

1	-1.192022000	-4.066322000	0.000000000	9	-3.135271134	4.341104521	0.000000000
1	1.192022000	-4.066322000	0.000000000	6	-1.462813858	1.921025828	0.000000000
1	-7.649514000	4.073731000	0.000000000	6	-0.705072922	0.759643722	0.000000000
1	-10.065369000	4.061963000	0.000000000	6	0.711908844	0.751446685	0.000000000
1	-3.228006000	4.066457000	0.000000000	6	1.511237178	1.885148554	0.000000000
1	1.192022000	4.066322000	0.000000000	6	0.709746982	3.065920808	0.000000000
1	-1.192022000	4.066322000	0.000000000	6	-0.668078528	3.102444007	0.000000000
6	3.728575000	3.104211000	0.000000000	1	-1.118287615	4.081389313	0.000000000
6	2.949715000	1.909506000	0.000000000	9	1.308609978	4.281725317	0.000000000
6	5.113834000	3.105279000	0.000000000	6	2.939909175	-1.944212677	0.000000000
6	3.716283000	0.756714000	0.000000000	6	2.988323313	1.862497643	0.000000000
6	5.895348000	1.912663000	0.000000000	6	3.748189815	0.701323656	0.000000000
6	5.131711000	0.757665000	0.000000000	6	3.740956187	-0.810629448	0.000000000
6	2.949715000	-1.909506000	0.000000000	6	3.737376475	-3.127154805	0.000000000
6	3.728575000	-3.104211000	0.000000000	6	5.115029275	-3.166994730	0.000000000
6	3.716283000	-0.756714000	0.000000000	6	5.910432071	-1.987660394	0.000000000
6	5.113834000	-3.105279000	0.000000000	6	5.158054730	-0.820744489	0.000000000
6	5.131711000	-0.757665000	0.000000000	6	5.165245744	0.694791010	0.000000000
6	5.895348000	-1.912663000	0.000000000	6	5.959943881	1.834229528	0.000000000
1	3.228006000	-4.066457000	0.000000000	6	5.157064838	3.012048217	0.000000000
1	5.612681000	-4.068455000	0.000000000	6	3.779234887	3.045768662	0.000000000
1	3.228006000	4.066457000	0.000000000	1	3.325819258	4.023232344	0.000000000
1	5.612681000	4.068455000	0.000000000	9	5.756305410	4.227501005	0.000000000
6	8.152808000	3.112808000	0.000000000	9	3.135271134	-4.341104521	0.000000000
6	7.373680000	1.914884000	0.000000000	1	5.564391968	-4.146616384	0.000000000
6	9.540987000	3.110193000	0.000000000	6	7.388359097	-2.013599962	0.000000000
6	8.129191000	0.756535000	0.000000000	6	8.167581092	-0.869661008	0.000000000
6	10.292442000	1.907576000	0.000000000	6	8.177151880	0.646124311	0.000000000
6	9.548543000	0.753633000	0.000000000	6	7.438432551	1.817103172	0.000000000
6	7.373680000	-1.914884000	0.000000000	6	8.239932155	3.002545488	0.000000000
6	8.152808000	-3.112808000	0.000000000	6	9.619999519	2.961545835	0.000000000
6	8.129191000	-0.756535000	0.000000000	6	10.362825248	1.757254965	0.000000000
6	9.540987000	-3.110193000	0.000000000	6	9.597887381	0.622663440	0.000000000
6	9.548543000	-0.753633000	0.000000000	6	9.588441758	-0.867601879	0.000000000
6	10.292442000	-1.907576000	0.000000000	6	10.316822339	-2.025946788	0.000000000
1	11.378107000	1.923255000	0.000000000	6	8.195712664	-3.198916030	0.000000000
1	7.649514000	-4.073731000	0.000000000	6	9.577095133	-3.227938726	0.000000000
1	10.065369000	-4.061963000	0.000000000	9	7.597459531	-4.412169823	0.000000000
1	11.378107000	-1.923255000	0.000000000	1	10.073268601	-4.190779573	0.000000000
1	7.649514000	4.073731000	0.000000000	35	12.208862824	-2.068782262	0.000000000
1	10.065369000	4.061963000	0.000000000	35	12.248230358	1.776727623	0.000000000
6	-5.113834000	3.105279000	0.000000000	9	10.291771350	4.123142026	0.000000000
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6	-9.584802000	1.914560000	0.000000000	6	10.455498507	3.006200062	0.000000000
6	-10.340436000	0.756486000	0.000000000	6	9.657873491	1.818316624	0.000000000
6	-11.759542000	0.753612000	0.000000000	6	10.400491085	0.649701267	0.000000000
6	-11.752031000	3.110078000	0.000000000	6	11.821253094	0.630705624	0.000000000
6	-5.939951000	3.104196000	0.000000000	6	11.816317599	-0.859574866	0.000000000
6	-7.342816000	0.757665000	0.000000000	6	10.395469674	-0.866020868	0.000000000
6	-5.160910000	1.909439000	0.000000000	6	12.548457725	-2.015432437	0.000000000
6	-5.927636000	0.756608000	0.000000000	6	11.812815524	-3.219929462	0.000000000
6	-12.503540000	1.907498000	0.000000000	6	10.431360484	-3.195146674	0.000000000
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6	-9.584802000	-1.914560000	0.000000000	6	8.141864011	-1.991796457	0.000000000
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6	-7.325328000	-3.105018000	0.000000000	6	5.207761693	1.849541986	0.000000000
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1	-13.589204000	-1.923301000	0.000000000	6	3.730649305	1.867398806	0.000000000
1	-12.276311000	-4.061934000	0.000000000	6	2.925731377	3.045862702	0.000000000
1	-9.860598000	-4.073576000	0.000000000	6	1.547775687	3.078562797	0.000000000
1	-7.824028000	-4.068279000	0.000000000	6	0.756853600	1.894807866	0.000000000
1	-5.439546000	-4.066599000	0.000000000	6	1.517976105	0.735347635	0.000000000
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6	-0.738046000	1.909863000	0.000000000	6	2.932499688	-0.780112838	0.000000000
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6	-2.918562000	0.756584000	0.000000000	6	3.693700317	-1.939410828	0.000000000
6	-2.903966000	3.103661000	0.000000000	6	2.902483899	-3.123377094	0.000000000
6	-3.684545000	1.909521000	0.000000000	6	1.524581646	-3.090764454	0.000000000
6	-0.738046000	-1.909863000	0.000000000	6	0.719973194	-1.912545168	0.000000000
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6	-2.918562000	-0.756584000	0.000000000	6	-2.932499688	0.780112838	0.000000000
1	-3.403492000	-4.066493000	0.000000000	6	-2.934819266	-0.731133146	0.000000000
1	-1.019279000	-4.066711000	0.000000000	6	-3.693700317	1.939410828	0.000000000
1	-9.860598000	4.073576000	0.000000000	6	-5.170933197	1.957427081	0.000000000
1	-12.276311000	4.061934000	0.000000000	6	-5.968510640	0.821369997	0.000000000
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6	1.518623000	3.103789000	0.000000000	6	-2.925731377	-3.045862702	0.000000000
6	0.738046000	1.909863000	0.000000000	6	-1.547775687	-3.078562797	0.000000000
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6	3.684545000	1.909521000	0.000000000	6	-5.972247396	3.137782918	0.000000000
6	2.918562000	0.756584000	0.000000000	6	-7.349959039	3.173525199	0.000000000
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6	2.918562000	-0.756584000	0.000000000	6	-7.373095300	-3.005373963	0.000000000
6	3.684545000	-1.909521000	0.000000000	6	-5.995242608	-3.035134293	0.000000000
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1	3.403492000	-4.066493000	0.000000000	6	-10.395469674	0.866020868	0.000000000
1	1.019279000	4.066711000	0.000000000	6	-10.400491085	-0.649701267	0.000000000
1	3.403492000	4.066493000	0.000000000	6	-11.816317599	0.859574866	0.000000000
6	5.939951000	3.104196000	0.000000000	6	-11.821253094	-0.630705624	0.000000000
6	5.160910000	1.909439000	0.000000000	6	-12.582676090	-1.767800681	0.000000000
6	7.325328000	3.105018000	0.000000000	6	-11.835732956	-2.969510194	0.000000000
6	5.927636000	0.756608000	0.000000000	6	-10.455498507	-3.006200062	0.000000000
6	8.106587000	1.912341000	0.000000000	6	-9.657873491	-1.818316624	0.000000000
6	7.342816000	0.757665000	0.000000000	6	-10.431360484	3.195146674	0.000000000
6	5.160910000	-1.909439000	0.000000000	6	-11.812815524	3.219929462	0.000000000
6	5.939951000	-3.104196000	0.000000000	6	-12.548457725	2.015432437	0.000000000
6	5.927636000	-0.756608000	0.000000000	35	-14.440662520	2.050163500	0.000000000
6	7.325328000	-3.105018000	0.000000000	1	-12.312151960	4.181187703	0.000000000
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1	5.439546000	-4.066599000	0.000000000	9	-5.373970470	4.353503771	0.000000000
1	7.824028000	-4.068279000	0.000000000	1	-3.355346755	4.101135699	0.000000000
1	5.439546000	4.066599000	0.000000000	9	-0.927849696	4.307478435	0.000000000
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6	12.503540000	1.907498000	0.000000000	1	9.998790699	3.982748761	0.000000000
6	11.759542000	0.753612000	0.000000000	9	12.503267831	4.133439119	0.000000000
6	10.340436000	0.756486000	0.000000000	35	14.467922420	1.794936697	0.000000000
6	10.363746000	3.112566000	0.000000000	35	14.440662520	-2.050163500	0.000000000
6	9.584802000	1.914560000	0.000000000	1	12.312151960	-4.181187703	0.000000000
6	12.503540000	-1.907498000	0.000000000	9	9.837016486	-4.410153861	0.000000000
6	11.759542000	-0.753612000	0.000000000	1	7.801827758	-4.152039369	0.000000000
6	9.584802000	-1.914560000	0.000000000	9	5.373970470	-4.353503771	0.000000000
6	10.363746000	-3.112566000	0.000000000	1	3.355346755	-4.101135699	0.000000000
6	11.752031000	-3.110078000	0.000000000	9	0.927849696	-4.307478435	0.000000000
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1	9.860598000	-4.073576000	0.000000000	9	-3.521274564	-4.263168957	0.000000000
1	12.276311000	-4.061934000	0.000000000	1	-5.539268275	-4.011473618	0.000000000
1	12.276311000	4.061934000	0.000000000	9	-7.969039011	-4.222281922	0.000000000
1	9.860598000	4.073576000	0.000000000	1	-9.998790699	-3.982748761	0.000000000
1	13.589204000	1.923301000	0.000000000	9	-12.503267831	-4.133439119	0.000000000
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6	-13.970684000	0.753678000	0.000000000	6	-12.625343934	-0.654728822	0.000000000
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6	-9.553391000	0.757456000	0.000000000	6	-12.623849866	0.861106487	0.000000000
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6	5.926022000	-0.756473000	0.000000000	6	3.723894328	1.880994983	0.000000000
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6	14.785697000	3.112537000	0.000000000	1	5.531252850	4.031045975	0.000000000
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9	-5.727938926	-4.266699233	0.000000000
6	-0.686376307	-3.071693097	0.000000000
6	0.691691754	-3.098373945	0.000000000
9	-1.277138016	-4.291269803	0.000000000
1	1.149017875	-4.074232882	0.000000000
6	3.764820524	-3.096281504	0.000000000
6	5.142951266	-3.122815641	0.000000000
6	8.216151109	-3.119845520	0.000000000
6	9.594234303	-3.146066433	0.000000000
1	10.051016743	-4.122070849	0.000000000
9	7.625688812	-4.339549616	0.000000000
1	5.600450543	-4.098641380	0.000000000
9	3.174245447	-4.315938076	0.000000000
10Bp_H			
6	-19.208558000	3.112794000	0.000000000
6	-16.950931000	1.912450000	0.000000000
6	-18.429326000	1.914789000	0.000000000
6	-19.184854000	0.756434000	0.000000000
6	-20.604151000	0.753623000	0.000000000
6	-20.596777000	3.110126000	0.000000000
6	-14.784014000	3.104060000	0.000000000
6	-16.187248000	0.757519000	0.000000000
6	-14.005431000	1.909059000	0.000000000
6	-14.772140000	0.756565000	0.000000000
6	-21.348063000	1.907501000	0.000000000
1	-22.433710000	1.923014000	0.000000000
6	-18.429326000	-1.914789000	0.000000000
6	-19.184854000	-0.756434000	0.000000000
6	-21.348063000	-1.907501000	0.000000000
6	-20.596777000	-3.110126000	0.000000000
6	-19.208558000	-3.112794000	0.000000000
6	-16.950931000	-1.912450000	0.000000000
6	-16.169351000	-3.105224000	0.000000000
6	-16.187248000	-0.757519000	0.000000000
6	-14.784014000	-3.104060000	0.000000000
6	-14.772140000	-0.756565000	0.000000000
6	-14.005431000	-1.909059000	0.000000000
6	-20.604151000	-0.753623000	0.000000000
1	-22.433710000	-1.923014000	0.000000000
1	-21.121073000	-4.061923000	0.000000000
1	-18.705278000	-4.073692000	0.000000000
1	-16.668189000	-4.068375000	0.000000000
1	-14.283400000	-4.066333000	0.000000000
6	-10.363345000	3.103728000	0.000000000
6	-9.582736000	1.909606000	0.000000000
6	-10.348253000	0.756603000	0.000000000
6	-11.763070000	0.756490000	0.000000000
6	-11.748669000	3.103438000	0.000000000
6	-12.529085000	1.909082000	0.000000000
6	-9.582736000	-1.909606000	0.000000000
6	-10.348253000	-0.756603000	0.000000000
6	-12.529085000	-1.909082000	0.000000000
6	-11.748669000	-3.103438000	0.000000000
6	-10.363345000	-3.103728000	0.000000000
6	-11.763070000	-0.756490000	0.000000000
1	-12.248339000	-4.066179000	0.000000000
1	-9.863976000	-4.066651000	0.000000000
1	-18.705278000	4.073692000	0.000000000
1	-21.121073000	4.061923000	0.000000000
1	-14.283400000	4.066333000	0.000000000
1	-9.863976000	4.066651000	0.000000000
1	-12.248339000	4.066179000	0.000000000
10Bp_F_Br			
6	-21.474803573	-1.800927083	0.000000000
6	-20.720320185	-2.997954207	0.000000000
6	-19.340014212	-3.026300717	0.000000000
6	-18.549691305	-1.833450815	0.000000000
6	-19.299527829	-0.669536687	0.000000000
6	-20.720468851	-0.659146160	0.000000000
6	-19.303557839	0.846246511	0.000000000
6	-20.724344638	0.831128043	0.000000000
6	-21.463686092	1.982362164	0.000000000
6	-20.735551319	3.191434813	0.000000000
6	-19.353908997	3.174972209	0.000000000
6	-18.535012807	1.997510368	0.000000000
6	-17.071296522	-1.835865781	0.000000000
6	-16.286925086	-0.689276667	0.000000000
6	-16.293329355	0.826241583	0.000000000
6	-17.056664736	1.986137522	0.000000000
6	-16.257874733	-3.006099053	0.000000000
6	-14.879939166	-3.027869454	0.000000000
6	-14.099467607	-1.837648709	0.000000000
6	-14.869883894	-0.683299858	0.000000000
6	-14.876043673	0.828672215	0.000000000
6	-14.084981777	1.969331111	0.000000000
6	-14.893715530	3.144715610	0.000000000
6	-16.271681911	3.172539220	0.000000000
6	-12.622331730	-1.846697885	0.000000000
6	-11.832893379	-0.705937428	0.000000000
6	-11.839226373	0.805344444	0.000000000
6	-12.607416691	1.960110934	0.000000000
6	-11.810627958	-3.020367195	0.000000000
6	-10.432624949	-3.045478946	0.000000000
6	-9.648212309	-1.857397575	0.000000000
6	-10.416043731	-0.702224752	0.000000000
6	-10.422129723	0.809271973	0.000000000
6	-11.822805466	3.148532385	0.000000000
6	-10.444726810	3.123559282	0.000000000
6	-9.632807505	1.950218973	0.000000000
6	-8.171297925	-1.866981726	0.000000000
6	-7.360123581	-3.040741571	0.000000000
6	-5.982098085	-3.066178431	0.000000000
6	-5.197597163	-1.878036470	0.000000000
6	-5.965148135	-0.722552949	0.000000000
6	-7.381945433	-0.725975866	0.000000000
6	-3.720614441	-1.887762941	0.000000000
6	-2.909470371	-3.061581646	0.000000000
6	-1.531427639	-3.087182588	0.000000000
6	-0.746753086	-1.899120436	0.000000000
6	-1.514245817	-0.743585186	0.000000000
6	-2.931094355	-0.746844863	0.000000000

6	-7.326085000	3.103815000	0.000000000	6	0.730314044	-1.908974301	0.000000000
6	-8.106565000	1.909579000	0.000000000	6	1.541517108	-3.082794281	0.000000000
6	-5.940744000	3.103800000	0.000000000	6	2.919603644	-3.108437427	0.000000000
6	-7.340784000	0.756618000	0.000000000	6	3.704332145	-1.920386527	0.000000000
6	-5.160399000	1.909541000	0.000000000	6	2.936811345	-0.764866146	0.000000000
6	-5.926090000	0.756651000	0.000000000	6	1.519929863	-0.768113669	0.000000000
6	-8.106565000	-1.909579000	0.000000000	6	-1.519929863	0.768113669	0.000000000
6	-7.326085000	-3.103815000	0.000000000	6	-2.936811345	0.764866146	0.000000000
6	-7.340784000	-0.756618000	0.000000000	6	-5.970956189	0.789144483	0.000000000
6	-5.940744000	-3.103800000	0.000000000	6	-7.387868658	0.785685102	0.000000000
6	-5.926090000	-0.756651000	0.000000000	6	1.514245817	0.743585186	0.000000000
6	-5.160399000	-1.909541000	0.000000000	6	2.931094355	0.746844863	0.000000000
1	-7.825772000	-4.066568000	0.000000000	6	-8.155594368	1.941010435	0.000000000
1	-5.441282000	-4.066635000	0.000000000	6	-7.371064069	3.129233260	0.000000000
1	-7.825772000	4.066568000	0.000000000	6	-5.992930607	3.103788897	0.000000000
1	-5.441282000	4.066635000	0.000000000	6	-5.181478940	1.930097761	0.000000000
6	-2.903855000	3.103809000	0.000000000	6	-3.704332145	1.920386527	0.000000000
6	-3.684242000	1.909544000	0.000000000	6	-2.919603644	3.108437427	0.000000000
6	-1.518535000	3.103889000	0.000000000	6	-1.541517108	3.082794281	0.000000000
6	-2.918553000	0.756652000	0.000000000	6	-0.730314044	1.908974301	0.000000000
6	-0.738084000	1.909626000	0.000000000	6	0.746753086	1.899120436	0.000000000
6	-1.503819000	0.756641000	0.000000000	6	1.531427639	3.087182588	0.000000000
6	-3.684242000	-1.909544000	0.000000000	6	2.909470371	3.061581646	0.000000000
6	-2.903855000	-3.103809000	0.000000000	6	3.720614441	1.887762941	0.000000000
6	-2.918553000	-0.756652000	0.000000000	6	5.181478940	-1.930097761	0.000000000
6	-1.518535000	-3.103889000	0.000000000	6	5.992930607	-3.103788897	0.000000000
6	-1.503819000	-0.756641000	0.000000000	6	7.371064069	-3.129233260	0.000000000
6	-0.738084000	-1.909626000	0.000000000	6	8.155594368	-1.941010435	0.000000000
1	-3.403438000	-4.066564000	0.000000000	6	7.387868658	-0.785685102	0.000000000
1	-1.018944000	-4.066715000	0.000000000	6	5.970956189	-0.789144483	0.000000000
1	-3.403438000	4.066564000	0.000000000	6	5.965148135	0.722552949	0.000000000
1	-1.018944000	4.066715000	0.000000000	6	7.381945433	0.725975866	0.000000000
6	-16.169351000	3.105224000	0.000000000	6	5.197597163	1.878036470	0.000000000
1	-16.668189000	4.068375000	0.000000000	6	5.982098085	3.066178431	0.000000000
6	2.903855000	3.103809000	0.000000000	6	7.360123581	3.040741571	0.000000000
6	5.160399000	1.909541000	0.000000000	6	8.171297925	1.866981726	0.000000000
6	3.684242000	1.909544000	0.000000000	6	9.648212309	1.857397575	0.000000000
6	2.918553000	0.756652000	0.000000000	6	10.416043731	0.702224752	0.000000000
6	1.503819000	0.756641000	0.000000000	6	10.422129723	-0.809271973	0.000000000
6	1.518535000	3.103889000	0.000000000	6	9.632807505	-1.950218973	0.000000000
6	7.326085000	3.103815000	0.000000000	6	10.444726810	-3.123559282	0.000000000
6	5.926090000	0.756651000	0.000000000	6	11.822805466	-3.148532385	0.000000000
6	8.106565000	1.909579000	0.000000000	6	12.607416691	-1.960110934	0.000000000
6	7.340784000	0.756618000	0.000000000	6	11.839226373	-0.805344444	0.000000000
6	0.738084000	1.909626000	0.000000000	6	11.832893379	0.705937428	0.000000000
6	3.684242000	-1.909544000	0.000000000	6	10.432624949	3.045478946	0.000000000
6	2.918553000	-0.756652000	0.000000000	6	11.810627958	3.020367195	0.000000000
6	0.738084000	-1.909626000	0.000000000	6	12.622331730	1.846697885	0.000000000
6	1.518535000	-3.103889000	0.000000000	6	14.099467607	1.837648709	0.000000000
6	2.903855000	-3.103809000	0.000000000	6	14.869883894	0.683299858	0.000000000
6	5.160399000	-1.909541000	0.000000000	6	14.876043673	-0.828672215	0.000000000
6	5.940744000	-3.103800000	0.000000000	6	14.084981777	-1.969331111	0.000000000
6	5.926090000	-0.756651000	0.000000000	6	14.893715530	-3.144715610	0.000000000
6	7.326085000	-3.103815000	0.000000000	6	16.271681911	-3.172539220	0.000000000
6	7.340784000	-0.756618000	0.000000000	6	17.056664736	-1.986137522	0.000000000
6	8.106565000	-1.909579000	0.000000000	6	16.293329355	-0.826241583	0.000000000
6	1.503819000	-0.756641000	0.000000000	6	16.286925086	0.689276667	0.000000000
1	1.018944000	-4.066715000	0.000000000	6	17.071296522	1.835865781	0.000000000
1	3.403438000	-4.066564000	0.000000000	6	16.257874733	3.006099053	0.000000000
1	5.441282000	-4.066635000	0.000000000	6	14.879939166	3.027869454	0.000000000
1	7.825772000	-4.066568000	0.000000000	6	18.535012807	-1.997510368	0.000000000
6	11.748669000	3.103438000	0.000000000	6	19.303557839	-0.846246511	0.000000000
6	12.529085000	1.909082000	0.000000000	6	19.299527829	0.669536687	0.000000000
6	11.763070000	0.756490000	0.000000000	6	18.549691305	1.833450815	0.000000000
6	10.348253000	0.756603000	0.000000000	6	19.353908997	-3.174972209	0.000000000
6	10.363345000	3.103728000	0.000000000	6	20.735551319	-3.191434813	0.000000000
6	9.582736000	1.909606000	0.000000000	6	21.463686092	-1.982362164	0.000000000
6	12.529085000	-1.909082000	0.000000000	6	20.724344638	-0.831128043	0.000000000
6	11.763070000	-0.756490000	0.000000000	6	20.720468851	0.659146160	0.000000000
6	9.582736000	-1.909606000	0.000000000	6	21.474803573	1.800927083	0.000000000
6	10.363345000	-3.103728000	0.000000000	6	20.720320185	2.997954207	0.000000000
6	11.748669000	-3.103438000	0.000000000	6	19.340014212	3.026300717	0.000000000
6	10.348253000	-0.756603000	0.000000000	35	23.359906573	1.840778795	0.000000000
1	9.863976000	-4.066651000	0.000000000	35	23.355940331	-2.004541424	0.000000000

1	12.248339000	-4.066179000	0.000000000	1	21.240819745	-4.149704914	0.000000000
1	3.403438000	4.066564000	0.000000000	9	18.767006805	-4.393483590	0.000000000
1	1.018944000	4.066715000	0.000000000	1	16.728735067	-4.148795009	0.000000000
1	7.825772000	4.066568000	0.000000000	9	14.302957702	-4.363999046	0.000000000
1	12.248339000	4.066179000	0.000000000	1	12.280552822	-4.124102398	0.000000000
1	9.863976000	4.066651000	0.000000000	9	9.855601177	-4.343878330	0.000000000
6	14.784014000	3.104060000	0.000000000	1	7.829337006	-4.104679719	0.000000000
6	14.005431000	1.909059000	0.000000000	9	5.403324966	-4.323893707	0.000000000
6	16.169351000	3.105224000	0.000000000	1	3.377739331	-4.083937248	0.000000000
6	14.772140000	0.756565000	0.000000000	9	0.951772697	-4.302849444	0.000000000
6	16.950931000	1.912450000	0.000000000	1	-1.073255808	-4.062651576	0.000000000
6	16.187248000	0.757519000	0.000000000	9	-3.499213782	-4.281636814	0.000000000
6	14.005431000	-1.909059000	0.000000000	1	-5.523792939	-4.041580040	0.000000000
6	14.784014000	-3.104060000	0.000000000	9	-7.949755124	-4.260825260	0.000000000
6	14.772140000	-0.756565000	0.000000000	1	-9.974310747	-4.020868597	0.000000000
6	16.169351000	-3.105224000	0.000000000	9	-12.398919547	-4.241108130	0.000000000
6	16.187248000	-0.757519000	0.000000000	1	-14.418864354	-4.001845944	0.000000000
6	16.950931000	-1.912450000	0.000000000	9	-16.846503581	-4.226465414	0.000000000
1	14.283400000	-4.066333000	0.000000000	1	-18.877808850	-4.000376472	0.000000000
1	16.668189000	-4.068375000	0.000000000	9	-21.380584043	-4.165969442	0.000000000
1	14.283400000	4.066333000	0.000000000	35	-23.359906573	-1.840778795	0.000000000
1	16.668189000	4.068375000	0.000000000	35	-23.355940331	2.004541424	0.000000000
6	19.208558000	3.112794000	0.000000000	1	-21.240819745	4.149704914	0.000000000
6	18.429326000	1.914789000	0.000000000	9	-18.767006805	4.393483590	0.000000000
6	20.596777000	3.110126000	0.000000000	1	-16.728735067	4.148795009	0.000000000
6	19.184854000	0.756434000	0.000000000	9	-14.302957702	4.363999046	0.000000000
6	21.348063000	1.907501000	0.000000000	1	-12.280552822	4.124102398	0.000000000
6	20.604151000	0.753623000	0.000000000	9	-9.855601177	4.343878330	0.000000000
6	18.429326000	-1.914789000	0.000000000	1	-7.829337006	4.104679719	0.000000000
6	19.208558000	-3.112794000	0.000000000	9	-5.403324966	4.323893707	0.000000000
6	19.184854000	-0.756434000	0.000000000	1	-3.377739331	4.083937248	0.000000000
6	20.596777000	-3.110126000	0.000000000	9	-0.951772697	4.302849444	0.000000000
6	20.604151000	-0.753623000	0.000000000	1	1.073255808	4.062651576	0.000000000
6	21.348063000	-1.907501000	0.000000000	9	3.499213782	4.281636814	0.000000000
1	22.433710000	1.923014000	0.000000000	1	5.523792939	4.041580040	0.000000000
1	18.705278000	-4.073692000	0.000000000	9	7.949755124	4.260825260	0.000000000
1	21.121073000	-4.061923000	0.000000000	1	9.974310747	4.020868597	0.000000000
1	22.433710000	-1.923014000	0.000000000	9	12.398919547	4.241108130	0.000000000
1	18.705278000	4.073692000	0.000000000	1	14.418864354	4.001845944	0.000000000
1	21.121073000	4.061923000	0.000000000	9	16.846503581	4.226465414	0.000000000
6	5.940744000	3.103800000	0.000000000	1	18.877808850	4.000376472	0.000000000
1	5.441282000	4.066635000	0.000000000	9	21.380584043	4.165969442	0.000000000

Table 2. The Cartesian coordinates of the optimized molecular structures of 2_m Bp-nanoribbons with zigzag edges (m=2-5) at the B3LYP/6-31G(d,p) level of theory

2_2Bp_H				2_2Bp_F_Br			
6	-1.898606000	0.733252000	0.000000000	6	1.232509264	2.780869209	0.000000000
6	-1.898606000	-0.733252000	0.000000000	6	3.270257862	0.984461607	0.000000000
6	-3.060826000	-1.522108000	0.000000000	6	6.337679339	-4.056441556	0.000000000
6	-3.066187000	-2.934733000	0.000000000	6	5.020498373	-4.577118980	0.000000000
6	-3.060826000	1.522108000	0.000000000	6	4.009006958	-3.660207078	0.000000000
6	-1.912190000	3.725214000	0.000000000	6	4.263080219	-2.257575862	0.000000000
6	-3.066187000	2.934733000	0.000000000	6	5.524775802	-1.686313702	0.000000000
6	-1.912190000	-3.725214000	0.000000000	6	6.552064447	-2.695401907	0.000000000
6	-5.720383000	-0.740123000	0.000000000	1	7.197537414	-4.715140857	0.000000000
6	-4.570795000	-1.505988000	0.000000000	35	4.739853045	-6.448768696	0.000000000
6	-5.729260000	-3.665448000	0.000000000	6	2.535722646	-3.404189740	0.000000000
6	-6.931984000	-2.902506000	0.000000000	6	2.766992414	-2.011736033	0.000000000
6	-6.927074000	-1.518732000	0.000000000	6	5.772824955	-0.225565054	0.000000000
6	-5.720383000	0.740123000	0.000000000	6	7.088376944	0.351669513	0.000000000
6	-6.927074000	1.518732000	0.000000000	6	7.295151501	1.712831572	0.000000000
6	-4.570795000	1.505988000	0.000000000	6	6.241210121	2.665812663	0.000000000
6	-6.931984000	2.902506000	0.000000000	6	4.989089014	2.121641171	0.000000000
6	-4.575451000	2.929163000	0.000000000	6	4.757698353	0.714928633	0.000000000
6	-5.729260000	3.665448000	0.000000000	1	7.968674012	-0.270535680	0.000000000
6	-4.575451000	-2.929163000	0.000000000	9	7.850623480	-2.316413217	0.000000000
1	-1.920348000	4.810201000	0.000000000	9	8.557456032	2.169064684	0.000000000
1	-7.885483000	-3.423476000	0.000000000	35	6.610434363	4.514409955	0.000000000
1	-7.884837000	-1.010241000	0.000000000	6	3.514373723	2.375672969	0.000000000

1	-7.884837000	1.010241000	0.000000000	6	1.993849519	0.402935213	0.000000000
1	-7.885483000	3.423476000	0.000000000	6	1.752770597	-1.039947538	0.000000000
1	-5.754211000	4.750758000	0.000000000	6	1.263330919	-3.977633349	0.000000000
6	1.898606000	-0.733252000	0.000000000	6	0.248233576	-3.032881407	0.000000000
6	3.060826000	-1.522108000	0.000000000	6	0.489341033	-1.634734482	0.000000000
6	1.912190000	-3.725214000	0.000000000	35	0.960552298	-5.839837499	0.000000000
6	0.756114000	-2.952104000	0.000000000	6	-1.232509264	-2.780869209	0.000000000
6	0.752726000	-1.532696000	0.000000000	6	-0.996957422	-1.382391306	0.000000000
6	1.898606000	0.733252000	0.000000000	6	-2.504227205	-3.336911319	0.000000000
6	-0.752726000	-1.532696000	0.000000000	6	-3.514373723	-2.375672969	0.000000000
6	0.752726000	1.532696000	0.000000000	6	-3.270257862	-0.984461607	0.000000000
6	-0.752726000	1.532696000	0.000000000	6	-1.993849519	-0.402935213	0.000000000
6	-0.756114000	-2.952104000	0.000000000	35	-2.833930714	-5.194146703	0.000000000
6	3.060826000	1.522108000	0.000000000	6	-4.989089014	-2.121641171	0.000000000
6	-0.756114000	2.952104000	0.000000000	6	-4.757698353	-0.714928633	0.000000000
6	0.756114000	2.952104000	0.000000000	6	-6.241210121	-2.665812663	0.000000000
6	3.066187000	2.934733000	0.000000000	6	-7.295151501	-1.712831572	0.000000000
6	1.912190000	3.725214000	0.000000000	6	-7.088376944	-0.351669513	0.000000000
6	3.066187000	-2.934733000	0.000000000	6	-5.772824955	0.225565054	0.000000000
1	1.920348000	4.810201000	0.000000000	35	-6.610434363	-4.514409955	0.000000000
6	5.720383000	-0.740123000	0.000000000	9	-8.557456032	-2.169064684	0.000000000
6	6.927074000	-1.518732000	0.000000000	1	-7.968674012	0.270535680	0.000000000
6	5.729260000	-3.665448000	0.000000000	6	-5.524775802	1.686313702	0.000000000
6	4.575451000	-2.929163000	0.000000000	6	-4.263080219	2.257575862	0.000000000
6	4.570795000	-1.505988000	0.000000000	6	-4.009006958	3.660207078	0.000000000
6	5.720383000	0.740123000	0.000000000	6	-5.020498373	4.577118980	0.000000000
6	4.570795000	1.505988000	0.000000000	6	-6.337679339	4.056441556	0.000000000
6	6.927074000	1.518732000	0.000000000	6	-6.552064447	2.695401907	0.000000000
6	4.575451000	2.929163000	0.000000000	6	-2.766992414	2.011736033	0.000000000
6	6.931984000	2.902506000	0.000000000	6	-2.535722646	3.404189740	0.000000000
6	5.729260000	3.665448000	0.000000000	6	-1.263330919	3.977633349	0.000000000
1	7.885483000	3.423476000	0.000000000	6	-0.248233576	3.032881407	0.000000000
1	7.884837000	-1.010241000	0.000000000	6	-0.489341033	1.634734482	0.000000000
1	7.884837000	1.010241000	0.000000000	6	-1.752770597	1.039947538	0.000000000
6	6.931984000	-2.902506000	0.000000000	6	0.996957422	1.382391306	0.000000000
1	7.885483000	-3.423476000	0.000000000	6	2.504227205	3.336911319	0.000000000
1	5.754211000	4.750758000	0.000000000	35	2.833930714	5.194146703	0.000000000
1	-1.920348000	-4.810201000	0.000000000	35	-0.960552298	5.839837499	0.000000000
1	-5.754211000	-4.750758000	0.000000000	35	-4.739853045	6.448768696	0.000000000
1	1.920348000	-4.810201000	0.000000000	1	-7.197537414	4.715140857	0.000000000
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6	-4.568494000	1.530223000	0.000000000	1	11.629905884	3.682337938	0.000000000
6	-10.748827000	2.902901000	0.000000000	6	10.682603409	3.156847618	0.000000000
6	-9.545950000	3.665282000	0.000000000	6	10.694250488	1.779524939	0.000000000
6	-10.744256000	1.519117000	0.000000000	6	9.529782700	0.931593782	0.000000000
6	-9.537888000	0.739808000	0.000000000	6	9.561294002	-0.549161504	0.000000000
6	-8.387546000	1.505391000	0.000000000	6	10.778380350	-1.314012463	0.000000000
6	-8.392254000	2.928737000	0.000000000	6	8.365623790	1.681673501	0.000000000
6	-6.883131000	2.933691000	0.000000000	6	6.849748267	1.659216124	0.000000000
6	-6.877950000	1.521744000	0.000000000	6	5.701784401	0.846725758	0.000000000
6	-5.714313000	0.732224000	0.000000000	6	5.728997969	-0.614775243	0.000000000
6	-4.573341000	2.950290000	0.000000000	6	6.908152258	-1.377977525	0.000000000
6	-5.727664000	3.723717000	0.000000000	6	8.419057655	-1.330020282	0.000000000
1	-9.569338000	4.750750000	0.000000000	6	8.440636836	-2.755962693	0.000000000
1	-11.702798000	3.423325000	0.000000000	6	10.781989106	-2.690135652	0.000000000
1	-11.702425000	1.011073000	0.000000000	6	9.598815981	-3.478093341	0.000000000
6	-9.537888000	-0.739808000	0.000000000	6	6.944330045	-2.788336529	0.000000000
6	-8.387546000	-1.505391000	0.000000000	6	5.802489482	-3.591123127	0.000000000
6	-6.877950000	-1.521744000	0.000000000	6	4.627602969	-2.854845509	0.000000000
6	-5.714313000	-0.732224000	0.000000000	6	4.599892353	-1.436081864	0.000000000
6	-4.568494000	-1.530223000	0.000000000	6	9.455462566	3.865140058	0.000000000
6	-5.727664000	-3.723717000	0.000000000	6	8.320914822	3.106768962	0.000000000
6	-6.883131000	-2.933691000	0.000000000	6	6.826172935	3.069108622	0.000000000
6	-8.392254000	-2.928737000	0.000000000	35	9.452058423	5.757919527	0.000000000
6	-9.545950000	-3.665282000	0.000000000	9	11.922496487	1.213296267	0.000000000
6	-10.748827000	-2.902901000	0.000000000	1	11.741435545	-0.829254202	0.000000000
6	-10.744256000	-1.519117000	0.000000000	9	11.963290985	-3.327547468	0.000000000
1	-11.702798000	-3.423325000	0.000000000	35	9.695043498	-5.361032799	0.000000000
1	-11.702425000	-1.011073000	0.000000000	35	5.859634133	-5.476867817	0.000000000
1	-5.734963000	4.808805000	0.000000000	6	3.091351651	-1.469394725	0.000000000
1	-9.569338000	-4.750750000	0.000000000	6	3.125723333	-2.883871078	0.000000000
6	-3.062346000	2.949077000	0.000000000	6	1.982757516	-3.677928110	0.000000000
6	-3.061853000	1.533520000	0.000000000	6	0.809742759	-2.931143551	0.000000000

6	-1.907263000	0.733880000	0.000000000	6	0.785239675	-1.515395213	0.000000000
6	-0.754084000	1.531592000	0.000000000	6	1.921484691	-0.694418161	0.000000000
6	-0.754938000	2.948695000	0.000000000	6	1.892505826	0.771394963	0.000000000
6	-1.907254000	3.731559000	0.000000000	6	3.031131526	1.593016182	0.000000000
6	-3.061853000	-1.533520000	0.000000000	6	4.540218793	1.620204611	0.000000000
6	-1.907263000	-0.733880000	0.000000000	6	5.651094233	3.823984364	0.000000000
6	-0.754084000	-1.531592000	0.000000000	6	4.509214023	3.039421917	0.000000000
6	-0.754938000	-2.948695000	0.000000000	6	3.007841568	3.007128714	0.000000000
6	-1.907254000	-3.731559000	0.000000000	35	5.629794029	5.710669273	0.000000000
6	-3.062346000	-2.949077000	0.000000000	6	1.833307478	3.754988989	0.000000000
6	-4.573341000	-2.950290000	0.000000000	6	0.691896900	2.962228539	0.000000000
1	-1.906760000	4.816575000	0.000000000	6	0.724847250	1.546027503	0.000000000
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1	-5.734963000	-4.808805000	0.000000000	6	-0.785239675	1.515395213	0.000000000
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6	0.754938000	2.948695000	0.000000000	6	-0.691896900	-2.962228539	0.000000000
6	1.907254000	3.731559000	0.000000000	6	-1.982757516	3.677928110	0.000000000
6	0.754084000	1.531592000	0.000000000	6	-3.125723333	2.883871078	0.000000000
6	1.907263000	0.733880000	0.000000000	6	-1.921484691	0.694418161	0.000000000
6	3.061853000	1.533520000	0.000000000	6	-3.091351651	1.469394725	0.000000000
6	3.062346000	2.949077000	0.000000000	35	-2.024537090	5.563861053	0.000000000
6	4.573341000	2.950290000	0.000000000	35	1.798229790	5.640961404	0.000000000
6	4.568494000	1.530223000	0.000000000	35	2.024537090	-5.563861053	0.000000000
6	5.714313000	0.732224000	0.000000000	6	-1.833307478	-3.754988989	0.000000000
6	6.883131000	2.933691000	0.000000000	6	-3.007841568	-3.007128714	0.000000000
6	5.727664000	3.723717000	0.000000000	6	-3.031131526	-1.593016182	0.000000000
1	1.906760000	4.816575000	0.000000000	6	-1.892505826	-0.771394963	0.000000000
6	1.907263000	-0.733880000	0.000000000	6	-4.540218793	-1.620204611	0.000000000
6	3.061853000	-1.533520000	0.000000000	6	-4.509214023	-3.039421917	0.000000000
6	4.568494000	-1.530223000	0.000000000	35	-1.798229790	-5.640961404	0.000000000
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6	6.877950000	-1.521744000	0.000000000	6	-4.599892353	1.436081864	0.000000000
6	5.727664000	-3.723717000	0.000000000	6	-5.728997969	0.614775243	0.000000000
6	4.573341000	-2.950290000	0.000000000	6	-5.701784401	-0.846725758	0.000000000
6	3.062346000	-2.949077000	0.000000000	6	-5.651094233	-3.823984364	0.000000000
6	1.907254000	-3.731559000	0.000000000	6	-6.826172935	-3.069108622	0.000000000
6	0.754938000	-2.948695000	0.000000000	6	-6.849748267	-1.659216124	0.000000000
6	0.754084000	-1.531592000	0.000000000	6	-6.908152258	1.377977525	0.000000000
1	5.734963000	4.808805000	0.000000000	6	-6.944330045	2.788336529	0.000000000
1	1.906760000	-4.816575000	0.000000000	6	-5.802489482	3.591123127	0.000000000
6	6.883131000	-2.933691000	0.000000000	35	-5.859634133	5.476867817	0.000000000
1	5.734963000	-4.808805000	0.000000000	6	-8.440636836	2.755962693	0.000000000
6	8.392254000	2.928737000	0.000000000	6	-8.419057655	1.330020282	0.000000000
6	9.545950000	3.665282000	0.000000000	6	-9.561294002	0.549161504	0.000000000
6	8.387546000	1.505391000	0.000000000	6	-9.529782700	-0.931593782	0.000000000
6	9.537888000	0.739808000	0.000000000	6	-8.365623790	-1.681673501	0.000000000
6	10.744256000	1.519117000	0.000000000	6	-8.320914822	-3.106768962	0.000000000
6	10.748827000	2.902901000	0.000000000	6	-9.455462566	-3.865140058	0.000000000
1	9.569338000	4.750750000	0.000000000	6	-10.682603409	-3.156847618	0.000000000
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6	10.744256000	-1.519117000	0.000000000	9	-11.922496487	-1.213296267	0.000000000
6	10.748827000	-2.902901000	0.000000000	1	-11.629905884	-3.682337938	0.000000000
6	9.545950000	-3.665282000	0.000000000	35	-9.452058423	-5.757919527	0.000000000
6	8.392254000	-2.928737000	0.000000000	35	-5.629794029	-5.710669273	0.000000000
6	8.387546000	-1.505391000	0.000000000	6	-9.598815981	3.478093341	0.000000000
1	9.569338000	-4.750750000	0.000000000	6	-10.781989106	2.690135652	0.000000000
1	11.702425000	1.011073000	0.000000000	6	-10.778380350	1.314012463	0.000000000
1	11.702798000	3.423325000	0.000000000	1	-11.741435545	0.829254202	0.000000000
1	11.702425000	-1.011073000	0.000000000	9	-11.963290985	3.327547468	0.000000000
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6	-13.362772000	3.665285000	0.000000000	6	13.140132448	3.811529316	0.000000000
6	-14.561202000	1.518966000	0.000000000	6	11.992472470	3.053566302	0.000000000
6	-13.354503000	0.739664000	0.000000000	6	12.028606560	1.627049279	0.000000000
6	-12.204388000	1.505387000	0.000000000	6	13.202900260	0.873016310	0.000000000
6	-12.209186000	2.928852000	0.000000000	6	14.357112290	1.713338387	0.000000000
6	-10.699933000	2.933470000	0.000000000	1	15.304437857	3.616476399	0.000000000
6	-10.694784000	1.521976000	0.000000000	35	13.145632324	5.701517029	0.000000000
6	-9.530729000	0.732034000	0.000000000	9	15.587772679	1.156163966	0.000000000
6	-8.390175000	2.950536000	0.000000000	6	13.239345833	-0.607174825	0.000000000
6	-9.544201000	3.723936000	0.000000000	6	14.455596322	-1.371577493	0.000000000

1	-13.386508000	4.750726000	0.000000000	6	14.458148184	-2.748722120	0.000000000
1	-15.519818000	3.423051000	0.000000000	6	13.275357866	-3.536075539	0.000000000
1	-15.519393000	1.010816000	0.000000000	6	12.116853246	-2.812578391	0.000000000
6	-13.354503000	-0.739664000	0.000000000	6	12.097409782	-1.387334276	0.000000000
6	-12.204388000	-1.505387000	0.000000000	6	10.589180652	-1.429606214	0.000000000
6	-10.694784000	-1.521976000	0.000000000	6	10.621311208	-2.842930245	0.000000000
6	-9.530729000	-0.732034000	0.000000000	9	15.639293597	-3.385204069	0.000000000
6	-8.385273000	-1.530167000	0.000000000	1	15.419491542	-0.888569014	0.000000000
6	-9.544201000	-3.723936000	0.000000000	35	13.369794055	-5.418283546	0.000000000
6	-10.699933000	-2.933470000	0.000000000	6	10.514997512	3.049636830	0.000000000
6	-12.209186000	-2.928852000	0.000000000	6	10.528035631	1.597060089	0.000000000
6	-13.362772000	-3.665285000	0.000000000	6	9.397249159	0.802327638	0.000000000
6	-14.565867000	-2.902542000	0.000000000	6	9.417767396	-0.660572539	0.000000000
6	-14.561202000	-1.518966000	0.000000000	6	9.374581892	3.808898587	0.000000000
1	-15.519818000	-3.423051000	0.000000000	6	8.194864502	3.032481792	0.000000000
1	-15.519393000	-1.010816000	0.000000000	6	8.209920368	1.586707305	0.000000000
1	-9.551625000	4.808991000	0.000000000	6	6.759465492	3.059823749	0.000000000
1	-13.386508000	-4.750726000	0.000000000	6	6.764046538	1.545723609	0.000000000
6	-6.879082000	2.948772000	0.000000000	35	9.367368057	5.694828180	0.000000000
6	-6.878691000	1.533884000	0.000000000	6	8.285452751	-1.478491985	0.000000000
6	-5.723584000	0.733518000	0.000000000	6	8.305797552	-2.901419529	0.000000000
6	-4.570821000	1.531199000	0.000000000	6	9.479833968	-3.642696633	0.000000000
6	-4.571770000	2.948725000	0.000000000	6	6.788118361	-1.499451751	0.000000000
6	-5.723406000	3.731658000	0.000000000	6	6.812168296	-2.926960682	0.000000000
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1	5.724409000	4.815603000	0.000000000	6	-8.399653756	1.486897759	0.000000000
1	1.908265000	-4.815529000	0.000000000	6	-9.564316022	3.667183327	0.000000000
6	8.388368000	2.948800000	0.000000000	6	-10.719937091	2.889976014	0.000000000
6	8.387355000	1.531137000	0.000000000	6	-10.706605730	1.476090136	0.000000000
6	9.540055000	0.733443000	0.000000000	6	-9.547449214	0.683367674	0.000000000
6	10.695307000	1.533931000	0.000000000	6	-12.222357782	2.883899623	0.000000000
6	10.695687000	2.948708000	0.000000000	6	-12.215412911	1.464499552	0.000000000
6	9.539893000	3.731688000	0.000000000	6	-13.386050699	3.636964028	0.000000000
6	8.387355000	-1.531137000	0.000000000	6	-14.540047495	2.850838018	0.000000000
6	9.540055000	-0.733443000	0.000000000	6	-14.524512812	1.440559615	0.000000000
6	10.695307000	-1.533931000	0.000000000	6	-13.356151899	0.659933047	0.000000000
6	10.695687000	-2.948708000	0.000000000	6	-16.036778819	2.840849079	0.000000000
6	9.539893000	-3.731688000	0.000000000	6	-16.035834733	1.414449795	0.000000000
6	8.388368000	-2.948800000	0.000000000	6	-17.184292209	3.579391192	0.000000000
6	6.878366000	-2.947302000	0.000000000	6	-18.379108272	2.808444704	0.000000000

1	9.539363000	4.816649000	0.000000000	6	-18.395340414	1.432760029	0.000000000
1	9.539363000	-4.816649000	0.000000000	6	-17.189128597	0.650321726	0.000000000
1	5.724409000	-4.815603000	0.000000000	9	-19.551123275	3.462966627	0.000000000
6	18.377808000	1.519075000	0.000000000	1	-19.365034414	0.961469017	0.000000000
6	12.206744000	2.950560000	0.000000000	35	-17.253464380	5.463800816	0.000000000
6	13.360694000	3.723952000	0.000000000	35	-13.415768715	5.523567283	0.000000000
6	12.201819000	1.530110000	0.000000000	35	-9.579037893	5.553797350	0.000000000
6	13.347279000	0.731989000	0.000000000	35	-5.757091973	5.573364602	0.000000000
6	14.511404000	1.522049000	0.000000000	6	-6.873610961	-1.566278487	0.000000000
6	14.516523000	2.933480000	0.000000000	6	-6.870318915	-2.980515432	0.000000000
6	16.025744000	2.928950000	0.000000000	6	-5.707476923	-3.745359407	0.000000000
6	16.020920000	1.505373000	0.000000000	35	-5.698935818	-5.632034484	0.000000000
6	17.171026000	0.739659000	0.000000000	6	-8.372219278	-2.990703179	0.000000000
6	18.382457000	2.902556000	0.000000000	6	-8.384201957	-1.573667265	0.000000000
6	17.179268000	3.665342000	0.000000000	6	-9.540000186	-0.782148403	0.000000000
1	13.368078000	4.809013000	0.000000000	6	-10.691199901	-1.587373165	0.000000000
6	13.347279000	-0.731989000	0.000000000	6	-12.200479973	-1.592044108	0.000000000
6	14.511404000	-1.522049000	0.000000000	6	-12.190222907	-3.011859008	0.000000000
6	16.020920000	-1.505373000	0.000000000	6	-10.688525041	-3.000997301	0.000000000
6	17.171026000	-0.739659000	0.000000000	6	-9.524602657	-3.766299680	0.000000000
6	18.377808000	-1.519075000	0.000000000	35	-9.518983136	-5.652869906	0.000000000
6	17.179268000	-3.665342000	0.000000000	6	-13.350365458	-0.801617598	0.000000000
6	16.025744000	-2.928950000	0.000000000	6	-14.510465832	-1.597482391	0.000000000
6	14.516523000	-2.933480000	0.000000000	6	-14.507390871	-3.007268401	0.000000000
6	13.360694000	-3.723952000	0.000000000	6	-13.343291194	-3.779375952	0.000000000
6	12.206744000	-2.950560000	0.000000000	35	-13.350683511	-5.666396662	0.000000000
6	12.201819000	-1.530110000	0.000000000	6	-16.026340598	-1.597601472	0.000000000
1	17.203123000	4.750788000	0.000000000	6	-16.002500091	-3.023444012	0.000000000
1	13.368078000	-4.809013000	0.000000000	6	-17.179286733	-0.830583149	0.000000000
6	18.382457000	-2.902556000	0.000000000	6	-18.356366953	-1.661424467	0.000000000
1	17.203123000	-4.750788000	0.000000000	6	-18.364822607	-3.038532834	0.000000000
1	19.335986000	1.010910000	0.000000000	6	-17.147944817	-3.764824070	0.000000000
1	19.336372000	3.423158000	0.000000000	35	-17.173162050	-5.657692295	0.000000000
1	19.335986000	-1.010910000	0.000000000	1	-19.319621764	-3.550250148	0.000000000
1	19.336372000	-3.423158000	0.000000000	9	-19.576158380	-1.076943247	0.000000000

Table 3. The Cartesian coordinates of the optimized molecular structures of 3_m Bp-sheets (m=1-3) at the B3LYP/6-31G(d,p) level of theory

3_1 Bp_H			3_1 Bp_F_Br				
6	-2.957375000	0.000000000	0.000000000	6	3.782701620	1.016269595	0.000000000
6	-1.495698000	0.000000000	0.000000000	6	-6.032941799	-3.585017927	0.000000000
6	-0.705612000	1.154511000	0.000000000	6	-5.311743820	-4.808178704	0.000000000
6	0.705612000	1.154511000	0.000000000	6	-3.935970691	-4.879360201	0.000000000
6	-3.745164000	1.154901000	0.000000000	6	-3.105736974	-3.707869368	0.000000000
6	-5.941085000	0.000000000	0.000000000	6	-3.823305868	-2.525014284	0.000000000
6	-5.160876000	1.156990000	0.000000000	6	-5.246913648	-2.467698641	0.000000000
6	1.495698000	0.000000000	0.000000000	6	-5.197882199	-0.972717467	0.000000000
6	-1.480454000	3.811360000	0.000000000	6	-3.782701620	-1.016269595	0.000000000
6	-0.710063000	2.664160000	0.000000000	6	-1.626534432	-3.758995613	0.000000000
6	1.480454000	3.811360000	0.000000000	6	-0.799032011	-2.644897602	0.000000000
6	0.691809000	5.007522000	0.000000000	6	-2.953985632	0.108952117	0.000000000
6	-0.691809000	5.007522000	0.000000000	6	-1.493849809	0.051994109	0.000000000
6	-2.960402000	3.812775000	0.000000000	6	-0.745951226	-1.132178813	0.000000000
6	-3.736327000	5.019094000	0.000000000	6	0.622449816	-2.688042572	0.000000000
6	-3.729414000	2.663094000	0.000000000	6	0.663976673	-1.179471851	0.000000000
6	-5.121491000	5.025271000	0.000000000	6	1.354466235	-3.865672490	0.000000000
6	-5.152183000	2.668131000	0.000000000	6	2.833220377	-3.920210557	0.000000000
6	-5.885851000	3.825264000	0.000000000	6	3.648651344	-2.801633943	0.000000000
6	0.710063000	2.664160000	0.000000000	6	3.705446574	-1.289535634	0.000000000
1	-7.026291000	0.000000000	0.000000000	6	2.953985632	-0.108952117	0.000000000
1	1.189360000	5.971464000	0.000000000	6	1.493849809	-0.051994109	0.000000000
1	-1.189360000	5.971464000	0.000000000	6	-0.847671767	-4.960015657	0.000000000
1	-3.226692000	5.976627000	0.000000000	6	0.527199951	-5.029509894	0.000000000
1	-5.640075000	5.980206000	0.000000000	6	3.612457604	-5.130648038	0.000000000
1	-6.971204000	3.851758000	0.000000000	6	4.989395094	-5.195907888	0.000000000
6	-1.480454000	-3.811360000	0.000000000	6	5.766021445	-4.012251093	0.000000000
6	-0.691809000	-5.007522000	0.000000000	6	5.072890530	-2.835351171	0.000000000
6	1.480454000	-3.811360000	0.000000000	6	5.119206139	-1.341269345	0.000000000
6	0.710063000	-2.664160000	0.000000000	6	5.928110381	-0.209542579	0.000000000
6	-0.710063000	-2.664160000	0.000000000	6	5.197882199	0.972717467	0.000000000
6	-2.960402000	-3.812775000	0.000000000	6	0.745951226	1.132178813	0.000000000

6	-0.705612000	-1.154511000	0.000000000	6	-0.663976673	1.179471851	0.000000000
6	-3.729414000	-2.663094000	0.000000000	6	-3.705446574	1.289535634	0.000000000
6	-3.745164000	-1.154901000	0.000000000	6	-5.119206139	1.341269345	0.000000000
6	0.705612000	-1.154511000	0.000000000	6	-5.928110381	0.209542579	0.000000000
6	-3.736327000	-5.019094000	0.000000000	6	-5.072890530	2.835351171	0.000000000
6	-5.160876000	-1.156990000	0.000000000	6	-3.648651344	2.801633943	0.000000000
6	-5.152183000	-2.668131000	0.000000000	6	-2.833220377	3.920210557	0.000000000
6	-5.121491000	-5.025271000	0.000000000	6	-1.354466235	3.865672490	0.000000000
6	-5.885851000	-3.825264000	0.000000000	6	-0.622449816	2.688042572	0.000000000
6	0.691809000	-5.007522000	0.000000000	6	0.799032011	2.644897602	0.000000000
1	-6.971204000	-3.851758000	0.000000000	6	1.626534432	3.758995613	0.000000000
6	5.941085000	0.000000000	0.000000000	6	3.105736974	3.707869368	0.000000000
6	5.160876000	1.156990000	0.000000000	6	3.823305868	2.525014284	0.000000000
6	2.957375000	0.000000000	0.000000000	6	5.246913648	2.467698641	0.000000000
6	3.745164000	1.154901000	0.000000000	6	6.032941799	3.585017927	0.000000000
6	5.885851000	3.825264000	0.000000000	6	5.311743820	4.808178704	0.000000000
6	5.121491000	5.025271000	0.000000000	6	3.935970691	4.879360201	0.000000000
6	5.152183000	2.668131000	0.000000000	6	0.847671767	4.960015657	0.000000000
6	3.736327000	5.019094000	0.000000000	6	-0.527199951	5.029509894	0.000000000
6	3.729414000	2.663094000	0.000000000	6	-3.612457604	5.130648038	0.000000000
6	2.960402000	3.812775000	0.000000000	6	-4.989395094	5.195907888	0.000000000
1	5.640075000	5.980206000	0.000000000	6	-5.766021445	4.012251093	0.000000000
1	3.226692000	5.976627000	0.000000000	35	-7.813637131	0.276584975	0.000000000
6	5.885851000	-3.825264000	0.000000000	35	-7.655841593	4.114532466	0.000000000
6	5.152183000	-2.668131000	0.000000000	1	-5.459810674	6.171618809	0.000000000
6	5.160876000	-1.156990000	0.000000000	9	-2.979252625	6.326186026	0.000000000
6	3.745164000	-1.154901000	0.000000000	1	-0.953388448	6.019431466	0.000000000
6	3.729414000	-2.663094000	0.000000000	9	1.479829684	6.158971596	0.000000000
6	3.736327000	-5.019094000	0.000000000	1	3.503271519	5.866705331	0.000000000
6	2.960402000	-3.812775000	0.000000000	9	6.011020044	5.953862678	0.000000000
6	5.121491000	-5.025271000	0.000000000	35	7.917941135	3.571512787	0.000000000
1	-1.189360000	-5.971464000	0.000000000	35	7.813637131	-0.276584975	0.000000000
1	-3.226692000	-5.976627000	0.000000000	35	7.655841593	-4.114532466	0.000000000
1	-5.640075000	-5.980206000	0.000000000	1	5.459810674	-6.171618809	0.000000000
1	1.189360000	-5.971464000	0.000000000	9	2.979252625	-6.326186026	0.000000000
1	7.026291000	0.000000000	0.000000000	1	0.953388448	-6.019431466	0.000000000
1	6.971204000	3.851758000	0.000000000	9	-1.479829684	-6.158971596	0.000000000
1	6.971204000	-3.851758000	0.000000000	1	-3.503271519	-5.866705331	0.000000000
1	3.226692000	-5.976627000	0.000000000	9	-6.011020044	-5.953862678	0.000000000
1	5.640075000	-5.980206000	0.000000000	35	-7.917941135	-3.571512787	0.000000000

3_2 Bp_H				3_2 Bp_F_Br			
6	-1.915693000	5.957199000	0.000000000	6	-6.265574118	-5.307095606	0.000000000
6	-3.070185000	5.166444000	0.000000000	6	-5.579305919	-6.551351212	0.000000000
6	-1.899671000	2.967438000	0.000000000	6	-4.206985149	-6.662480267	0.000000000
6	-3.062266000	3.753891000	0.000000000	6	-3.342894314	-5.514113619	0.000000000
6	-5.738192000	5.885307000	0.000000000	6	-4.026577515	-4.311647178	0.000000000
6	-6.937549000	5.116965000	0.000000000	6	-5.448527383	-4.213125411	0.000000000
6	-4.580525000	5.154814000	0.000000000	6	-5.355417161	-2.719639468	0.000000000
6	-6.927344000	3.733227000	0.000000000	6	-3.945139886	-2.804384243	0.000000000
6	-4.570483000	3.731190000	0.000000000	6	-6.054753620	-1.514204428	0.000000000
6	-5.717235000	2.959479000	0.000000000	6	-5.217508432	-0.406833639	0.000000000
1	-7.893497000	5.633582000	0.000000000	6	-3.802638619	-0.502210743	0.000000000
1	-7.882977000	3.220239000	0.000000000	6	-3.081501182	-1.700374347	0.000000000
6	-1.899671000	-2.967438000	0.000000000	6	-5.119882725	1.091260982	0.000000000
6	-1.900389000	-1.503027000	0.000000000	6	-3.703380544	1.002552490	0.000000000
6	-3.057561000	-0.704844000	0.000000000	6	-5.805939571	2.296179686	0.000000000
6	-3.057561000	0.704844000	0.000000000	6	-4.954847233	3.401655316	0.000000000
6	-3.062266000	-3.753891000	0.000000000	6	-3.546776769	3.304268811	0.000000000
6	-1.915693000	-5.957199000	0.000000000	6	-2.832682559	2.095379311	0.000000000
6	-3.070185000	-5.166444000	0.000000000	6	-4.862207608	4.894074624	0.000000000
6	-1.900389000	1.503027000	0.000000000	6	-3.439104847	4.813848724	0.000000000
6	-5.713409000	-1.480344000	0.000000000	6	-5.517513292	6.091478503	0.000000000
6	-4.567082000	-0.710520000	0.000000000	6	-4.703294580	7.250821237	0.000000000
6	-5.713409000	1.480344000	0.000000000	6	-3.330018462	7.141183608	0.000000000
6	-6.911438000	0.690863000	0.000000000	6	-2.588593979	5.905687219	0.000000000
6	-6.911438000	-0.690863000	0.000000000	1	-5.143025989	8.240774674	0.000000000
6	-5.717235000	-2.959479000	0.000000000	9	-2.658678500	8.315403765	0.000000000
6	-6.927344000	-3.733227000	0.000000000	35	-7.403124568	6.254346094	0.000000000
6	-4.570483000	-3.731190000	0.000000000	35	-7.687879410	2.431990648	0.000000000
6	-6.937549000	-5.116965000	0.000000000	35	-7.938020677	-1.403615859	0.000000000
6	-4.580525000	-5.154814000	0.000000000	35	-8.149762997	-5.242878634	0.000000000
6	-5.738192000	-5.885307000	0.000000000	9	-6.312530570	-7.675741690	0.000000000
6	-4.567082000	0.710520000	0.000000000	1	-3.802776658	-7.661900215	0.000000000

1	-1.924716000	-7.042266000	0.000000000	6	-1.622351756	-1.802275758	0.000000000
1	-7.874786000	1.189364000	0.000000000	6	-0.754946917	-0.706439813	0.000000000
1	-7.874786000	-1.189364000	0.000000000	6	-0.656755906	0.798359902	0.000000000
1	-7.882977000	-3.220239000	0.000000000	6	0.754946917	0.706439813	0.000000000
1	-7.893497000	-5.633582000	0.000000000	6	0.656755906	-0.798359902	0.000000000
1	-5.767862000	-6.970494000	0.000000000	6	1.372987099	-1.998562174	0.000000000
6	1.915693000	5.957199000	0.000000000	6	0.502226111	-3.101503843	0.000000000
6	0.757111000	5.186106000	0.000000000	6	-0.904564076	-3.011009787	0.000000000
6	-0.757111000	5.186106000	0.000000000	6	-1.004591979	-4.521277331	0.000000000
6	-0.752590000	3.766779000	0.000000000	6	0.415607231	-4.608086849	0.000000000
6	0.752590000	3.766779000	0.000000000	6	1.112132958	-5.806172074	0.000000000
6	3.062266000	3.753891000	0.000000000	6	0.249029725	-6.945438734	0.000000000
6	1.899671000	2.967438000	0.000000000	6	-1.122174644	-6.833861956	0.000000000
6	1.900389000	-1.503027000	0.000000000	6	-1.865613099	-5.608911534	0.000000000
6	3.057561000	-0.704844000	0.000000000	9	-1.790400191	-8.012783589	0.000000000
6	1.900389000	1.503027000	0.000000000	1	0.644639842	-7.948066039	0.000000000
6	0.752792000	0.708011000	0.000000000	6	-1.372987099	1.998562174	0.000000000
6	0.752792000	-0.708011000	0.000000000	6	-0.502226111	3.101503843	0.000000000
6	1.899671000	-2.967438000	0.000000000	6	0.904564076	3.011009787	0.000000000
6	-0.752792000	-0.708011000	0.000000000	6	1.622351756	1.802275758	0.000000000
6	0.752590000	-3.766779000	0.000000000	6	-0.415607231	4.608086849	0.000000000
6	-0.752590000	-3.766779000	0.000000000	6	-1.112132958	5.806172074	0.000000000
6	-0.752792000	0.708011000	0.000000000	6	1.004591979	4.521277331	0.000000000
6	3.062266000	-3.753891000	0.000000000	6	1.865613099	5.608911534	0.000000000
6	-0.757111000	-5.186106000	0.000000000	6	1.122174644	6.833861956	0.000000000
6	0.757111000	-5.186106000	0.000000000	6	-0.249029725	6.945438734	0.000000000
6	3.070185000	-5.166444000	0.000000000	1	-0.644639842	7.948066039	0.000000000
6	1.915693000	-5.957199000	0.000000000	9	1.790400191	8.012783589	0.000000000
6	3.057561000	0.704844000	0.000000000	6	3.342894314	5.514113619	0.000000000
1	1.924716000	-7.042266000	0.000000000	6	3.081501182	1.700374347	0.000000000
6	3.070185000	5.166444000	0.000000000	6	3.945139886	2.804384243	0.000000000
6	5.738192000	5.885307000	0.000000000	6	4.026577515	4.311647178	0.000000000
6	4.580525000	5.154814000	0.000000000	6	4.206985149	6.662480267	0.000000000
6	6.937549000	5.116965000	0.000000000	6	5.579305919	6.551351212	0.000000000
6	4.570483000	3.731190000	0.000000000	6	6.265574118	5.307095606	0.000000000
6	6.927344000	3.733227000	0.000000000	6	5.448527383	4.213125411	0.000000000
6	5.717235000	2.959479000	0.000000000	6	5.355417161	2.719639468	0.000000000
1	7.882977000	3.220239000	0.000000000	6	2.588593979	-5.905687219	0.000000000
1	7.893497000	5.633582000	0.000000000	6	3.439104847	-4.813848724	0.000000000
6	5.713409000	-1.480344000	0.000000000	6	3.546776769	-3.304268811	0.000000000
6	6.911438000	-0.690863000	0.000000000	6	2.832682559	-2.095379311	0.000000000
6	5.713409000	1.480344000	0.000000000	6	3.703380544	-1.002552490	0.000000000
6	4.567082000	0.710520000	0.000000000	6	3.802638619	0.502210743	0.000000000
6	4.567082000	-0.710520000	0.000000000	6	5.217508432	0.406833639	0.000000000
6	5.717235000	-2.959479000	0.000000000	6	6.054753620	1.514204428	0.000000000
6	4.570483000	-3.731190000	0.000000000	6	5.119882725	-1.091260982	0.000000000
6	6.927344000	-3.733227000	0.000000000	6	5.805939571	-2.296179686	0.000000000
6	4.580525000	-5.154814000	0.000000000	6	4.954847233	-3.401655316	0.000000000
6	6.937549000	-5.116965000	0.000000000	6	4.862207608	-4.894074624	0.000000000
6	5.738192000	-5.885307000	0.000000000	6	5.517513292	-6.091478503	0.000000000
1	7.893497000	-5.633582000	0.000000000	6	4.703294580	-7.250821237	0.000000000
1	7.874786000	-1.189364000	0.000000000	6	3.330018462	-7.141183608	0.000000000
1	7.882977000	-3.220239000	0.000000000	9	2.658678500	-8.315403765	0.000000000
6	6.911438000	0.690863000	0.000000000	1	5.143025989	-8.240774674	0.000000000
1	7.874786000	1.189364000	0.000000000	35	7.403124568	-6.254346094	0.000000000
1	5.767862000	-6.970494000	0.000000000	35	7.687879410	-2.431990648	0.000000000
1	-1.924716000	7.042266000	0.000000000	35	7.938020677	1.403615859	0.000000000
1	-5.767862000	6.970494000	0.000000000	35	8.149762997	5.242878634	0.000000000
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1	5.767862000	6.970494000	0.000000000	1	3.802776658	7.661900215	0.000000000
3_3 Bp_H				3_3 Bp_F_Br			
6	-9.525605000	1.479762000	0.000000000	6	-10.496307685	-5.650378418	0.000000000
6	-8.378337000	0.710557000	0.000000000	6	-10.539060258	-4.273944798	0.000000000
6	-9.525605000	-1.479762000	0.000000000	6	-9.392634549	-3.399901994	0.000000000
6	-10.723596000	-0.690569000	0.000000000	6	-8.213743125	-4.124307186	0.000000000
6	-10.723596000	0.690569000	0.000000000	6	-8.136446301	-5.547888315	0.000000000
6	-9.531704000	2.957376000	0.000000000	6	-9.253467915	-6.331538540	0.000000000
6	-10.742369000	3.730663000	0.000000000	35	-9.207766399	-8.223928731	0.000000000
6	-8.385367000	3.729332000	0.000000000	1	-11.431568360	-6.196941935	0.000000000
6	-10.753410000	5.114310000	0.000000000	9	-11.780287354	-3.736519001	0.000000000
6	-8.396674000	5.152696000	0.000000000	6	-9.456603670	-1.922388020	0.000000000
6	-9.554356000	5.883093000	0.000000000	6	-8.343274083	-1.097350646	0.000000000
6	-8.378337000	-0.710557000	0.000000000	6	-8.414713595	0.324169012	0.000000000

1	-9.583567000	6.968336000	0.000000000	6	-9.591429747	1.058705810	0.000000000
6	-5.709392000	1.503025000	0.000000000	6	-10.726563986	0.183212883	0.000000000
6	-4.562391000	0.708472000	0.000000000	6	-10.685272257	-1.190984104	0.000000000
6	-5.709392000	-1.503025000	0.000000000	1	-11.637807211	-1.695266861	0.000000000
6	-6.867990000	-0.704206000	0.000000000	9	-11.972449108	0.716328780	0.000000000
6	-6.867990000	0.704206000	0.000000000	6	-9.663007660	2.536501459	0.000000000
6	-5.712139000	2.965805000	0.000000000	6	-8.544731625	3.349866983	0.000000000
6	-6.877093000	3.752302000	0.000000000	6	-8.605631888	4.774356822	0.000000000
6	-4.568046000	3.766763000	0.000000000	6	-9.783376745	5.464201657	0.000000000
6	-6.886849000	5.164138000	0.000000000	6	-10.943844983	4.643093977	0.000000000
6	-4.576484000	5.186738000	0.000000000	6	-10.901408393	3.267675497	0.000000000
6	-5.733202000	5.957137000	0.000000000	1	-11.849760023	2.755206972	0.000000000
6	-4.562391000	-0.708472000	0.000000000	9	-12.142817377	5.246938779	0.000000000
1	-5.743133000	7.042112000	0.000000000	35	-9.930950544	7.344101202	0.000000000
6	-9.554356000	-5.883093000	0.000000000	6	-7.111208285	4.846695508	0.000000000
6	-10.753410000	-5.114310000	0.000000000	6	-7.037924035	3.437110149	0.000000000
6	-10.742369000	-3.730663000	0.000000000	6	-5.991217076	5.678109609	0.000000000
6	-8.385367000	-3.729332000	0.000000000	6	-4.798434374	4.970973948	0.000000000
6	-9.531704000	-2.957376000	0.000000000	6	-4.734057758	3.553270844	0.000000000
6	-8.396674000	-5.152696000	0.000000000	6	-5.842146331	2.701720822	0.000000000
6	-5.733202000	-5.957137000	0.000000000	6	-3.227289968	3.626960691	0.000000000
6	-6.886849000	-5.164138000	0.000000000	6	-3.298419077	5.040245320	0.000000000
6	-4.576484000	-5.186738000	0.000000000	6	-2.038182769	2.882759800	0.000000000
6	-6.877093000	-3.752302000	0.000000000	6	-0.923723062	3.733436660	0.000000000
6	-4.568046000	-3.766763000	0.000000000	6	-0.984482067	5.147647708	0.000000000
6	-5.712139000	-2.965805000	0.000000000	6	-2.176730018	5.863686400	0.000000000
6	1.905668000	2.975842000	0.000000000	35	-2.265579400	7.748420267	0.000000000
6	1.903791000	1.509680000	0.000000000	35	-6.095596674	7.562121420	0.000000000
6	0.753968000	0.707732000	0.000000000	6	0.584124525	3.801815375	0.000000000
6	0.753968000	-0.707732000	0.000000000	6	0.516114207	5.216772139	0.000000000
6	0.753612000	3.775189000	0.000000000	6	1.769926478	3.055504399	0.000000000
6	1.909990000	5.973116000	0.000000000	6	2.888206941	3.904351199	0.000000000
6	0.755678000	5.192247000	0.000000000	6	2.830299866	5.317077997	0.000000000
6	1.903791000	-1.509680000	0.000000000	6	1.638001323	6.036578851	0.000000000
6	-1.903791000	1.509680000	0.000000000	35	1.557399393	7.921563803	0.000000000
6	-0.753968000	0.707732000	0.000000000	6	4.329849672	5.385205252	0.000000000
6	-1.903791000	-1.509680000	0.000000000	6	4.396068055	3.966593830	0.000000000
6	-3.055356000	-0.706714000	0.000000000	6	5.576981606	3.220814075	0.000000000
6	-3.055356000	0.706714000	0.000000000	6	6.701581727	4.064778569	0.000000000
6	-1.905668000	2.975842000	0.000000000	6	6.643402741	5.473858496	0.000000000
6	-3.061843000	3.773427000	0.000000000	6	5.450659731	6.199173194	0.000000000
6	-0.753612000	3.775189000	0.000000000	35	5.382863886	8.085015485	0.000000000
6	-3.064556000	5.188925000	0.000000000	6	8.136446301	5.547888315	0.000000000
6	-0.755678000	5.192247000	0.000000000	6	8.213743125	4.124307186	0.000000000
6	-1.909990000	5.973116000	0.000000000	6	9.392634549	3.399901994	0.000000000
6	-0.753968000	-0.707732000	0.000000000	6	10.539060258	4.273944798	0.000000000
1	1.911154000	7.058058000	0.000000000	6	10.496307685	5.650378418	0.000000000
1	-1.911154000	7.058058000	0.000000000	6	9.253467915	6.331538540	0.000000000
6	5.709392000	1.503025000	0.000000000	35	9.207766399	8.223928731	0.000000000
6	6.867990000	0.704206000	0.000000000	1	11.431568360	6.196941935	0.000000000
6	5.709392000	-1.503025000	0.000000000	9	11.780287354	3.736519001	0.000000000
6	4.562391000	-0.708472000	0.000000000	6	9.456603670	1.922388020	0.000000000
6	4.562391000	0.708472000	0.000000000	6	10.685272257	1.190984104	0.000000000
6	5.712139000	2.965805000	0.000000000	6	8.343274083	1.097350646	0.000000000
6	3.055356000	0.706714000	0.000000000	6	8.414713595	-0.324169012	0.000000000
6	4.568046000	3.766763000	0.000000000	6	9.591429747	-1.058705810	0.000000000
6	3.061843000	3.773427000	0.000000000	6	10.726563986	-0.183212883	0.000000000
6	3.055356000	-0.706714000	0.000000000	1	11.637807211	1.695266861	0.000000000
6	6.877093000	3.752302000	0.000000000	9	11.972449108	-0.716328780	0.000000000
6	3.064556000	5.188925000	0.000000000	6	9.663007660	-2.536501459	0.000000000
6	4.576484000	5.186738000	0.000000000	6	10.901408393	-3.267675497	0.000000000
6	6.886849000	5.164138000	0.000000000	6	8.544731625	-3.349866983	0.000000000
6	5.733202000	5.957137000	0.000000000	6	8.605631888	-4.774356822	0.000000000
6	6.867990000	-0.704206000	0.000000000	6	9.783376745	-5.464201657	0.000000000
1	5.743133000	7.042112000	0.000000000	6	10.943844983	-4.643093977	0.000000000
6	9.525605000	1.479762000	0.000000000	9	12.142817377	-5.246938779	0.000000000
6	10.723596000	0.690569000	0.000000000	1	11.849760023	-2.755206972	0.000000000
6	9.525605000	-1.479762000	0.000000000	35	9.930950544	-7.344101202	0.000000000
6	8.378337000	-0.710557000	0.000000000	6	7.111208285	-4.846695508	0.000000000
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6	9.531704000	2.957376000	0.000000000	6	5.842146331	-2.701720822	0.000000000
6	8.385367000	3.729332000	0.000000000	6	5.779508856	-1.240524356	0.000000000
6	10.742369000	3.730663000	0.000000000	6	4.595032639	-0.499795433	0.000000000
6	8.396674000	5.152696000	0.000000000	6	4.530078817	0.914446952	0.000000000

6	10.753410000	5.114310000	0.000000000	6	5.642181729	1.759679679	0.000000000
6	9.554356000	5.883093000	0.000000000	6	6.836482286	1.015657881	0.000000000
1	11.709912000	5.630040000	0.000000000	6	6.902440125	-0.391489668	0.000000000
1	11.686850000	1.189172000	0.000000000	6	4.734057758	-3.553270844	0.000000000
1	11.697836000	3.217453000	0.000000000	6	3.227289968	-3.626960691	0.000000000
6	10.723596000	-0.690569000	0.000000000	6	2.038182769	-2.882759800	0.000000000
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1	9.583567000	6.968336000	0.000000000	6	3.088038111	-0.567161543	0.000000000
6	1.909990000	-5.973116000	0.000000000	6	3.023566211	0.844536721	0.000000000
6	0.755678000	-5.192247000	0.000000000	6	0.785705566	-0.672011487	0.000000000
6	1.905668000	-2.975842000	0.000000000	6	0.721287382	0.740872573	0.000000000
6	0.753612000	-3.775189000	0.000000000	6	1.835225774	1.592241470	0.000000000
6	-1.909990000	-5.973116000	0.000000000	6	3.298419077	-5.040245320	0.000000000
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6	-3.061843000	-3.773427000	0.000000000	35	6.095596674	-7.562121420	0.000000000
6	-0.753612000	-3.775189000	0.000000000	6	2.176730018	-5.863686400	0.000000000
6	-1.905668000	-2.975842000	0.000000000	6	0.984482067	-5.147647708	0.000000000
6	5.733202000	-5.957137000	0.000000000	6	0.923723062	-3.733436660	0.000000000
6	4.576484000	-5.186738000	0.000000000	35	2.265579400	-7.748420267	0.000000000
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