

Supporting Information

Graphyne and Graphdiyne: Theoretical insight into ground and excited state properties

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Ground state optimized coordinates of gr1 and gr2 structures

Gr1:

C 6.0 -2.2240741960 2.1478985302 0.6554256856
C 6.0 -3.6394840079 2.1435941110 0.4928361356
C 6.0 -4.3384427059 0.9082166450 0.3697865375
C 6.0 -3.6177026546 -0.3207563405 0.3684582901
C 6.0 -2.2022924461 -0.3164517628 0.5310442865
C 6.0 -1.5033340786 0.9189255826 0.6540971584
C 6.0 1.0167166942 7.8831470838 1.2819353880
C 6.0 -6.9814271173 7.8547568055 0.4441886167
C 6.0 -10.9185118180 0.8854237179 -0.3305509805
C 6.0 -6.8584962671 -6.0560054909 -0.2580316266
C 6.0 1.1396454246 -6.0276168705 0.5797440584
C 6.0 5.0767387098 0.9417198583 1.3543997386
C 6.0 2.4370383308 7.8993736426 1.4319308159
C 6.0 3.1056745664 9.1295174093 1.5653279517
C 6.0 2.3983990637 10.3288532896 1.5526249263
C 6.0 1.0135866629 10.3289102921 1.4073644344
C 6.0 0.3051834797 9.1215642933 1.2709692646
C 6.0 -6.2918281919 9.0981244768 0.5804484352
C 6.0 -7.0215317630 10.3003889183 0.5657373489
C 6.0 -8.4062604702 10.2905446493 0.4200135689
C 6.0 -9.0922929139 9.0863032332 0.2859660435
C 6.0 -8.4019505556 7.8609615122 0.2953597388
C 6.0 -11.6492600632 2.1125749874 -0.3441398074
C 6.0 -13.0476039615 2.0847037409 -0.4923964958
C 6.0 -13.7250325587 0.8755247279 -0.6257499981

C 6.0 -13.0262824453 -0.3288092545 -0.6141731754
C 6.0 -11.6275328216 -0.3468140132 -0.4682348645
C 6.0 -8.2788200037 -6.0722337826 -0.4080071676
C 6.0 -8.9474529406 -7.3023766030 -0.5414297316
C 6.0 -8.2401714443 -8.5017095084 -0.5287776357
C 6.0 -6.8553568713 -8.5017647292 -0.3835379530
C 6.0 -6.1469576129 -7.2944199778 -0.2471114237
C 6.0 0.4500402797 -7.2709873251 0.4435413700
C 6.0 1.1797335827 -8.4732567886 0.4583480115
C 6.0 2.5644582884 -8.4634147860 0.6041098232
C 6.0 3.2504973758 -7.2591703561 0.7380963798
C 6.0 2.5601652811 -6.0338235905 0.7286069577
C 6.0 5.8074948182 -0.2854275089 1.3679186391
C 6.0 7.2058446041 -0.2575528011 1.5161193063
C 6.0 7.8832705810 0.9516254658 1.6494928729
C 6.0 7.1845120740 2.1559552809 1.6379910773
C 6.0 5.7857571965 2.1739568682 1.4921029103
H 1.0 4.1847811194 9.1262988470 1.6784719333
H 1.0 2.9300528226 11.2699297872 1.6567838543
H 1.0 0.4597234516 11.2618714276 1.3972111255
H 1.0 -6.4841953430 11.2372032609 0.6702928413
H 1.0 -8.9545192748 11.2278047055 0.4107185947
H 1.0 -10.1712783973 9.0754703385 0.1721416491
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H 1.0 -13.5514212866 -1.2726204452 -0.7177716246
H 1.0 -10.0265615075 -7.2991596566 -0.6545547164
H 1.0 -8.7718222979 -9.4427851165 -0.6329593922

H	1.0	-6.3014890083	-9.4347235285	-0.3734236264
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H	1.0	3.1127088707	-9.4006788832	0.6134806452
H	1.0	4.3294802019	-7.2483388860	0.8519461097
H	1.0	7.7476326086	-1.1975940599	1.5246043532
H	1.0	8.9631876389	0.9554363546	1.7630448709
H	1.0	7.7096484953	3.0997657339	1.7416084151
C	6.0	-1.1036677144	9.1367216689	1.1243043624
C	6.0	-2.3190876656	9.1537129438	0.9983133079
C	6.0	-3.6682861905	9.1489110084	0.8572562481
C	6.0	-4.8833305456	9.1232713583	0.7291227476
C	6.0	-4.3517729862	3.3588222587	0.4912446707
C	6.0	-4.9691707605	4.4148836471	0.4780302478
C	6.0	-5.6521029296	5.5820998356	0.4675167575
C	6.0	-6.2696931457	6.6379602682	0.4565774154
C	6.0	0.3265361645	6.6614279369	1.1464175980
C	6.0	-0.2723591027	5.6013185415	1.0286431051
C	6.0	-0.9346200869	4.4292391824	0.9000324837
C	6.0	-1.5333203433	3.3691595770	0.7799937718
C	6.0	5.0879600101	3.4066677348	1.4818199217
C	6.0	4.4893997169	4.4720581811	1.4730722167
C	6.0	3.8045586711	5.6429955784	1.4606062274
C	6.0	3.1694394816	6.6869516871	1.4469164630
C	6.0	3.6747258031	0.9367577457	1.2072706452
C	6.0	2.4581312128	0.9324438003	1.0797650105
C	6.0	1.1133058591	0.9277576997	0.9372090650
C	6.0	-0.1036204491	0.9233289366	0.8119481131
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C 6.0 -4.3084574323 -1.5420177164 0.2438985351
C 6.0 -4.9071599629 -2.6020971768 0.1238699161
C 6.0 -5.5694223157 -3.7741767415 -0.0047317806
C 6.0 -6.1683173838 -4.8342865976 -0.1225031134
C 6.0 5.1315288656 -1.5229450283 1.2329274505
C 6.0 4.5518359931 -2.5924264889 1.1164230287
C 6.0 3.8877312765 -3.7680472019 0.9855132013
C 6.0 3.2710951239 -4.8163488963 0.8662171569
C 6.0 -5.7381568208 0.9038130304 0.2119400241
C 6.0 -8.2999084902 0.8946964088 -0.0558765273
C 6.0 -9.5165020987 0.8903837197 -0.1833915340
C 6.0 -9.1128737810 6.6434898466 0.1576884962
C 6.0 -9.7295046875 5.5951903330 0.0383462233
C 6.0 -10.3936047040 4.4195718300 -0.0926072969
C 6.0 -10.9732944709 3.3500919002 -0.2091411806
C 6.0 -0.9584530099 -7.2961318219 0.2948256379
C 6.0 -2.1734939024 -7.3217683137 0.1666587845
C 6.0 -3.5226890975 -7.3265686452 0.0255699170
C 6.0 -4.7381067627 -7.3095769537 -0.1004431889
C 6.0 -6.9550834369 0.8993827383 0.0866821459
C 6.0 -9.0112247234 -4.8598136036 -0.4229638407
C 6.0 -9.6463445484 -3.8158578492 -0.4366510269
C 6.0 -10.3311842579 -2.6449197675 -0.4491286552
C 6.0 -10.9297416431 -1.5795278687 -0.4578991179

Gr2:

C 6.0 -2.2240741960 2.1478985302 0.6554256856
C 6.0 -3.6394840079 2.1435941110 0.4928361356
C 6.0 -4.3384427059 0.9082166450 0.3697865375
C 6.0 -3.6177026546 -0.3207563405 0.3684582901
C 6.0 -2.2022924461 -0.3164517628 0.5310442865
C 6.0 -1.5033340786 0.9189255826 0.6540971584
C 6.0 1.0167166942 7.8831470838 1.2819353880
C 6.0 -6.9814271173 7.8547568055 0.4441886167
C 6.0 -10.9185118180 0.8854237179 -0.3305509805
C 6.0 -6.8584962671 -6.0560054909 -0.2580316266
C 6.0 1.1396454246 -6.0276168705 0.5797440584
C 6.0 5.0767387098 0.9417198583 1.3543997386
C 6.0 2.4370383308 7.8993736426 1.4319308159
C 6.0 3.1056745664 9.1295174093 1.5653279517
C 6.0 2.3983990637 10.3288532896 1.5526249263
C 6.0 1.0135866629 10.3289102921 1.4073644344
C 6.0 0.3051834797 9.1215642933 1.2709692646
C 6.0 -6.2918281919 9.0981244768 0.5804484352
C 6.0 -7.0215317630 10.3003889183 0.5657373489
C 6.0 -8.4062604702 10.2905446493 0.4200135689
C 6.0 -9.0922929139 9.0863032332 0.2859660435
C 6.0 -8.4019505556 7.8609615122 0.2953597388
C 6.0 -11.6492600632 2.1125749874 -0.3441398074
C 6.0 -13.0476039615 2.0847037409 -0.4923964958
C 6.0 -13.7250325587 0.8755247279 -0.6257499981
C 6.0 -13.0262824453 -0.3288092545 -0.6141731754
C 6.0 -11.6275328216 -0.3468140132 -0.4682348645

C	6.0	-8.2788200037	-6.0722337826	-0.4080071676
C	6.0	-8.9474529406	-7.3023766030	-0.5414297316
C	6.0	-8.2401714443	-8.5017095084	-0.5287776357
C	6.0	-6.8553568713	-8.5017647292	-0.3835379530
C	6.0	-6.1469576129	-7.2944199778	-0.2471114237
C	6.0	0.4500402797	-7.2709873251	0.4435413700
C	6.0	1.1797335827	-8.4732567886	0.4583480115
C	6.0	2.5644582884	-8.4634147860	0.6041098232
C	6.0	3.2504973758	-7.2591703561	0.7380963798
C	6.0	2.5601652811	-6.0338235905	0.7286069577
C	6.0	5.8074948182	-0.2854275089	1.3679186391
C	6.0	7.2058446041	-0.2575528011	1.5161193063
C	6.0	7.8832705810	0.9516254658	1.6494928729
C	6.0	7.1845120740	2.1559552809	1.6379910773
C	6.0	5.7857571965	2.1739568682	1.4921029103
H	1.0	4.1847811194	9.1262988470	1.6784719333
H	1.0	2.9300528226	11.2699297872	1.6567838543
H	1.0	0.4597234516	11.2618714276	1.3972111255
H	1.0	-6.4841953430	11.2372032609	0.6702928413
H	1.0	-8.9545192748	11.2278047055	0.4107185947
H	1.0	-10.1712783973	9.0754703385	0.1721416491
H	1.0	-13.5893854166	3.0247482613	-0.5009391275
H	1.0	-14.8049451959	0.8717165154	-0.7393441196
H	1.0	-13.5514212866	-1.2726204452	-0.7177716246
H	1.0	-10.0265615075	-7.2991596566	-0.6545547164
H	1.0	-8.7718222979	-9.4427851165	-0.6329593922
H	1.0	-6.3014890083	-9.4347235285	-0.3734236264
H	1.0	0.6423923976	-9.4100732261	0.3538359156

H	1.0	3.1127088707	-9.4006788832	0.6134806452
H	1.0	4.3294802019	-7.2483388860	0.8519461097
H	1.0	7.7476326086	-1.1975940599	1.5246043532
H	1.0	8.9631876389	0.9554363546	1.7630448709
H	1.0	7.7096484953	3.0997657339	1.7416084151
C	6.0	-1.1036677144	9.1367216689	1.1243043624
C	6.0	-2.3190876656	9.1537129438	0.9983133079
C	6.0	-3.6682861905	9.1489110084	0.8572562481
C	6.0	-4.8833305456	9.1232713583	0.7291227476
C	6.0	-4.3517729862	3.3588222587	0.4912446707
C	6.0	-4.9691707605	4.4148836471	0.4780302478
C	6.0	-5.6521029296	5.5820998356	0.4675167575
C	6.0	-6.2696931457	6.6379602682	0.4565774154
C	6.0	0.3265361645	6.6614279369	1.1464175980
C	6.0	-0.2723591027	5.6013185415	1.0286431051
C	6.0	-0.9346200869	4.4292391824	0.9000324837
C	6.0	-1.5333203433	3.3691595770	0.7799937718
C	6.0	5.0879600101	3.4066677348	1.4818199217
C	6.0	4.4893997169	4.4720581811	1.4730722167
C	6.0	3.8045586711	5.6429955784	1.4606062274
C	6.0	3.1694394816	6.6869516871	1.4469164630
C	6.0	3.6747258031	0.9367577457	1.2072706452
C	6.0	2.4581312128	0.9324438003	1.0797650105
C	6.0	1.1133058591	0.9277576997	0.9372090650
C	6.0	-0.1036204491	0.9233289366	0.8119481131
C	6.0	0.4279173381	-4.8108174703	0.5673009071
C	6.0	-0.1896698797	-3.7549554324	0.5563473329
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C 6.0 4.5518359931 -2.5924264889 1.1164230287
C 6.0 3.8877312765 -3.7680472019 0.9855132013
C 6.0 3.2710951239 -4.8163488963 0.8662171569
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