

Supporting Information for:

Charge Transfer Induced Magic Cluster Formation of Azaborine Heterocycles on Noble Metal Surfaces

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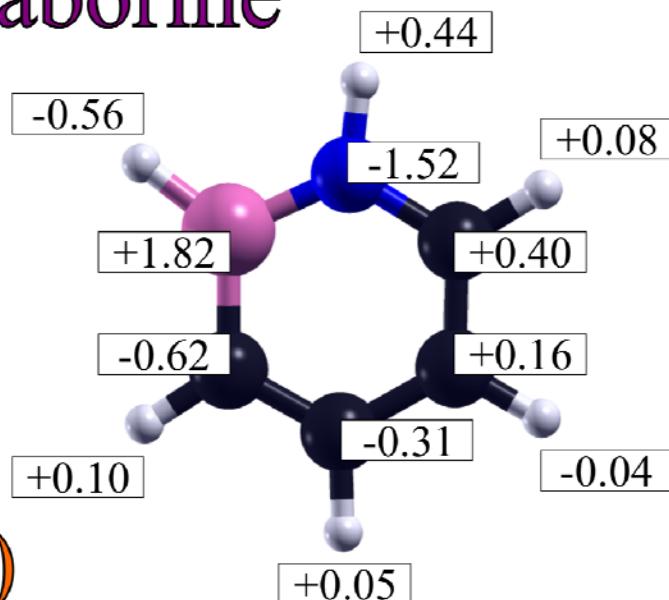
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Section S1. Bader Charges of 1,2-Azaborine:

Free Azaborine

Bader
Charge
Analysis



$\text{Cu}(111)$

$\text{Au}(111)$

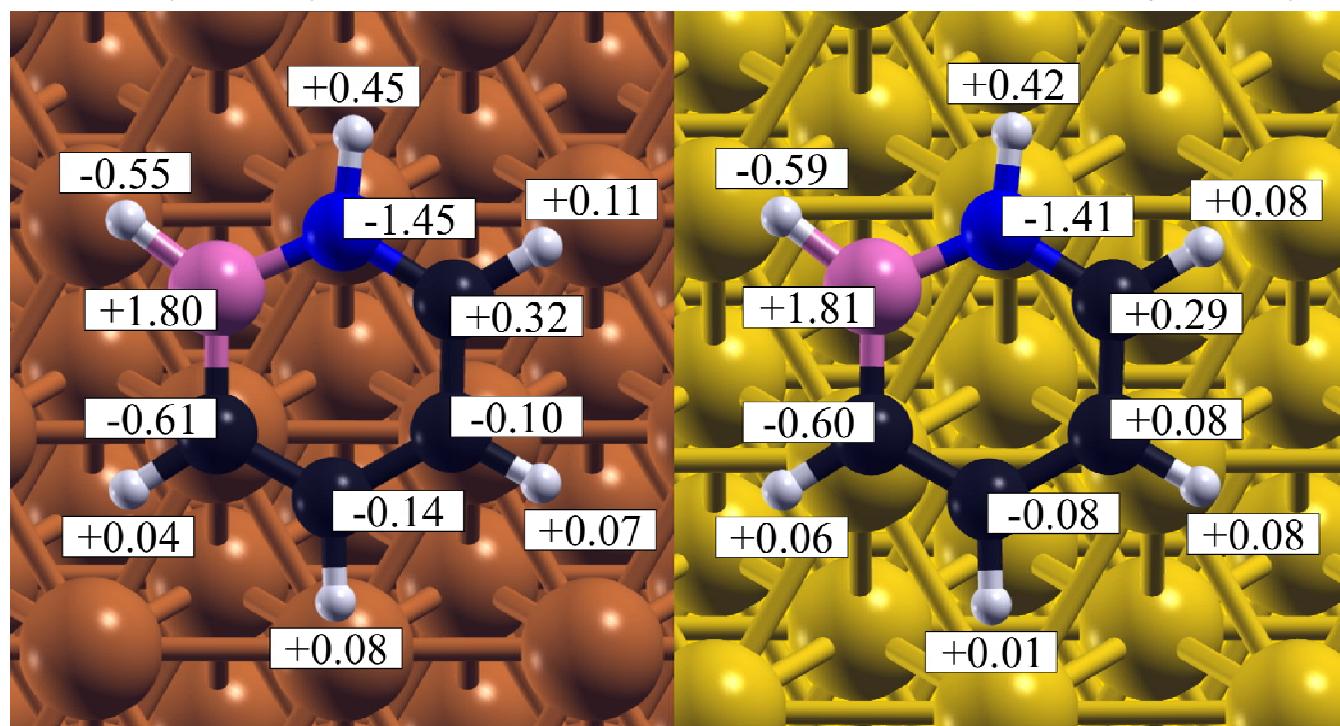


Figure S1: The Bader charges (units of e) of the atoms within 1,2-azaborine in the gas phase along with 1,2-azaborine adsorbed on Cu(111) and Au(111) as calculated with VASP. The total 1,2-azaborine charge is neutral, $+0.02\text{ e}$, and $+0.15\text{ e}$ in the gas-phase, Cu(111), and Au(111) systems, respectively. The hydrogen, boron, carbon, nitrogen, copper, and gold atoms are colored white, pink, black, blue, orange, and yellow, respectively.

Section S2. Pauli Repulsion and Charge Transfer Between 1,2-Azaborine and Cu(111)/Au(111):

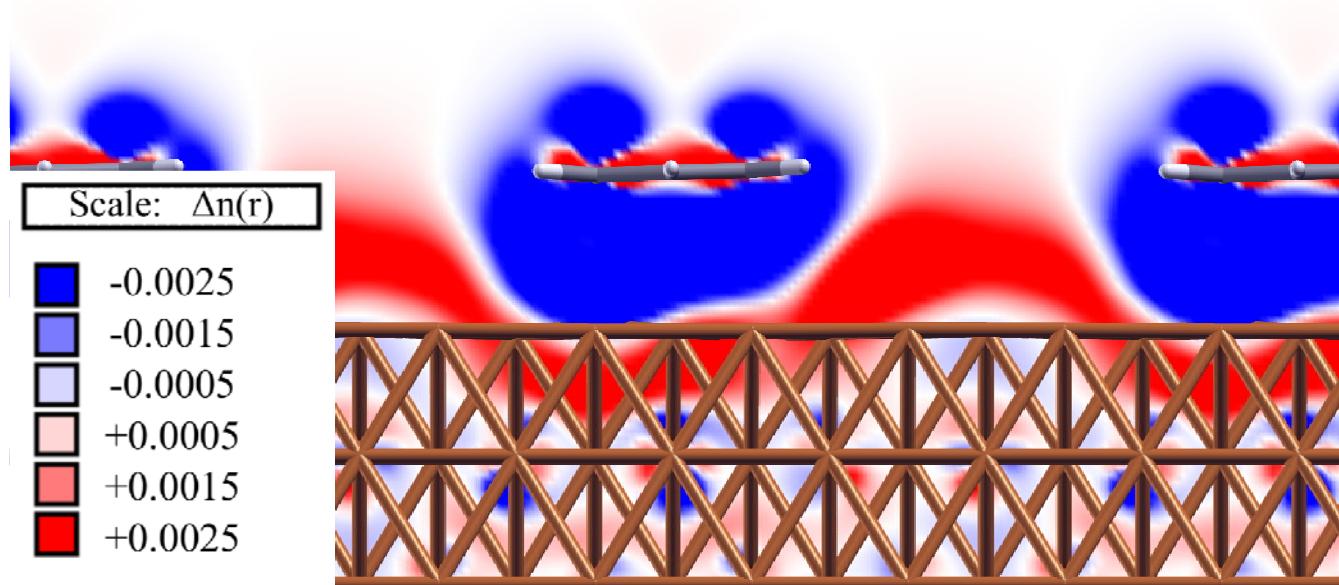


Figure S2: A contour plot (scale in $e/\text{\AA}^3$ is given in the left corner) of the CDD calculated for the adsorption of 1,2-azaborine on the Cu(111) surface. The depletion of charge between the molecule and the surface (blue region) is indicative of Pauli repulsion. The red regions represent charge gain.

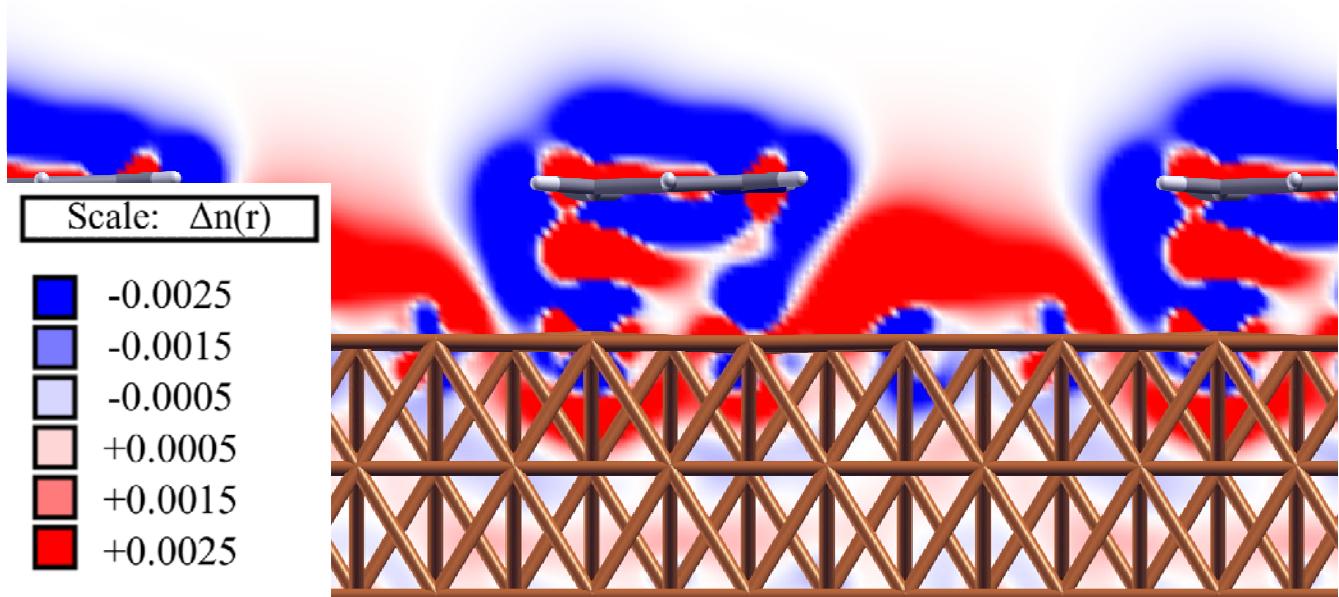


Figure S3: The same as Figure S2, but for a different cut plane. The red region between the molecule and the surface suggests some charge transfer from 1,2-azaborine to the surface.

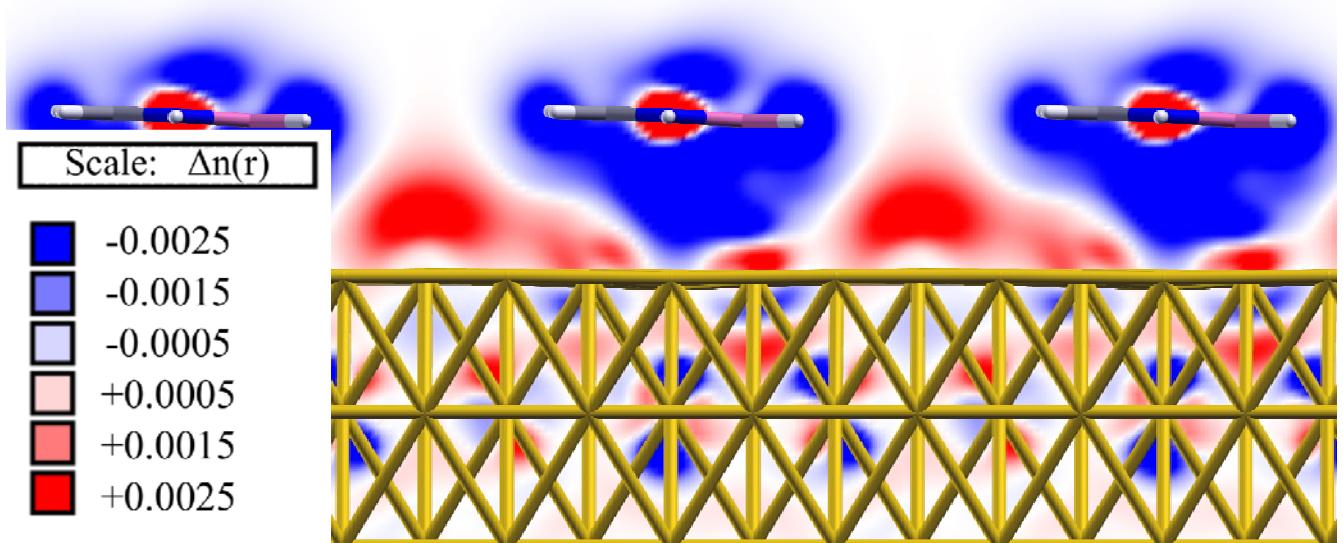


Figure S4: The same as Figure S2, but for 1,2-azaborine adsorbed to the Au(111) surface.

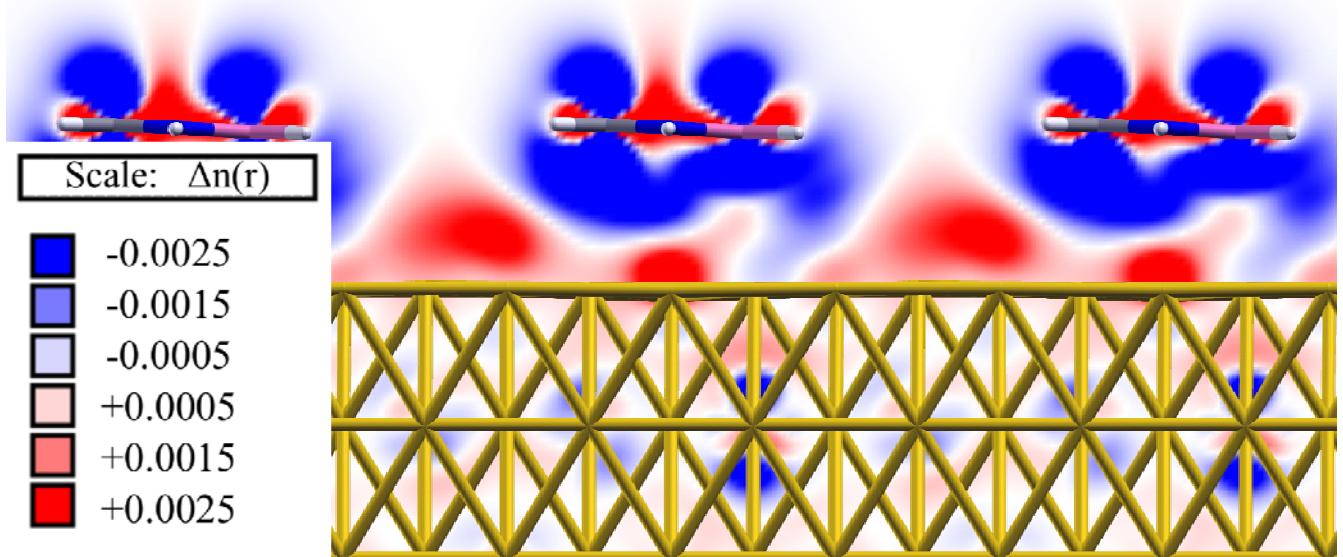


Figure S5: Same as Figure S4, except the red region between the molecule and the surface is indicative of charge transfer from 1,2-azaborine to the surface on a different cut plane.

Section S3. Projected Densities of States of 1,2-Azaborine on Cu(111) and Au(111):

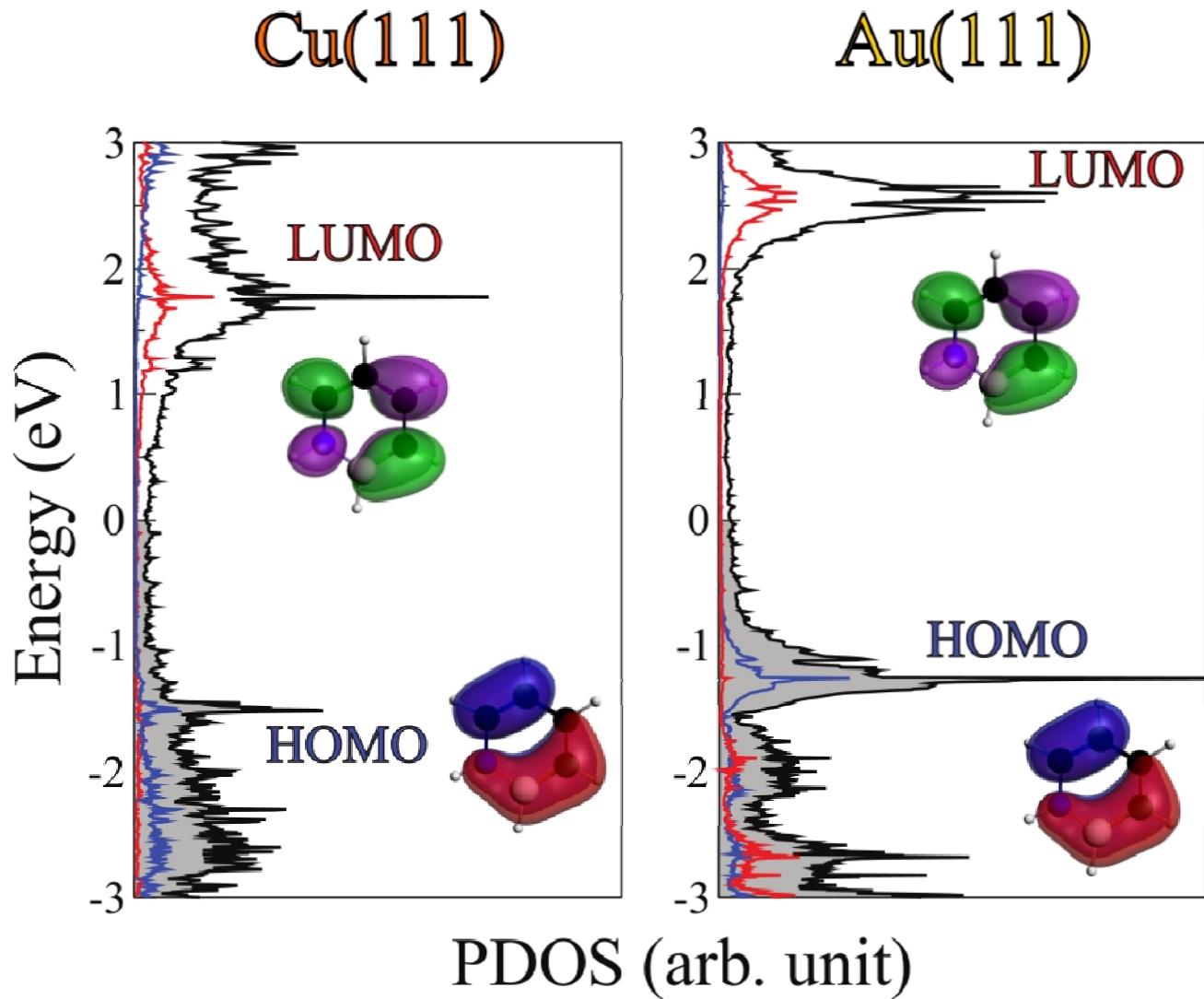


Figure S6: The PDOS (arbitrary units) of 1,2-azaborine on the Cu(111) and Au(111) surfaces (black line), where the Fermi level has been set to zero. The blue lines correspond to the PDOS of the H atom that is bonded to the boron atom and the hydrogen that is bonded to the carbon across from the boron atom. The red lines correspond to the PDOS of the H atom that is bonded to the nitrogen atom and the H atom that is bonded to the carbon atom across from the nitrogen atom. An isosurface (isovalue of +/- 0.03 au) of the HOMO and LUMO of the gas phase molecule (as calculated with ADF) is shown in the inset.

Section S4. Change in Work Function due to 1,2-Azaborine Adsorption to Cu(111) and Au(111):

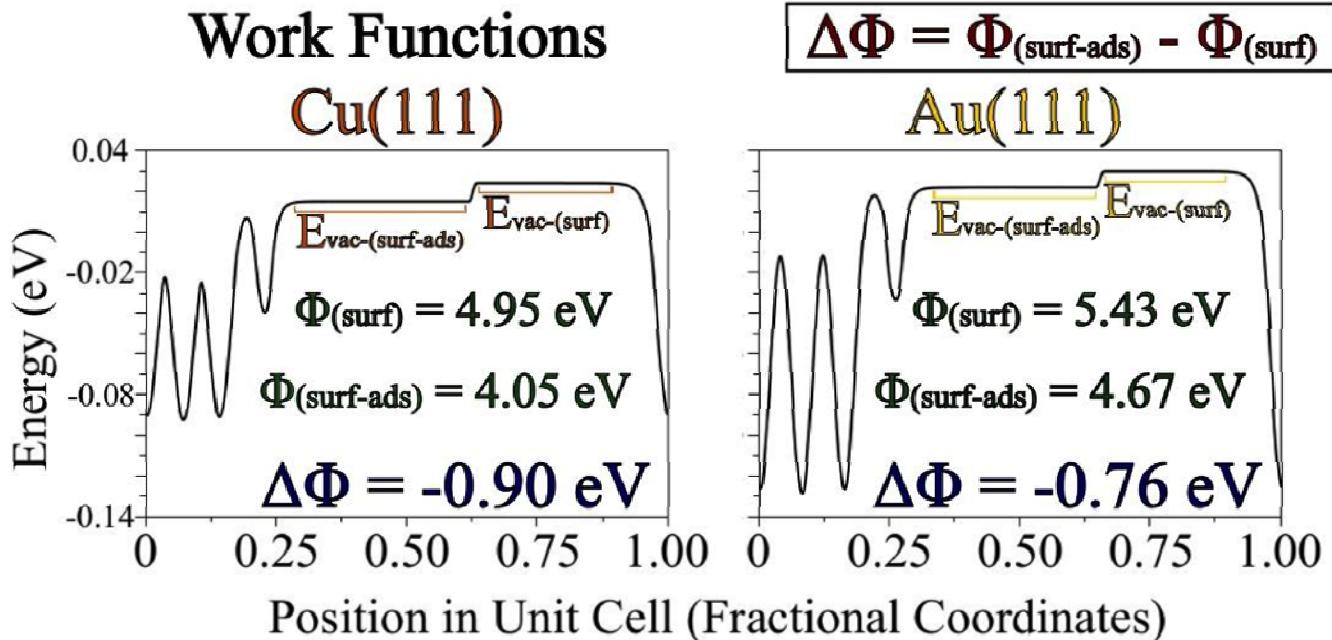


Figure S7: The planar averaged local potential as a function of the z-axis for the 1,2-azaborine monomer adsorbed to (left) Cu(111) and (right) Au(111) as calculated with vdW-DF-optPBE. The formula used to calculate the change in the workfunction ($\Delta\Phi$) is provided in the top right hand corner. The workfunction for each component was calculated via $\Phi = E_{\text{vac}} - E_f$.

Section S5. Coordinates (POSCAR Format):

Isolated 1,2-Azaborine Monomer:

N C B H

1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

N C B H
1 4 1 6

Direct

0.1356370443034473 0.1549892961858806 0.2306526095463582
0.2586154296076398 0.2208417600110706 0.2280042086197298
0.1973846559060310 0.2569211950061991 0.2311474640691507
0.1373958826329082 0.2234644691484186 0.2324070888598905
0.2599204463074489 0.1517978167173735 0.2258628402293511
0.1946180750458149 0.1135934221404560 0.2272055303498973
0.304916708222371 0.2498362736708259 0.2273386485901348
0.1972793312783149 0.3113344643217955 0.2324887862611567
0.0893557959149683 0.1341719661484098 0.2320075597357411
0.0897318495902201 0.2495245180593392 0.2349731667229205
0.1870652098242246 0.0542382955461346 0.2258758202791848
0.3085324939167232 0.1273675012440619 0.2232992767364722

Isolated 1,2-Azaborine Dimer:

N C B H

1.00000000000000
20.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 20.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 30.0000000000000000

N C B H
2 8 2 12

Direct

0.3912832469087641 0.2041816215104348 0.2308026669977284
0.4476387793112329 0.3880605557545649 0.2308026669977284
0.2669258189978224 0.2060569741224419 0.2260132591261541
0.3902032161371924 0.1358312740455488 0.2326372407386485
0.3305883206514805 0.1016453392218448 0.2312570011320792
0.2690322179925101 0.1369787927825939 0.2279531747461072
0.5719962072321791 0.3861852035875636 0.2260132591261541
0.4487188098378094 0.4564109032244460 0.2326372407386485
0.5083337052035178 0.4905968382631532 0.2312570011320792
0.5698898079874939 0.4552633849224094 0.2279531747461072
0.3317769830686495 0.2443614262719851 0.2273423242888676
0.5071450432963550 0.3478807512030155 0.2273423242888676
0.2182727040893007 0.2304113444976580 0.2234323391752106

0.3374011118084472	0.3039835977548349	0.2256538862424364
0.4382790428382500	0.1104537075157368	0.2350031454125467
0.4373421843909318	0.2258012094953313	0.2317026829013369
0.3311732423961236	0.0473065327352440	0.2325962047205338
0.2229499452241982	0.1077059625398561	0.2268690745183449
0.6206493222356931	0.3618308333873400	0.2234323391752106
0.5015209147715534	0.2882585796951618	0.2256538862424364
0.4006429830417523	0.4817884695842607	0.2350031454125467
0.4015798419040701	0.3664409676046662	0.2317026829013369
0.5077487832588783	0.5449356447497540	0.2325962047205338
0.6159720806558112	0.4845362153301424	0.2268690745183449

Isolated 1,2-Azaborine Trimer:

N C B H

1.000000000000000			
20.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	20.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	30.0000000000000000	

N	C	B	H
3	12	3	18

Direct

0.3958415233909335	0.1937168124077209	0.2296693495382901
0.4564373923432591	0.3890498077499276	0.2319885070311998
0.2266927555613258	0.3685122691102458	0.2311650636354457
0.2715144340954180	0.1971404956357151	0.2235538468840695
0.2726296298757403	0.1281968225532226	0.2274559473879652
0.3335690048217125	0.0922733110570657	0.2321689652806588
0.3936992679037015	0.1256147336946518	0.2332100457987758
0.5788674970223381	0.4557042725904393	0.2282060874605197
0.5176727233106844	0.4912729383754200	0.2321518193681880
0.4579418830176269	0.4573467403167317	0.2339957761216969
0.5805603934876170	0.3866088372550078	0.2261542869136372
0.1603032485243433	0.4909326707559073	0.2280893493636018
0.1246694647672194	0.4296611903570765	0.2326290965657581
0.1585740140997906	0.3699422118705493	0.2343247532272414
0.2293194334590747	0.4926792221501432	0.2248887006864308
0.3371684761401383	0.2345562426708450	0.2244366765521851
0.5155150608467134	0.3483582128174516	0.2279634238375711
0.2671768505873964	0.4274924082737779	0.2259443192603608
0.2225703354294651	0.2207647246525156	0.2196240908563441
0.3452559483595798	0.2935841164481078	0.2212015147302690
0.2261284603316424	0.0994985933642479	0.2269518762559244
0.4420432862938408	0.2150853235521387	0.2306069933741444
0.3332513563854537	0.0380836696661224	0.2349610260090107
0.4412176759567762	0.0995776128992233	0.2366314873550777
0.6249717031694687	0.4849419085895393	0.2267378010943795

0.5170696716004860	0.5456216322914971	0.2335948964224675
0.4099247820913162	0.3684121139788221	0.2328445340402923
0.4100630563436040	0.4827919086853794	0.2368336873716155
0.5088410724538596	0.2886928087856136	0.2263322414355484
0.6292084665965338	0.3623660967249990	0.2230951768771436
0.1310255273942328	0.5370641321360096	0.2271477840333336
0.0703972655950771	0.4293809864818261	0.2349552252209103
0.2483045461517775	0.3225868587398965	0.2324092930001289
0.1330755647760906	0.3220835009564309	0.2379831003124651
0.3259401752427767	0.4196582966511674	0.2224009303602142
0.2534933616929639	0.5413237999445712	0.2214783263371115

Isolated 1,2-Azaborine Tetramer:

N C B H

1.000000000000000			
20.0000000000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	20.0000000000000000	0.0000000000000000	
0.0000000000000000	0.0000000000000000	30.0000000000000000	

N	C	B	H
4	16	4	24

Direct

0.2251319805366539	0.3703397265126048	0.2312275899916688
0.3861259384430397	0.1896851686371303	0.2318758242503048
0.4526398621972898	0.3969142684343431	0.2318806303570550
0.6130031774707457	0.2130332490661142	0.2298001063587864
0.2269108592229444	0.4946328168767844	0.2246918171272605
0.1579135340090962	0.4922662580241835	0.2282594160806626
0.1228183771762216	0.4307941003972967	0.2331576267549718
0.1570622555269047	0.3712384671971316	0.2347297262458150
0.2626096052488040	0.1970716857521751	0.2232564365547205
0.2615201632493107	0.1279751582345017	0.2269923136647566
0.3209695422334474	0.0900825836644825	0.2328182476180439
0.3819850324636789	0.1216958816241955	0.2350403126951036
0.5767620240574058	0.4597171321657429	0.2274233042643803
0.5168748225700703	0.4971100704818984	0.2323320572376646
0.4561139715183287	0.4649950041403702	0.2342466202294710
0.5764723094775077	0.3905345863982145	0.2246436414347974
0.6764924797608209	0.0890278770906395	0.2285294078095606
0.7133740582416296	0.1494184380189277	0.2335983997478238
0.6808677220093381	0.2100059623887471	0.2344197662500930
0.6076382453766697	0.0888578906958541	0.2238888501649282
0.2650694612092662	0.4295569816671864	0.2255705791874786
0.3292795117738615	0.2324975665508165	0.2256619863825031
0.5101704254851260	0.3545571847913239	0.2269710028760234
0.5715466849151016	0.1549850755841799	0.2237642160752742
0.2506560565981755	0.5434290780918115	0.2208803693995866

0.3238844334041058 0.4223219480602237 0.2216061883187457
 0.1283326342503610 0.5382064654789438 0.2273551392741733
 0.0685962731888969 0.4303315959723069 0.2358831683127867
 0.2471376184246557 0.3245902559757031 0.2325722286674951
 0.1319425383555776 0.3232701348836862 0.2387795386332054
 0.2145361294774978 0.2219495782348712 0.2182046102711674
 0.3398391761114694 0.2913123153349489 0.2226076204092920
 0.2142253838349980 0.1006451972926524 0.2253982706431074
 0.4332438390286821 0.2088294438550086 0.2331458786907497
 0.3191433346161535 0.0359040558921088 0.2355213877227086
 0.4287705204803459 0.0946952825779290 0.2391717380028822
 0.6238124445091169 0.4874098249128282 0.2257891323303645
 0.5181167613152294 0.5514265791976480 0.2342096550066774
 0.4056629147636906 0.3773550162585365 0.2329538797961764
 0.4090118001649993 0.4917338859272942 0.2375268956945490
 0.5000924797153757 0.2955271275359413 0.2250481647402527
 0.6248487152679097 0.3659137137841661 0.2204811054431230
 0.7046323364145042 0.0421838745746358 0.2283115236818877
 0.7675170714313785 0.1483457596399589 0.2369538317676135
 0.5923001052992656 0.2594132133989952 0.2306473293993381
 0.7072773780020425 0.2572810127670908 0.2384112343021425
 0.5131448166712288 0.1637822472928633 0.2186565398963231
 0.5823726258660729 0.0407929760900326 0.2201506902365114

1,2-Azaborine Monomer on Cu(111):

Cu N C B H

1.000000000000000				
10.320000000000003	0.000000000000000	0.000000000000000		
0.000000000000000	8.935999999999999	0.000000000000000		
0.000000000000000	0.000000000000000	30.000000000000000		

Cu	N	C	B	H
48	1	4	1	6

Direct

0.3749309999999966 0.7499779999999987 0.000000000000000
 0.1249770000000012 0.2499930000000035 0.000000000000000
 0.2499540000000025 0.4999850000000023 0.000000000000000
 0.000000000000000 0.4999850000000023 0.000000000000000
 0.1249770000000012 0.5833159999999964 0.0702059999999989
 0.2499540000000025 0.8333089999999999 0.0702059999999989
 0.000000000000000 0.8333089999999999 0.0702059999999989
 0.1249770000000012 0.7499779999999987 0.000000000000000
 0.1230762772554712 0.9190970646274508 0.1387501957717276
 0.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 0.3333239999999975 0.0702059999999989
 0.9979663515837345 0.6679629821766468 0.1389086618765418
 0.8748390000000015 0.7499779999999987 0.000000000000000

0.6248849999999990	0.2499930000000035	0.0000000000000000
0.7498620000000003	0.4999850000000023	0.0000000000000000
0.4999079999999978	0.4999850000000023	0.0000000000000000
0.6248849999999990	0.5833159999999964	0.0702059999999989
0.7498620000000003	0.8333089999999999	0.0702059999999989
0.4999079999999978	0.8333089999999999	0.0702059999999989
0.6248849999999990	0.7499779999999987	0.0000000000000000
0.6278525624198537	0.9191111388793374	0.1390485203628984
0.4999079999999978	0.0000000000000000	0.0000000000000000
0.2499540000000025	0.0000000000000000	0.0000000000000000
0.3749309999999966	0.083331000000012	0.0702059999999989
0.4999079999999978	0.333323999999975	0.0702059999999989
0.2499540000000025	0.333323999999975	0.0702059999999989
0.3749309999999966	0.2499930000000035	0.0000000000000000
0.3761591564369908	0.4122862839947601	0.1391714131924431
0.5033423782126789	0.6705634508598379	0.1372932792808186
0.2496789092904095	0.6694170716532142	0.1415698211334586
0.3749309999999966	0.5833159999999964	0.0702059999999989
0.3756301700526308	0.9182524030625814	0.1400069569944975
0.2492206007844189	0.1652595406826194	0.1390954945483998
0.9994708625728421	0.1677959422447799	0.1399091802975505
0.1249770000000012	0.083331000000012	0.0702059999999989
0.1237863584354102	0.4165228628293036	0.1382077840300298
0.7498620000000003	0.0000000000000000	0.0000000000000000
0.8748390000000015	0.083331000000012	0.0702059999999989
0.7498620000000003	0.333323999999975	0.0702059999999989
0.8748390000000015	0.2499930000000035	0.0000000000000000
0.8748762585120460	0.4175130766741475	0.1399673804110790
0.7516027037476647	0.6678774768347040	0.1394160045688295
0.8748390000000015	0.5833159999999964	0.0702059999999989
0.8748677419830670	0.9179978545923149	0.1400623780887003
0.7505734504557537	0.1680219120618105	0.1400403963874908
0.5017385104097301	0.1653126950957997	0.1391809625261260
0.6248849999999990	0.083331000000012	0.0702059999999989
0.6268284961880042	0.4169173962615389	0.1383547240424789
0.4958811754741035	0.6629411701668602	0.2260500505749192
0.2539235139456579	0.5172533477886674	0.2250011793951359
0.3726755364200116	0.4356629668451646	0.2264464173560725
0.4905885575367464	0.5101137501376414	0.2276055834429442
0.2526624738259287	0.6736181466484936	0.2216105315191044
0.3812696695630677	0.7576663713955369	0.2212387309979817
0.1633721604153493	0.4541461284880555	0.2272383222442400
0.3721160720569401	0.3141605026985133	0.2289903835167593
0.5866114838520744	0.7082135183985443	0.2260842988657714
0.5822630641100375	0.4498841441176538	0.2296103686553295
0.3957804527391389	0.8908583139842037	0.2222248021904107

0.1592241033180954 0.7305197052753485 0.2237022762666783

1,2-Azaborine Dimer on Cu(111):

Cu N C B H

1.000000000000000
12.9000000000000004 0.000000000000000 0.000000000000000
0.000000000000000 13.403999999999999 0.000000000000000
0.000000000000000 0.000000000000000 30.000000000000000

Cu N C B H
90 2 8 2 12

Direct

0.7999220000000022 0.6666680000000014 0.000000000000000
0.899903999999994 0.8333280000000016 0.000000000000000
0.7999220000000022 0.000000000000000 0.000000000000000
0.899903999999994 0.499985999999998 0.000000000000000
0.7999220000000022 0.333323999999975 0.000000000000000
0.899903999999994 0.1666620000000023 0.000000000000000
0.699869999999971 0.8333280000000016 0.000000000000000
0.5998900000000020 0.6666680000000014 0.000000000000000
0.2999439999999964 0.8333280000000016 0.000000000000000
0.199961999999993 0.6666680000000014 0.000000000000000
0.3999260000000007 0.6666680000000014 0.000000000000000
0.499907999999978 0.8333280000000016 0.000000000000000
0.000000000000000 0.6666680000000014 0.000000000000000
0.099981999999971 0.8333280000000016 0.000000000000000
0.699869999999971 0.1666620000000023 0.000000000000000
0.5998900000000020 0.000000000000000 0.000000000000000
0.299943999999964 0.1666620000000023 0.000000000000000
0.1999640000000014 0.000000000000000 0.000000000000000
0.3999260000000007 0.000000000000000 0.000000000000000
0.4999060000000028 0.499985999999998 0.000000000000000
0.3999260000000007 0.333323999999975 0.000000000000000
0.5998900000000020 0.333323999999975 0.000000000000000
0.4999060000000028 0.1666620000000023 0.000000000000000
0.699869999999971 0.499985999999998 0.000000000000000
0.000000000000000 0.000000000000000 0.000000000000000
0.099981999999971 0.499985999999998 0.000000000000000
0.000000000000000 0.333323999999975 0.000000000000000
0.1999640000000014 0.333323999999975 0.000000000000000
0.099981999999971 0.1666620000000023 0.000000000000000
0.299943999999964 0.499985999999998 0.000000000000000
0.899903999999994 0.7222220000000021 0.070205999999989
0.7999220000000022 0.8888820000000024 0.070205999999989
0.899903999999994 0.0555540000000008 0.070205999999989
0.7999220000000022 0.2222160000000031 0.070205999999989
0.7999220000000022 0.5555400000000006 0.070205999999989

0.8999039999999994	0.3888760000000033	0.0702059999999989
0.4999079999999978	0.7222220000000021	0.0702059999999989
0.5998900000000020	0.8888820000000024	0.0702059999999989
0.6998699999999971	0.7222220000000021	0.0702059999999989
0.0999819999999971	0.7222220000000021	0.0702059999999989
0.1999640000000014	0.8888820000000024	0.0702059999999989
0.3999260000000007	0.8888820000000024	0.0702059999999989
0.2999439999999964	0.7222220000000021	0.0702059999999989
0.0000000000000000	0.8888820000000024	0.0702059999999989
0.4999060000000028	0.0555540000000008	0.0702059999999989
0.6998699999999971	0.3888760000000033	0.0702059999999989
0.5998900000000020	0.2222160000000031	0.0702059999999989
0.6998699999999971	0.0555540000000008	0.0702059999999989
0.0999819999999971	0.0555540000000008	0.0702059999999989
0.2999439999999964	0.3888760000000033	0.0702059999999989
0.1999619999999993	0.2222160000000031	0.0702059999999989
0.3999260000000007	0.2222160000000031	0.0702059999999989
0.2999439999999964	0.0555540000000008	0.0702059999999989
0.3999260000000007	0.5555400000000006	0.0702059999999989
0.5998900000000020	0.5555400000000006	0.0702059999999989
0.4999060000000028	0.3888760000000033	0.0702059999999989
0.0000000000000000	0.2222160000000031	0.0702059999999989
0.0000000000000000	0.5555400000000006	0.0702059999999989
0.1999640000000014	0.5555400000000006	0.0702059999999989
0.0999819999999971	0.3888760000000033	0.0702059999999989
0.4025531981647390	0.4458336843582273	0.1377009819312747
0.9002747271529188	0.9450787557947677	0.1399561832204270
0.9000156752058430	0.2780048021680770	0.1399698874204702
0.0998884530856401	0.9445276478419089	0.1400203772548991
0.0994483618681912	0.2769279412231924	0.1386701125207495
0.5002672503387799	0.9447757391104901	0.1394707541893396
0.5012221504895535	0.2771540989862871	0.1390165349067303
0.9001719429630910	0.6112512352912560	0.1397741732877904
0.0991415843943386	0.6128683972113009	0.1391453336502266
0.8004173577608356	0.4445952365098051	0.1401099500175818
0.5015117324500693	0.6122584238862743	0.1385993908894534
0.0001170168574660	0.7783403388946439	0.1401395969905366
0.9999520997755837	0.1111005181291915	0.1400851364343936
0.2000028394393567	0.7783251522733607	0.1399716099442543
0.1998236386484820	0.1097041979336026	0.1395600995265767
0.2999691732577290	0.9444703935125602	0.1400963223837977
0.3011100630854529	0.2751270782718720	0.1391612797611330
0.3995458993491354	0.7786878258771708	0.1387839180290840
0.4007289734955179	0.1094863001037325	0.1397797056982455
0.6016219954867807	0.4441851593774899	0.1393931325702695
0.8016996690732441	0.7784246383272162	0.1390673399200324

0.8003243211607511 0.1116088845549115 0.1400444093575999
 0.7011067755155054 0.9459686950045452 0.1389229243057244
 0.7005261453112652 0.2778249209784747 0.1401899463656378
 0.3007742563025388 0.6122722840165764 0.1398408378405236
 0.6011086182999463 0.7786246380784689 0.1380735002713180
 0.6004378389035381 0.1113472091183638 0.1400526504739688
 0.7006431352481215 0.6109846578947469 0.1398150580119690
 0.9990125099842118 0.4448841245479684 0.1389881929462575
 0.2004371655988848 0.4457245036912383 0.1421576439071259
 0.5008548702719153 0.7144826364607013 0.2418966156429363
 0.3955488719135403 0.4454552357848840 0.2308339866247024
 0.6942422440274569 0.7083398289293754 0.2363893123469154
 0.2014349962291391 0.4483515148385990 0.2239583336829725
 0.6925428060503336 0.8120072885997587 0.2383070588728984
 0.2048749577866573 0.3446021055257162 0.2293004509238656
 0.5978176136349944 0.8662392310850251 0.2405733764647735
 0.3004809110352724 0.2922980609784176 0.2326572168246486
 0.5042478009936460 0.8164565873197063 0.2420214531704374
 0.3935298947718380 0.3437831468502281 0.2337439011718843
 0.5922456461489034 0.6523906905010222 0.2382032441663142
 0.3030144155495904 0.5058984744891433 0.2243108732106975
 0.5821809225037242 0.5634548006958227 0.2386436268671446
 0.3113539318514285 0.5951758190325975 0.2240146924504529
 0.7694200930763202 0.6711829995017311 0.2343146594918863
 0.1256982127867516 0.4846396301931648 0.2247238684140243
 0.4284012205581291 0.6843223884630945 0.2420039609605169
 0.4673207685761938 0.4773294678378690 0.2320657052203501
 0.7647230099947251 0.8547512296585396 0.2374476611430509
 0.1331781899818409 0.3013127479440669 0.2315150143067299
 0.5981006680112131 0.9474645384397533 0.2404986123529298
 0.3015496078478890 0.2114722718089084 0.2361332463849521
 0.4304201005572637 0.8559299716024142 0.2428635383186162
 0.4676773039391833 0.3056726701681640 0.2374005254815401

1,2-Azaborine Trimer on Cu(111):

Cu N C B H

1.000000000000000		
15.480000000000004	0.000000000000000	0.000000000000000
0.000000000000000	17.871999999999999	0.000000000000000
0.000000000000000	0.000000000000000	30.000000000000000

Cu N C B H

144 3 12 3 18

Direct

0.8332679999999968	0.750000000000000	0.000000000000000
0.9165869999999998	0.8749970000000005	0.000000000000000
0.8332679999999968	0.500000999999975	0.000000000000000

0.9165869999999998	0.6249960000000030	0.0000000000000000
0.8332679999999968	0.0000000000000000	0.0000000000000000
0.9165869999999998	0.3749899999999968	0.0000000000000000
0.8332679999999968	0.2499930000000035	0.0000000000000000
0.9165869999999998	0.1249960000000030	0.0000000000000000
0.6666019999999975	0.7500000000000000	0.0000000000000000
0.7499180000000010	0.8749970000000005	0.0000000000000000
0.5832249999999988	0.8749970000000005	0.0000000000000000
0.4999079999999978	0.7500000000000000	0.0000000000000000
0.2499529999999979	0.8749970000000005	0.0000000000000000
0.1666370000000015	0.7500000000000000	0.0000000000000000
0.3332720000000009	0.7500000000000000	0.0000000000000000
0.4165899999999993	0.8749970000000005	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.0000000000000000
0.0833179999999984	0.8749970000000005	0.0000000000000000
0.6666019999999975	0.5000009999999975	0.0000000000000000
0.7499200000000030	0.6249960000000030	0.0000000000000000
0.6666019999999975	0.0000000000000000	0.0000000000000000
0.7499200000000030	0.3749899999999968	0.0000000000000000
0.6666019999999975	0.2499930000000035	0.0000000000000000
0.7499200000000030	0.1249960000000030	0.0000000000000000
0.5832249999999988	0.6249960000000030	0.0000000000000000
0.4999079999999978	0.5000009999999975	0.0000000000000000
0.2499529999999979	0.6249960000000030	0.0000000000000000
0.1666349999999994	0.5000009999999975	0.0000000000000000
0.3332720000000009	0.5000009999999975	0.0000000000000000
0.4165899999999993	0.6249960000000030	0.0000000000000000
0.0000000000000000	0.5000009999999975	0.0000000000000000
0.0833179999999984	0.6249960000000030	0.0000000000000000
0.5832249999999988	0.1249960000000030	0.0000000000000000
0.4999079999999978	0.0000000000000000	0.0000000000000000
0.2499529999999979	0.1249960000000030	0.0000000000000000
0.1666370000000015	0.0000000000000000	0.0000000000000000
0.3332720000000009	0.0000000000000000	0.0000000000000000
0.4165879999999973	0.3749899999999968	0.0000000000000000
0.3332720000000009	0.2499930000000035	0.0000000000000000
0.4999079999999978	0.2499930000000035	0.0000000000000000
0.4165879999999973	0.1249960000000030	0.0000000000000000
0.5832249999999988	0.3749899999999968	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0833179999999984	0.3749899999999968	0.0000000000000000
0.0000000000000000	0.2499930000000035	0.0000000000000000
0.1666370000000015	0.2499930000000035	0.0000000000000000
0.0833179999999984	0.1249960000000030	0.0000000000000000
0.2499529999999979	0.3749899999999968	0.0000000000000000
0.9165869999999998	0.7916659999999993	0.070205999999989

0.8332679999999968	0.9166620000000023	0.0702059999999989
0.9165869999999998	0.5416669999999968	0.0702059999999989
0.8332679999999968	0.6666620000000023	0.0702059999999989
0.9165869999999998	0.0416659999999993	0.0702059999999989
0.8332679999999968	0.1666620000000023	0.0702059999999989
0.8332679999999968	0.4166549999999987	0.0702059999999989
0.9165869999999998	0.2916570000000007	0.0702059999999989
0.7499180000000010	0.7916659999999993	0.0702059999999989
0.6666019999999975	0.9166620000000023	0.0702059999999989
0.4165899999999993	0.7916659999999993	0.0702059999999989
0.4999079999999978	0.9166620000000023	0.0702059999999989
0.5832249999999988	0.7916659999999993	0.0702059999999989
0.0833179999999984	0.7916659999999993	0.0702059999999989
0.1666349999999994	0.9166620000000023	0.0702059999999989
0.3332720000000009	0.9166620000000023	0.0702059999999989
0.2499529999999979	0.7916659999999993	0.0702059999999989
0.0000000000000000	0.9166620000000023	0.0702059999999989
0.7499200000000030	0.5416669999999968	0.0702059999999989
0.6666019999999975	0.6666620000000023	0.0702059999999989
0.7499200000000030	0.0416659999999993	0.0702059999999989
0.6666019999999975	0.1666620000000023	0.0702059999999989
0.6666019999999975	0.4166549999999987	0.0702059999999989
0.7499200000000030	0.2916570000000007	0.0702059999999989
0.4165899999999993	0.5416669999999968	0.0702059999999989
0.4999079999999978	0.6666620000000023	0.0702059999999989
0.5832249999999988	0.5416669999999968	0.0702059999999989
0.0833179999999984	0.5416669999999968	0.0702059999999989
0.1666370000000015	0.6666620000000023	0.0702059999999989
0.3332720000000009	0.6666620000000023	0.0702059999999989
0.2499529999999979	0.5416669999999968	0.0702059999999989
0.0000000000000000	0.6666620000000023	0.0702059999999989
0.4165879999999973	0.0416659999999993	0.0702059999999989
0.5832249999999988	0.2916570000000007	0.0702059999999989
0.4999079999999978	0.1666620000000023	0.0702059999999989
0.5832249999999988	0.0416659999999993	0.0702059999999989
0.0833179999999984	0.0416659999999993	0.0702059999999989
0.2499529999999979	0.2916570000000007	0.0702059999999989
0.1666349999999994	0.1666620000000023	0.0702059999999989
0.3332720000000009	0.1666620000000023	0.0702059999999989
0.2499529999999979	0.0416659999999993	0.0702059999999989
0.3332720000000009	0.4166549999999987	0.0702059999999989
0.4999079999999978	0.4166549999999987	0.0702059999999989
0.4165879999999973	0.2916570000000007	0.0702059999999989
0.0000000000000000	0.1666620000000023	0.0702059999999989
0.0000000000000000	0.4166549999999987	0.0702059999999989
0.1666370000000015	0.4166549999999987	0.0702059999999989

0.0833179999999984	0.2916570000000007	0.0702059999999989
0.3343153991988004	0.3338768618401105	0.1384185418376163
0.9166396577503946	0.9583674170576444	0.1398880871738584
0.9166371257493324	0.7084726982651048	0.1398153431442282
0.9168114111643817	0.2082213178974612	0.1397511237793978
0.7501114093732255	0.9583287290838385	0.1399152709621703
0.0834998088544836	0.9580204900308686	0.1399126329860820
0.7500892965929040	0.7085793219242049	0.1398362107604427
0.7504156950916823	0.2081160700729043	0.1391522482161989
0.0834364538728423	0.7083464639871906	0.1398348733092689
0.0830852803072517	0.2076333118369149	0.1389775877769921
0.4166068080352474	0.9579603460551027	0.1399246456891774
0.4166126941418398	0.7084274632726775	0.1397463476702328
0.4166892768534467	0.2076496509919679	0.1391415505054852
0.9164079359069817	0.4585267338093857	0.1400139682357775
0.7504256890926655	0.4586954738914528	0.1395912457775310
0.0826546371600756	0.4591364591219644	0.1393170452919392
0.6663805997701289	0.3343249898676035	0.1383023078420038
0.4173980025559416	0.4587272834206857	0.1393229578267920
0.0000716828478815	0.8333543389558429	0.1398668473381548
0.9999604112861391	0.5834458746729183	0.1398196405292040
0.0000019604204340	0.0829735873799535	0.1400685506485999
0.8336010680203501	0.8334152317386625	0.1397993095333163
0.1666112659044572	0.8331507460169902	0.1398859466864835
0.8337701323376905	0.5833947629719560	0.1400437863772268
0.8336325592811491	0.0830472418033139	0.1397914199638350
0.1665897691950065	0.5832946087852520	0.1399058635795214
0.1664368367333537	0.0823593906431839	0.1396900829299739
0.2500426394781528	0.9578999006857742	0.1398874908208114
0.2500288630498133	0.7083936507997279	0.1398493123855289
0.2502746328123848	0.2070085380146622	0.1392930681763431
0.3334821756884239	0.8331681067428889	0.1399452410526578
0.3332092824795936	0.5834440664001974	0.1391647159332621
0.3336960212904216	0.0822970466160271	0.1398200302558124
0.5001565154253740	0.3332986961546425	0.1392902676340739
0.6666733635301298	0.8334712884557192	0.1398762534691897
0.6675859255282148	0.5835508248464052	0.1394539856731001
0.6666299959711850	0.0825216130736806	0.1393805847008593
0.5835250208913294	0.9583187621525582	0.1399696313235026
0.5837200425139528	0.7087668578940196	0.1392545641858973
0.5836592624001185	0.2083663255613359	0.1405508005502654
0.2502128982749525	0.4586012516137927	0.1398878342136314
0.5000591506814729	0.8334302839777976	0.1398304271328499
0.5005358877590211	0.5831411794418813	0.1388499154291480
0.5000149605418542	0.0827542072304013	0.1397658804758422
0.5839006666197903	0.4586549367192418	0.1392630265891270

0.9992880978393828 0.3335193567537615 0.1392762259612539
 0.8334451435653421 0.3335958411113253 0.1396195148283965
 0.1662435061065253 0.3339264356801550 0.1415409229814841
 0.6352328220571266 0.3458545812893234 0.2434195260768135
 0.4109937626739040 0.5516509894805566 0.2458004986074371
 0.3242722917564294 0.3297599849429318 0.2378676570294544
 0.6267645703891915 0.2064357662911647 0.2375447590710991
 0.5721209623992252 0.5463092763906303 0.2414102829755436
 0.1630899533972183 0.3373705134260234 0.2321292286128127
 0.7164045341480261 0.2063423913816322 0.2411243998907793
 0.5714326305850150 0.6238399058841821 0.2443231001489465
 0.1620971207218957 0.2597952337050629 0.2366054909823774
 0.7646753189548505 0.2738241884610702 0.2442721519531545
 0.4928789417667190 0.6648602915399593 0.2468699140879309
 0.2398715158753149 0.2177820126682022 0.2394349698114624
 0.7232507379713340 0.3421499920835913 0.2454447273725151
 0.4144277129523033 0.6280282566003663 0.2473387533281652
 0.3189574282459233 0.2535846017448122 0.2404007747843977
 0.5801917214327759 0.2810080381967239 0.2383610523015065
 0.4866675893057391 0.5048684116959947 0.2417526067792650
 0.2495169953193610 0.3777293989327219 0.2323208649250574
 0.5039032540177715 0.2913995318856024 0.2370309103544841
 0.4762647908077966 0.4383855892973116 0.2405339503431705
 0.2602895637008515 0.4442501972050508 0.2309084404268233
 0.5937159575482767 0.1525630414838943 0.2353128382637024
 0.6353108238080551 0.5193599472503081 0.2385063108733689
 0.1012219396905323 0.3667076597178465 0.2310827266417732
 0.6092572232961047 0.3980953982799775 0.2440913476468367
 0.3507054301278458 0.5288060075888836 0.2454415536500321
 0.3852918907064051 0.3512318725124928 0.2386939484838138
 0.7522479699189191 0.1536158566461054 0.2411975672021001
 0.6320444650715515 0.6552823061918573 0.2439134488286356
 0.1009787960159017 0.2291110393436711 0.2374684362321346
 0.8349514844831987 0.2723500288522374 0.2456795483647625
 0.4936812244506186 0.7257269048621851 0.2479466581763958
 0.2382538806168029 0.1570472768786217 0.2417891233625227
 0.7585623054150616 0.3948268921666127 0.2474582548683983
 0.3532127703359791 0.6579796246469627 0.2487169088922201
 0.3795266437781777 0.2229511914757154 0.2432078241227060

1,2-Azaborine Tetramer on Cu(111):

Cu N C B H

1.00000000000000		
15.480000000000004	0.000000000000000	0.000000000000000
0.000000000000000	17.871999999999999	0.000000000000000
0.000000000000000	0.000000000000000	30.000000000000000

Cu N C B H
 144 4 16 4 24

Direct

0.2499529999999979	0.3749899999999968	0.0000000000000000
0.0833179999999984	0.1249960000000030	0.0000000000000000
0.1666370000000015	0.2499930000000035	0.0000000000000000
0.0000000000000000	0.2499930000000035	0.0000000000000000
0.0833179999999984	0.3749899999999968	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5832249999999988	0.3749899999999968	0.0000000000000000
0.4165879999999973	0.1249960000000030	0.0000000000000000
0.4999079999999978	0.2499930000000035	0.0000000000000000
0.3332720000000009	0.2499930000000035	0.0000000000000000
0.4165879999999973	0.3749899999999968	0.0000000000000000
0.3332720000000009	0.0000000000000000	0.0000000000000000
0.1666370000000015	0.0000000000000000	0.0000000000000000
0.2499529999999979	0.1249960000000030	0.0000000000000000
0.4999079999999978	0.0000000000000000	0.0000000000000000
0.5832249999999988	0.1249960000000030	0.0000000000000000
0.0833179999999984	0.6249960000000030	0.0000000000000000
0.0000000000000000	0.5000009999999975	0.0000000000000000
0.4165899999999993	0.6249960000000030	0.0000000000000000
0.3332720000000009	0.5000009999999975	0.0000000000000000
0.1666349999999994	0.5000009999999975	0.0000000000000000
0.2499529999999979	0.6249960000000030	0.0000000000000000
0.4999079999999978	0.5000009999999975	0.0000000000000000
0.5832249999999988	0.6249960000000030	0.0000000000000000
0.7499200000000030	0.1249960000000030	0.0000000000000000
0.6666019999999975	0.2499930000000035	0.0000000000000000
0.7499200000000030	0.3749899999999968	0.0000000000000000
0.6666019999999975	0.0000000000000000	0.0000000000000000
0.7499200000000030	0.6249960000000030	0.0000000000000000
0.6666019999999975	0.5000009999999975	0.0000000000000000
0.0833179999999984	0.8749970000000005	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.0000000000000000
0.4165899999999993	0.8749970000000005	0.0000000000000000
0.3332720000000009	0.7500000000000000	0.0000000000000000
0.1666370000000015	0.7500000000000000	0.0000000000000000
0.2499529999999979	0.8749970000000005	0.0000000000000000
0.4999079999999978	0.7500000000000000	0.0000000000000000
0.5832249999999988	0.8749970000000005	0.0000000000000000
0.7499180000000010	0.8749970000000005	0.0000000000000000
0.6666019999999975	0.7500000000000000	0.0000000000000000
0.9165869999999998	0.1249960000000030	0.0000000000000000
0.8332679999999968	0.2499930000000035	0.0000000000000000
0.9165869999999998	0.3749899999999968	0.0000000000000000

0.8332679999999968	0.0000000000000000	0.0000000000000000
0.9165869999999998	0.6249960000000030	0.0000000000000000
0.8332679999999968	0.500000999999975	0.0000000000000000
0.9165869999999998	0.8749970000000005	0.0000000000000000
0.8332679999999968	0.7500000000000000	0.0000000000000000
0.0833179999999984	0.2916570000000007	0.0702059999999989
0.1666370000000015	0.4166549999999987	0.0702059999999989
0.0000000000000000	0.4166549999999987	0.0702059999999989
0.0000000000000000	0.1666620000000023	0.0702059999999989
0.4165879999999973	0.2916570000000007	0.0702059999999989
0.4999079999999978	0.4166549999999987	0.0702059999999989
0.3332720000000009	0.4166549999999987	0.0702059999999989
0.2499529999999979	0.0416659999999993	0.0702059999999989
0.3332720000000009	0.1666620000000023	0.0702059999999989
0.1666349999999994	0.1666620000000023	0.0702059999999989
0.2499529999999979	0.2916570000000007	0.0702059999999989
0.0833179999999984	0.0416659999999993	0.0702059999999989
0.5832249999999988	0.0416659999999993	0.0702059999999989
0.4999079999999978	0.1666620000000023	0.0702059999999989
0.5832249999999988	0.2916570000000007	0.0702059999999989
0.4165879999999973	0.0416659999999993	0.0702059999999989
0.0000000000000000	0.6666620000000023	0.0702059999999989
0.2499529999999979	0.5416669999999968	0.0702059999999989
0.3332720000000009	0.6666620000000023	0.0702059999999989
0.1666370000000015	0.6666620000000023	0.0702059999999989
0.0833179999999984	0.5416669999999968	0.0702059999999989
0.5832249999999988	0.5416669999999968	0.0702059999999989
0.4999079999999978	0.6666620000000023	0.0702059999999989
0.4165899999999993	0.5416669999999968	0.0702059999999989
0.7499200000000030	0.2916570000000007	0.0702059999999989
0.666601999999975	0.4166549999999987	0.0702059999999989
0.666601999999975	0.1666620000000023	0.0702059999999989
0.7499200000000030	0.0416659999999993	0.0702059999999989
0.666601999999975	0.6666620000000023	0.0702059999999989
0.7499200000000030	0.5416669999999968	0.0702059999999989
0.0000000000000000	0.9166620000000023	0.0702059999999989
0.2499529999999979	0.7916659999999993	0.0702059999999989
0.3332720000000009	0.9166620000000023	0.0702059999999989
0.1666349999999994	0.9166620000000023	0.0702059999999989
0.0833179999999984	0.7916659999999993	0.0702059999999989
0.5832249999999988	0.7916659999999993	0.0702059999999989
0.4999079999999978	0.9166620000000023	0.0702059999999989
0.4165899999999993	0.7916659999999993	0.0702059999999989
0.666601999999975	0.9166620000000023	0.0702059999999989
0.7499180000000010	0.7916659999999993	0.0702059999999989
0.9165869999999998	0.2916570000000007	0.0702059999999989

0.8332679999999968	0.4166549999999987	0.0702059999999989
0.8332679999999968	0.1666620000000023	0.0702059999999989
0.9165869999999998	0.0416659999999993	0.0702059999999989
0.8332679999999968	0.6666620000000023	0.0702059999999989
0.9165869999999998	0.5416669999999968	0.0702059999999989
0.8332679999999968	0.9166620000000023	0.0702059999999989
0.9165869999999998	0.7916659999999993	0.0702059999999989
0.3336101426319615	0.3333181225240551	0.1409423225932755
0.0838055457528100	0.2082045022686714	0.1398131787283816
0.0829849160790985	0.7087428467180743	0.1392863152754629
0.7501519042042020	0.2084267499770576	0.1406769317302050
0.7501652207251581	0.7088038959401857	0.1392795767758130
0.0835595710452566	0.9583330081486565	0.1399251478521322
0.7501031705176331	0.9582062038738925	0.1399851948987560
0.9171656010757019	0.2080853420147051	0.1391902872929265
0.9166082568927578	0.7085701404269074	0.1399713249425929
0.9166654147030115	0.9583472667357071	0.1399270598616127
0.4169266410934185	0.2066353117690127	0.1390769026613938
0.4171156628135364	0.7086340676754048	0.1395344344166389
0.4165649332278605	0.9579181180096157	0.1399421219506465
0.0832365003212630	0.4579340991261489	0.1398252319014190
0.7501474421772301	0.4586065307427845	0.1395000592495634
0.9169352531355699	0.4586697146166969	0.1397702449556988
0.6667465376643307	0.3333004835249511	0.1393764168879983
0.4169281170589585	0.4583510172272085	0.1396229247825147
0.1665571763609108	0.0829879458045681	0.1400780052219943
0.1653421186725552	0.5827939664603932	0.1392088897269659
0.8335550038821822	0.0825176409436139	0.1392995511491790
0.8340481929545689	0.5835393408291694	0.1394890968162272
0.1665901362082991	0.8333582553057752	0.1398029550576467
0.8335377169761244	0.8334306635930275	0.1399291428482456
0.0002266147896108	0.0830181751159387	0.1397378798745947
0.9994467906574727	0.5833807475718800	0.1397039525204278
0.0000351252970958	0.8334620292966406	0.1399008723617925
0.2497467200006653	0.2076036677566719	0.1389599536550818
0.2500842879302354	0.7082327228212293	0.1395935001179467
0.2499435898036353	0.9579476877581357	0.1399788427128144
0.3332762657227235	0.0821971870663845	0.1396838638665585
0.3341515982480701	0.5832424325994623	0.1398249365139819
0.3335439378048903	0.8332881340274980	0.1397911095499182
0.5006007582248415	0.3335229113724765	0.1387032207345271
0.6664934216855372	0.0826919787932070	0.1396871611187223
0.6669099919362296	0.5833204220216075	0.1389021737934257
0.6666524826659099	0.8333504881318348	0.1398984213212771
0.5835814903663206	0.2076321961024092	0.1391120193573485
0.5834344170726737	0.7084537503054307	0.1397929246809539

0.5835648892626040	0.9579320472581898	0.1399438585819084
0.2497440250677343	0.4582693044178825	0.1386920725411542
0.5001627805927740	0.0822269189747260	0.1397669853839147
0.5001206071823177	0.5833147792097648	0.1391534356222763
0.5001394816613285	0.8332499562778821	0.1400172705459113
0.5840398232003068	0.4584661895107018	0.1394978981276083
0.1661186320720205	0.3332951056403672	0.1395252028073202
0.8336388062330116	0.3343221484685870	0.1384238998512188
0.0001773781460130	0.3335602966727720	0.1397121095593263
0.7995377993097037	0.3382276171582959	0.2445504807541639
0.4926268362167079	0.3155443705849308	0.2399299070692820
0.5817204311155137	0.5476257964768081	0.2484884329898591
0.2771406529671410	0.5207631994321744	0.2472192054894080
0.7912046618646968	0.1989765974437745	0.2380699050104553
0.3315987130661995	0.3235957151590156	0.2341752557792631
0.7422677773263899	0.5388729238351146	0.2435700420819771
0.2836641103985968	0.6597902133984093	0.2392443965747546
0.8808954570111993	0.1988062837908799	0.2413752971864298
0.3302777724274577	0.2460285792071488	0.2387551799846079
0.7439341850509607	0.6164203230286276	0.2457349977340328
0.1939170596990252	0.6593286640968898	0.2401138536677436
0.9292428587414747	0.2662496095814362	0.2448110378176693
0.4078383060040451	0.2039438214956348	0.2418145909767162
0.6665417728498753	0.6590875711716890	0.2477618266534094
0.1465287090041656	0.5911817098796348	0.2427142149978465
0.8875656609256453	0.3344734267480405	0.2463551708185179
0.4871419727617194	0.2394769489247324	0.2424563434899483
0.5872482666404082	0.6238893914380697	0.2491893681531181
0.1890244693756173	0.5235839580444974	0.2462131304795250
0.7445579955202604	0.2734410362221453	0.2393656318225155
0.4182050764435488	0.3636124299248067	0.2343314402619470
0.6557841914045781	0.4990756843161961	0.2445994750532492
0.3313807396597142	0.5860590652862498	0.2427344395268065
0.6683044521750929	0.2836650398551015	0.2383334235007268
0.4306163374028031	0.4298204699962511	0.2327418715514256
0.6431550768487426	0.4328005986312320	0.2440342075278039
0.4077779047303096	0.5771148930478489	0.2439077509373249
0.7582181297050141	0.1450688877812070	0.2358028510142063
0.2690752282774866	0.3517799048951460	0.2316449129603839
0.8047128260797578	0.5105500616175291	0.2409451160833385
0.3164875487702759	0.7138090213211044	0.2371833141019408
0.7732997027800010	0.3904098386878658	0.2455823425556218
0.5537137268288959	0.3369363056872032	0.2403660117219104
0.5205348385593709	0.5266110675142741	0.2489004804295263
0.3038196194418958	0.4689026555067031	0.2496689536184533
0.9168098811097067	0.1461032214805655	0.2412461150714904

0.2690109838729242 0.2155512703589721 0.2392732819725509
 0.8052573451675329 0.6467657241605309 0.2448875805259760
 0.1573619410927378 0.7116016815131516 0.2382464509251463
 0.9995056899291441 0.2649270237152095 0.2463919152528149
 0.4058209982572833 0.1432062835227086 0.2442585169681522
 0.6689273169891194 0.7199236720626772 0.2483574098014572
 0.0762262678491936 0.5915954827749133 0.2419848109126335
 0.9226026992456582 0.3872330274821749 0.2488988985466989
 0.5475326037534103 0.2085059249901917 0.2451195470583798
 0.5267784505055886 0.6549403428835419 0.2505947562902548
 0.1544035094640606 0.4705374939675266 0.2480649932409378

1,2-Azaborine Monomer on Au(111):

Au N C B H

1.00000000000000		
8.90399999999999	0.00000000000000	0.00000000000000
0.00000000000000	10.27999999999999	0.00000000000000
0.00000000000000	0.00000000000000	30.00000000000000

Au N C B H
36 1 4 1 6

Direct

0.1666510000000017 0.7500369999999990 0.0000000000000000
 0.00000000000000 0.5000250000000008 0.0000000000000000
 0.00000000000000 0.8333749999999966 0.0807709999999986
 0.4999540000000025 0.7500369999999990 0.0000000000000000
 0.8332570000000032 0.7500369999999990 0.0000000000000000
 0.666604999999970 0.5000250000000008 0.0000000000000000
 0.666604999999970 0.8333749999999966 0.0807709999999986
 0.1666510000000017 0.2500119999999981 0.0000000000000000
 0.4999540000000025 0.2500119999999981 0.0000000000000000
 0.3333030000000008 0.0000000000000000 0.0000000000000000
 0.3333030000000008 0.5000250000000008 0.0000000000000000
 0.1666510000000017 0.5833620000000010 0.0807709999999986
 0.4999540000000025 0.5833620000000010 0.0807709999999986
 0.3333030000000008 0.3333500000000029 0.0807709999999986
 0.3333030000000008 0.8333749999999966 0.0807709999999986
 0.1656336398520608 0.9164764055517978 0.162747330836864
 0.4999783035291969 0.9148985143852570 0.1615900878001568
 0.3308999267393631 0.6688501828626272 0.1624180580528503
 0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.1666510000000017 0.0833370000000002 0.0807709999999986
 0.0000000000000000 0.3333500000000029 0.0807709999999986
 0.1635189254805667 0.4194683480447452 0.1618281543748310
 0.0004034062947227 0.1666175425290177 0.1624083441855362
 0.9982916970411182 0.6679401702114944 0.1632885865589415
 0.8332570000000032 0.2500119999999981 0.0000000000000000

0.8332570000000032 0.5833620000000010 0.080770999999986
 0.8333817442000964 0.9154826875201962 0.1628116043285033
 0.6666049999999970 0.0000000000000000 0.0000000000000000
 0.4999540000000025 0.0833370000000002 0.080770999999986
 0.8332570000000032 0.0833370000000002 0.080770999999986
 0.6666049999999970 0.3333500000000029 0.080770999999986
 0.4982553364859399 0.4210403486591119 0.1586303432572933
 0.8340413091735996 0.4187074115845490 0.1618127664770910
 0.6707558376940170 0.1661151681217063 0.1601980512274395
 0.6661663765290911 0.6673901541750027 0.1630675031904048
 0.3319034303213186 0.1674388450669895 0.1617446699463798
 0.4998906254133786 0.4000607602486923 0.2599026917617451
 0.3615296189540871 0.1878827495391278 0.2568226552364976
 0.6334536260439663 0.3349065318337026 0.2613591185045081
 0.6368691786976797 0.2004193595827033 0.2610874803153251
 0.5011880703505298 0.1275748132518544 0.2598532959191715
 0.3547760675243197 0.3358213870623814 0.2570395599621378
 0.2613991673296567 0.1265421040940993 0.2568591460047287
 0.2447067213092424 0.4027058674552251 0.2565932559366289
 0.7358158912633783 0.3931339099171325 0.2619306573992617
 0.5072230731165774 0.4990162938430487 0.2589994223858980
 0.7451998899497525 0.1516570255890386 0.2625401325046326
 0.5102944675122743 0.0215109057921907 0.2603450346159519

1,2-Azaborine Dimer on Au(111):

Au N C B H

1.00000000000000				
14.83999999999999	0.0000000000000000	0.0000000000000000		
0.0000000000000000	15.41999999999999	0.0000000000000000		
0.0000000000000000	0.0000000000000000	30.0000000000000000		

Au	N	C	B	H
90	2	8	2	12

Direct

0.5999330000000000 0.6666669999999968 0.0000000000000000
 0.7999140000000011 0.6666669999999968 0.0000000000000000
 0.8999049999999968 0.8333409999999972 0.0000000000000000
 0.6999229999999983 0.8333409999999972 0.0000000000000000
 0.5999330000000000 0.0000000000000000 0.0000000000000000
 0.7999140000000011 0.3333500000000029 0.0000000000000000
 0.7999140000000011 0.0000000000000000 0.0000000000000000
 0.8999049999999968 0.1666749999999979 0.0000000000000000
 0.6999229999999983 0.1666749999999979 0.0000000000000000
 0.8999049999999968 0.5000250000000008 0.0000000000000000
 0.5999330000000000 0.3333500000000029 0.0000000000000000
 0.6999229999999983 0.5000250000000008 0.0000000000000000
 0.3999629999999996 0.6666669999999968 0.0000000000000000

0.4999540000000025	0.8333409999999972	0.0000000000000000
0.0000000000000000	0.6666669999999968	0.0000000000000000
0.1999819999999985	0.6666669999999968	0.0000000000000000
0.2999719999999968	0.8333409999999972	0.0000000000000000
0.0999910000000028	0.8333409999999972	0.0000000000000000
0.3999629999999996	0.0000000000000000	0.0000000000000000
0.4999540000000025	0.1666749999999979	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.1999819999999985	0.3333500000000029	0.0000000000000000
0.1999819999999985	0.0000000000000000	0.0000000000000000
0.2999719999999968	0.1666749999999979	0.0000000000000000
0.0999910000000028	0.1666749999999979	0.0000000000000000
0.3999629999999996	0.3333500000000029	0.0000000000000000
0.4999540000000025	0.5000250000000008	0.0000000000000000
0.2999719999999968	0.5000250000000008	0.0000000000000000
0.0000000000000000	0.3333500000000029	0.0000000000000000
0.0999910000000028	0.5000250000000008	0.0000000000000000
0.8999049999999968	0.7222250000000017	0.0807709999999986
0.5999330000000000	0.8888999999999996	0.0807709999999986
0.6999229999999983	0.7222250000000017	0.0807709999999986
0.7999140000000011	0.8888999999999996	0.0807709999999986
0.8999049999999968	0.0555579999999978	0.0807709999999986
0.5999330000000000	0.2222330000000028	0.0807709999999986
0.6999229999999983	0.0555579999999978	0.0807709999999986
0.7999140000000011	0.5555829999999986	0.0807709999999986
0.7999140000000011	0.2222330000000028	0.0807709999999986
0.8999049999999968	0.3889080000000007	0.0807709999999986
0.6999229999999983	0.3889080000000007	0.0807709999999986
0.5999330000000000	0.5555829999999986	0.0807709999999986
0.3999629999999996	0.8888999999999996	0.0807709999999986
0.4999540000000025	0.7222250000000017	0.0807709999999986
0.2999719999999968	0.7222250000000017	0.0807709999999986
0.0000000000000000	0.8888999999999996	0.0807709999999986
0.0999910000000028	0.7222250000000017	0.0807709999999986
0.1999819999999985	0.8888999999999996	0.0807709999999986
0.3999629999999996	0.2222330000000028	0.0807709999999986
0.4999540000000025	0.0555579999999978	0.0807709999999986
0.2999719999999968	0.0555579999999978	0.0807709999999986
0.4999540000000025	0.3889080000000007	0.0807709999999986
0.0000000000000000	0.2222330000000028	0.0807709999999986
0.0999910000000028	0.0555579999999978	0.0807709999999986
0.1999819999999985	0.5555829999999986	0.0807709999999986
0.1999819999999985	0.2222330000000028	0.0807709999999986
0.2999719999999968	0.3889080000000007	0.0807709999999986
0.0999910000000028	0.3889080000000007	0.0807709999999986
0.3999629999999996	0.5555829999999986	0.0807709999999986

0.0000000000000000	0.5555829999999986	0.0807709999999986
0.8996701060593395	0.9453745187377152	0.1622999061743258
0.9001144978608764	0.2782076681695216	0.1624291466614309
0.2995570484676122	0.9460357716534133	0.1617630665536964
0.2982440510338904	0.2777275524271943	0.1620302810792396
0.4007895301224167	0.7786920164446229	0.1616617998320038
0.3994851518498805	0.1112552771500859	0.1621434037673311
0.9002356997955872	0.6120428250520362	0.1625841979937519
0.2981636358721218	0.6097574840366562	0.1590750508705980
0.8006495279323715	0.7791799189074879	0.1623915821625772
0.8000181532596002	0.1115658719336423	0.1628633201596656
0.1975693103427716	0.7792484616928164	0.1610838647330084
0.1986288326484242	0.1115330435989463	0.1622645659471971
0.5005817356084634	0.9458711110229032	0.1623071883130365
0.4995672453636786	0.2781922606409637	0.1614599662338279
0.7002233442383812	0.9457162816569848	0.1625800281616492
0.7018258214184812	0.2781741955236683	0.1610742030028049
0.0989876487512689	0.9453442347933532	0.1626286908824213
0.0989101705664694	0.2778735654758933	0.1624248403075370
0.6018316054509754	0.7794068688453279	0.1618352846075268
0.6004162100465393	0.1113508355894481	0.1619487052569113
0.9989067122658781	0.7787198735445457	0.1626240745156267
0.9990915636120477	0.1115849246704101	0.1626198445114824
0.8011647496509440	0.4460263118164818	0.1620765897728660
0.1981451877447640	0.4436025397279124	0.1627437781888119
0.7009904265476194	0.6131988606786010	0.1626172993527319
0.0989086639698087	0.6115142894739733	0.1620969144588713
0.5000759718785304	0.6118059354366920	0.1610523308705964
0.9995795067104467	0.4448440900387567	0.1627524243984766
0.3986544541734887	0.4440319112477908	0.1613609181177225
0.6013160102574844	0.4472667623414424	0.1592978312583142
0.3284392055249725	0.6145415242681693	0.2630293066817018
0.5743904756261600	0.4560102743533960	0.2638446315544627
0.4077328657370742	0.7575644453344381	0.2585791851917207
0.4952109352391929	0.3129858312073424	0.2604964759753727
0.3235019158391452	0.7961954441886121	0.2631137384251261
0.5797014636625519	0.2746233380277303	0.2642819092401183
0.2434697301695152	0.7459370913157315	0.2660307261775259
0.2475576327918816	0.6564459477070699	0.2660620518660863
0.6598578074016643	0.3250070448047495	0.2666431341541795
0.6556218418833311	0.4144677515332376	0.2663785583360436
0.4137035163861498	0.6593470419057752	0.2586060045864471
0.4890174434430818	0.4111130560875580	0.2601957687295666
0.4812333347978281	0.6169908022166837	0.2568769502996417
0.4670692130645477	0.7992905291283421	0.2571180343571342
0.4213512110444526	0.4532360692516448	0.2587831495506023

0.4361671209448517 0.2707832666150765 0.2593187284178313
 0.3256330411719333 0.5484808381179604 0.2626721193232555
 0.5770205753878557 0.5220312942630940 0.2631477049042346
 0.3168928267486635 0.8667603374744530 0.2638093836540918
 0.5865497573804461 0.2040064512295530 0.2648778319728819
 0.1872820913202418 0.6162707065522852 0.2678997912292331
 0.7157988500926749 0.4547877614117581 0.2679036053531831
 0.1779063882710048 0.7770832232491429 0.2687351365976980
 0.7255155651292071 0.2937786704990160 0.2688637189652781

1,2-Azaborine Trimer on Au(111):

Au N C B H

1.000000000000000		
17.807999999999998	0.000000000000000	0.000000000000000
0.000000000000000	20.559999999999987	0.000000000000000
0.000000000000000	0.000000000000000	30.000000000000000

Au N C B H

144 3 12 3 18

Direct

0.0833259999999996 0.3750190000000018 0.000000000000000
 0.000000000000000 0.2500130000000027 0.000000000000000
 0.2499770000000012 0.3750190000000018 0.000000000000000
 0.4166280000000029 0.3750190000000018 0.000000000000000
 0.3333030000000008 0.2500130000000027 0.000000000000000
 0.0833259999999996 0.1250059999999991 0.000000000000000
 0.2499770000000012 0.1250059999999991 0.000000000000000
 0.1666519999999991 0.000000000000000 0.000000000000000
 0.1666519999999991 0.2500130000000027 0.000000000000000
 0.000000000000000 0.000000000000000 0.000000000000000
 0.4166280000000029 0.1250059999999991 0.000000000000000
 0.3333030000000008 0.000000000000000 0.000000000000000
 0.0833259999999996 0.6250059999999991 0.000000000000000
 0.2499770000000012 0.6250059999999991 0.000000000000000
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1,2-Azaborine Tetramer on Au(111):

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Au N C B H

144 4 16 4 24

Direct

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0.6800832034678805	0.5117157144082825	0.2645374962468381
0.4123893153543250	0.2249127667133237	0.2648666998095237
0.0625201802737152	0.2215568322338370	0.2672672594622583
0.2701876211092866	0.6069531086192939	0.2677277426608526
0.6912694630833869	0.5784352402453408	0.2670296682957698
0.4805158231188429	0.1922463237563150	0.2682025058117858
0.1234976241021570	0.1770008046565721	0.2699397012348115
0.2023350838985181	0.5711021764312250	0.2708725409045130
0.6298499096017380	0.6222870308068877	0.2708181750134813

0.1966309640422779	0.1992819121471925	0.2711275562785360
0.2035018069102463	0.5039782444538332	0.2715096210728376
0.5571343626500465	0.5995051816576833	0.2723335141633427
0.5496563076411363	0.2264459108141637	0.2710859185859036
0.5505278800159346	0.2935914069763399	0.2714584677999312
0.1541047109636793	0.3134778613119806	0.2664461217129457
0.3418688319345762	0.5025304796021928	0.2646402778032382
0.6005235514840308	0.4857857579159557	0.2656330947099832
0.4121755445282602	0.2986721924571327	0.2654379161004812
0.1729983470306067	0.3691962342771333	0.2664745966744775
0.3962116646509486	0.4678521406599856	0.2629990050995801
0.5822743062971654	0.4298280340165519	0.2643621526359254
0.0251330498456142	0.3198410993386318	0.2629467349298693
0.3888995882054900	0.6072001294059888	0.2610573654162636
0.7293114779834866	0.4803293199988943	0.2613089546652105
0.3586503773625367	0.3343008966645584	0.2641119326621748
0.3618622595705006	0.1950949013035412	0.2626771876501977
0.2670152761958349	0.2766636895448329	0.2708116623154950
0.2651552614650825	0.4215655032003056	0.2691643381596123
0.4872355558779375	0.5216877312225421	0.2706815960076909
0.4916356114221969	0.3775536631345204	0.2691705701805560
0.0057539917760892	0.2012809349473486	0.2665569361453066
0.2663382573154394	0.6600158001344667	0.2674257702519540
0.7479423186037408	0.5988405824346117	0.2658904047864183
0.4823453069571570	0.1391014705143050	0.2680554395052823
0.2441759397128678	0.1660992517523212	0.2731959649704621
0.1523639522822933	0.4750388712000770	0.2734187843381619
0.5093311467798003	0.6323043616147572	0.2747226403187284
0.6025257242810795	0.3213769869863015	0.2731204643115746
0.1134702761609034	0.1247502010470640	0.2708127184878393
0.1484500942446729	0.5959682195198326	0.2727400190376130
0.6395760105547907	0.6745329281732850	0.2720576197875317
0.6027601971411727	0.2003637190844643	0.2729529968782813

Section S6. Coordinates (XYZ Format):**Azaborine Monomer:**

12

C	-5.329166	1.066582	0.000000
C	-6.296171	0.013786	0.000000
C	-5.891215	-1.301791	0.000000
N	-4.550062	-1.621494	0.000000
B	-3.486730	-0.633503	0.000000
C	-3.965587	0.810208	0.000000
H	-5.705902	2.095941	0.000000
H	-7.363934	0.238127	0.000000
H	-4.331950	-2.614006	0.000000
H	-6.604440	-2.128872	0.000000
H	-2.354430	-1.038657	0.000000
H	-3.283611	1.666367	0.000000

Azaborine Dimer:

24

C	-0.348665	-6.009915	0.000000
C	0.518719	-4.876407	0.000000
C	-0.003695	-3.600529	0.000000
N	-1.361275	-3.397201	0.000000
B	-2.321391	-4.477334	0.000000
C	-1.730621	-5.873768	0.000000
H	0.116151	-7.002629	0.000000
H	1.602312	-5.003517	0.000000
H	-1.654646	-2.420677	0.000000
H	0.632206	-2.713131	0.000000
H	-3.496569	-4.199793	0.000000
H	-2.338505	-6.783961	0.000000
C	-5.428826	1.166463	0.000000
C	-6.293980	0.031271	0.000000
C	-5.768929	-1.243477	0.000000
N	-4.410988	-1.443996	0.000000
B	-3.452949	-0.362055	0.000000
C	-4.046593	1.033079	0.000000
H	-5.895625	2.158231	0.000000
H	-7.377818	0.156174	0.000000
H	-4.115762	-2.419971	0.000000
H	-6.402945	-2.132210	0.000000
H	-2.277293	-0.637632	0.000000
H	-3.440668	1.944545	0.000000

Azaborine Trimer 1:

36

N	2.971789	3.180269	0.000000
N	4.363701	-1.522676	0.000000
N	0.448011	-1.128203	0.000000
C	2.663135	4.516292	0.000000
C	5.409923	3.735279	0.000000
C	3.660984	5.468020	0.000000
C	5.032706	5.071951	0.000000
C	5.715109	-1.282099	0.000000
C	4.803650	-3.988465	0.000000
C	6.616443	-2.325899	0.000000
C	6.157200	-3.676625	0.000000
C	-0.866190	-1.515179	0.000000
C	-0.252866	1.273595	0.000000
C	-1.876802	-0.575843	0.000000
C	-1.564965	0.815405	0.000000
B	4.325287	2.674220	0.000000
B	3.799946	-2.853201	0.000000
B	0.868328	0.252204	0.000000
H	2.183086	2.538882	0.000000
H	4.470545	1.481030	0.000000
H	1.604799	4.785036	0.000000
H	6.480109	3.504200	0.000000
H	3.385673	6.523759	0.000000
H	5.787639	5.866852	0.000000
H	3.774849	-0.691523	0.000000
H	2.598901	-2.969288	0.000000
H	6.031861	-0.238467	0.000000
H	4.517670	-5.045049	0.000000
H	7.684044	-2.100537	0.000000
H	6.914459	-4.469297	0.000000
H	1.138058	-1.880158	0.000000
H	2.052428	0.467857	0.000000
H	-1.070851	-2.587490	0.000000
H	-0.104279	2.359374	0.000000
H	-2.913841	-0.914036	0.000000
H	-2.402982	1.521512	0.000000

Azaborine Trimer 2:

36

C	-3.608669	-7.611639	0.000000
C	-2.187949	-7.746560	0.000000
C	-1.382609	-6.626795	0.000000

N	-1.931592	-5.370544	0.000000
B	-3.354422	-5.128486	0.000000
C	-4.227459	-6.367612	0.000000
H	-4.203756	-8.532152	0.000000
H	-1.722001	-8.733036	0.000000
H	-1.265476	-4.597669	0.000000
H	-0.292954	-6.693776	0.000000
H	-3.713991	-3.979828	0.000000
H	-5.321760	-6.338162	0.000000
C	2.997142	-1.386436	0.000000
C	2.439124	-0.072991	0.000000
C	1.070914	0.101971	0.000000
N	0.227613	-0.979078	0.000000
B	0.692682	-2.345442	0.000000
C	2.198030	-2.523013	0.000000
H	4.089994	-1.470883	0.000000
H	3.084556	0.806631	0.000000
H	-0.770024	-0.765394	0.000000
H	0.611426	1.092197	0.000000
H	-0.145098	-3.210255	0.000000
H	2.693488	-3.499135	0.000000
C	-5.568481	1.291694	0.000000
C	-6.514245	0.222960	0.000000
C	-6.083256	-1.087261	0.000000
N	-4.744656	-1.382320	0.000000
B	-3.710538	-0.375342	0.000000
C	-4.198354	1.059827	0.000000
H	-5.962989	2.314333	0.000000
H	-7.586037	0.426864	0.000000
H	-4.505693	-2.374242	0.000000
H	-6.779106	-1.928361	0.000000
H	-2.572150	-0.768085	0.000000
H	-3.531877	1.928213	0.000000

Azaborine Timer 3:

36

C	-3.924257	-7.045617	0.000000
C	-2.650745	-7.689847	0.000000
C	-1.491748	-6.942651	0.000000
N	-1.543936	-5.571736	0.000000
B	-2.780317	-4.822297	0.000000
C	-4.044099	-5.662049	0.000000
H	-4.814081	-7.685448	0.000000
H	-2.577337	-8.778221	0.000000
H	-0.645777	-5.093949	0.000000

H	-0.503352	-7.406097	0.000000
H	-2.695979	-3.626415	0.000000
H	-5.056263	-5.241513	0.000000
C	0.360716	-2.316032	0.000000
C	0.446047	-0.891517	0.000000
C	1.674868	-0.269179	0.000000
N	2.834376	-1.006103	0.000000
B	2.865863	-2.454344	0.000000
C	1.496363	-3.114803	0.000000
H	-0.644977	-2.745157	0.000000
H	-0.458932	-0.284172	0.000000
H	3.697302	-0.467649	0.000000
H	1.772199	0.818488	0.000000
H	3.941844	-2.992551	0.000000
H	1.378253	-4.204835	0.000000
C	-5.570337	0.944866	0.000000
C	-6.537057	-0.106113	0.000000
C	-6.130799	-1.423957	0.000000
N	-4.797440	-1.745451	0.000000
B	-3.737631	-0.760337	0.000000
C	-4.206736	0.684251	0.000000
H	-5.944524	1.975450	0.000000
H	-7.604709	0.118629	0.000000
H	-4.574403	-2.738539	0.000000
H	-6.845230	-2.249848	0.000000
H	-2.607465	-1.161866	0.000000
H	-3.521505	1.538504	0.000000

Azaborine Trimer 4:

36

C	-3.430733	-7.804540	0.000000
C	-2.105758	-7.275099	0.000000
C	-1.899117	-5.911543	0.000000
N	-2.959066	-5.039650	0.000000
B	-4.336735	-5.476936	0.000000
C	-4.546707	-6.978295	0.000000
H	-3.540925	-8.895231	0.000000
H	-1.240674	-7.940248	0.000000
H	-2.713847	-4.049812	0.000000
H	-0.899759	-5.475414	0.000000
H	-5.206317	-4.640971	0.000000
H	-5.535855	-7.447007	0.000000
C	1.181205	0.039860	0.000000
C	2.584001	-0.227946	0.000000
C	3.043495	-1.526924	0.000000

N	2.161706	-2.581636	0.000000
B	0.723091	-2.419892	0.000000
C	0.241703	-0.980826	0.000000
H	0.867086	1.090230	0.000000
H	3.308685	0.587660	0.000000
H	2.584858	-3.506511	0.000000
H	4.108988	-1.764916	0.000000
H	0.049432	-3.416805	0.000000
H	-0.813978	-0.709244	0.000000
C	-4.681293	0.979761	0.000000
C	-5.971340	0.369704	0.000000
C	-6.089715	-1.004174	0.000000
N	-4.975049	-1.803078	0.000000
B	-3.626280	-1.285849	0.000000
C	-3.514085	0.227356	0.000000
H	-4.640229	2.075227	0.000000
H	-6.876310	0.978998	0.000000
H	-5.148589	-2.808052	0.000000
H	-7.060915	-1.502786	0.000000
H	-2.720404	-2.078410	0.000000
H	-2.562347	0.767514	0.000000

Azaborine Trimer 5:

36

N	-2.712518	3.671563	0.000000
N	4.376993	-1.649210	0.000000
N	0.744325	-1.491071	0.000000
C	-4.061745	3.418386	0.000000
C	-3.165957	6.128379	0.000000
C	-4.970533	4.454095	0.000000
C	-4.516525	5.808798	0.000000
C	5.665396	-1.172997	0.000000
C	5.249039	-3.996813	0.000000
C	6.737751	-2.038398	0.000000
C	6.525275	-3.450074	0.000000
C	-0.511045	-2.043158	0.000000
C	-0.262131	0.800966	0.000000
C	-1.633673	-1.242927	0.000000
C	-1.502749	0.177334	0.000000
B	-2.143648	5.003049	0.000000
B	4.058543	-3.058657	0.000000
B	0.984011	-0.066178	0.000000
H	-2.110898	2.853821	0.000000
H	-0.943888	5.094919	0.000000
H	-4.376578	2.372789	0.000000

H	-2.889603	7.187685	0.000000
H	-6.036923	4.222857	0.000000
H	-5.279312	6.596309	0.000000
H	3.649605	-0.935469	0.000000
H	2.895760	-3.384811	0.000000
H	5.795385	-0.089221	0.000000
H	5.154820	-5.087175	0.000000
H	7.748016	-1.626656	0.000000
H	7.411206	-4.095348	0.000000
H	1.512756	-2.162153	0.000000
H	2.126040	0.322851	0.000000
H	-0.576090	-3.132913	0.000000
H	-0.210434	1.894935	0.000000
H	-2.618585	-1.711736	0.000000
H	-2.436449	0.752077	0.000000

Azaborine Trimer – Mixed Chirality 1:

48

C	-8.104440	-6.961752	0.000000
C	-6.968498	-7.826247	0.000000
C	-5.693996	-7.298943	0.000000
N	-5.498541	-5.942004	0.000000
B	-6.578668	-4.983402	0.000000
C	-7.973351	-5.578923	0.000000
H	-9.095519	-7.430155	0.000000
H	-7.092989	-8.910125	0.000000
H	-4.530519	-5.631487	0.000000
H	-4.804972	-7.932313	0.000000
H	-6.285292	-3.817999	0.000000
H	-8.887720	-4.976826	0.000000
C	2.021141	2.211285	0.000000
C	0.882613	3.072392	0.000000
C	-0.390206	2.541747	0.000000
N	-0.582057	1.184348	0.000000
B	0.500834	0.228855	0.000000
C	1.893897	0.828044	0.000000
H	3.010913	2.682558	0.000000
H	1.004139	4.156696	0.000000
H	-1.548949	0.870146	0.000000
H	-1.280959	3.172904	0.000000
H	0.211097	-0.937722	0.000000
H	2.809859	0.228385	0.000000
C	-0.520951	-6.223535	0.000000
C	0.515458	-5.245853	0.000000
C	0.203707	-3.901742	0.000000

N	-1.102025	-3.486464	0.000000
B	-2.225470	-4.394092	0.000000
C	-1.864835	-5.868273	0.000000
H	-0.222790	-7.278199	0.000000
H	1.564227	-5.545897	0.000000
H	-1.237105	-2.476642	0.000000
H	0.969769	-3.125171	0.000000
H	-3.329091	-3.909115	0.000000
H	-2.591490	-6.687825	0.000000
C	-5.552720	1.473521	0.000000
C	-6.592219	0.499272	0.000000
C	-6.284513	-0.845788	0.000000
N	-4.980235	-1.265156	0.000000
B	-3.854075	-0.361233	0.000000
C	-4.210130	1.113859	0.000000
H	-5.847307	2.529092	0.000000
H	-7.640046	0.802419	0.000000
H	-4.848360	-2.275364	0.000000
H	-7.053130	-1.619783	0.000000
H	-2.752485	-0.850288	0.000000
H	-3.480962	1.930977	0.000000

Azaborine Trimer – Mixed Chirality 2:

48

C	4.736380	-1.916734	0.000000
C	5.518899	-0.724668	0.000000
C	4.903465	0.509347	0.000000
N	3.535629	0.612068	0.000000
B	2.655931	-0.534044	0.000000
C	3.347642	-1.882815	0.000000
H	5.271482	-2.873248	0.000000
H	6.608718	-0.772646	0.000000
H	3.174753	1.566295	0.000000
H	5.471318	1.441730	0.000000
H	1.463664	-0.333469	0.000000
H	2.819866	-2.839310	0.000000
C	-0.604335	5.066402	0.000000
C	-1.450586	3.917388	0.000000
C	-0.907739	2.650398	0.000000
N	0.454072	2.473402	0.000000
B	1.394750	3.570748	0.000000
C	0.779984	4.955932	0.000000
H	-1.086979	6.050592	0.000000
H	-2.535309	4.030123	0.000000
H	0.762307	1.502253	0.000000

H	-1.523374	1.751888	0.000000
H	2.575494	3.315834	0.000000
H	1.371294	5.876963	0.000000
C	-0.402084	-5.845726	0.000000
C	0.444429	-4.696910	0.000000
C	-0.098119	-3.429795	0.000000
N	-1.459893	-3.252515	0.000000
B	-2.400820	-4.349642	0.000000
C	-1.786371	-5.734954	0.000000
H	0.080338	-6.830022	0.000000
H	1.529124	-4.809916	0.000000
H	-1.767874	-2.281304	0.000000
H	0.517704	-2.531420	0.000000
H	-3.581503	-4.094473	0.000000
H	-2.377888	-6.655847	0.000000
C	-5.742492	1.137912	0.000000
C	-6.525477	-0.053728	0.000000
C	-5.910619	-1.287909	0.000000
N	-4.542924	-1.391238	0.000000
B	-3.662782	-0.245616	0.000000
C	-4.353873	1.103376	0.000000
H	-6.277137	2.094587	0.000000
H	-7.615195	-0.005291	0.000000
H	-4.182566	-2.345586	0.000000
H	-6.478830	-2.219979	0.000000
H	-2.470694	-0.446755	0.000000
H	-3.825738	2.059565	0.000000

Azaborine Trimer – Mixed Chirality 3:

48

C	4.665805	1.590334	0.000000
C	4.554643	3.012409	0.000000
C	3.311506	3.611525	0.000000
N	2.171398	2.853935	0.000000
B	2.170719	1.409501	0.000000
C	3.546761	0.766344	0.000000
H	5.675131	1.162738	0.000000
H	5.446392	3.640810	0.000000
H	1.289648	3.362215	0.000000
H	3.190884	4.696750	0.000000
H	1.095847	0.869347	0.000000
H	3.724096	-0.315437	0.000000
C	-1.408989	6.517097	0.000000
C	-2.830835	6.403674	0.000000
C	-3.427988	5.159684	0.000000

N	-2.668749	4.020829	0.000000
B	-1.224403	4.022512	0.000000
C	-0.583255	5.399396	0.000000
H	-0.982960	7.527009	0.000000
H	-3.460706	7.294241	0.000000
H	-3.175396	3.138165	0.000000
H	-4.512969	5.037526	0.000000
H	-0.682474	2.948474	0.000000
H	0.498173	5.578436	0.000000
C	-0.259109	-4.486890	0.000000
C	1.162971	-4.374739	0.000000
C	1.761260	-3.131178	0.000000
N	1.003103	-1.991450	0.000000
B	-0.441315	-1.991810	0.000000
C	-1.083768	-3.368253	0.000000
H	-0.686029	-5.496539	0.000000
H	1.792105	-5.266003	0.000000
H	1.510841	-1.109355	0.000000
H	2.846449	-3.009982	0.000000
H	-0.982493	-0.917191	0.000000
H	-2.165447	-3.546122	0.000000
C	-6.328493	0.432623	0.000000
C	-6.213848	-0.989198	0.000000
C	-4.969201	-1.585176	0.000000
N	-3.831017	-0.824727	0.000000
B	-3.833851	0.619737	0.000000
C	-5.211493	1.259487	0.000000
H	-7.338905	0.857715	0.000000
H	-7.104021	-1.619793	0.000000
H	-2.948065	-1.330845	0.000000
H	-4.845786	-2.670092	0.000000
H	-2.760081	1.162161	0.000000
H	-5.391481	2.340830	0.000000

Azaborine Trimer – Mixed Chirality 4:

48

C	5.503838	0.578263	0.000000
C	5.390289	2.000134	0.000000
C	4.146164	2.597136	0.000000
N	3.007351	1.837644	0.000000
B	3.009024	0.393214	0.000000
C	4.386194	-0.247587	0.000000
H	6.513849	0.152356	0.000000
H	6.280961	2.629994	0.000000
H	2.124766	2.344430	0.000000

H	4.023747	3.682141	0.000000
H	1.935098	-0.148684	0.000000
H	4.565473	-1.329025	0.000000
C	-0.578257	5.503841	0.000000
C	-2.000128	5.390301	0.000000
C	-2.597138	4.146180	0.000000
N	-1.837653	3.007362	0.000000
B	-0.393223	3.009026	0.000000
C	0.247587	4.386192	0.000000
H	-0.152343	6.513850	0.000000
H	-2.629982	6.280977	0.000000
H	-2.344445	2.124780	0.000000
H	-3.682144	4.023769	0.000000
H	0.148669	1.935096	0.000000
H	1.329025	4.565465	0.000000
C	0.578257	-5.503841	0.000000
C	2.000128	-5.390301	0.000000
C	2.597138	-4.146180	0.000000
N	1.837653	-3.007362	0.000000
B	0.393223	-3.009026	0.000000
C	-0.247587	-4.386192	0.000000
H	0.152343	-6.513850	0.000000
H	2.629982	-6.280977	0.000000
H	2.344445	-2.124780	0.000000
H	3.682144	-4.023769	0.000000
H	-0.148669	-1.935096	0.000000
H	-1.329025	-4.565465	0.000000
C	-5.503838	-0.578263	0.000000
C	-5.390289	-2.000134	0.000000
C	-4.146164	-2.597136	0.000000
N	-3.007351	-1.837644	0.000000
B	-3.009024	-0.393214	0.000000
C	-4.386194	0.247587	0.000000
H	-6.513849	-0.152356	0.000000
H	-6.280961	-2.629994	0.000000
H	-2.124766	-2.344430	0.000000
H	-4.023747	-3.682141	0.000000
H	-1.935098	0.148684	0.000000
H	-4.565473	1.329025	0.000000

Azaborine Tetramer 1:

48

C	-8.104440	-6.961752	0.000000
C	-6.968498	-7.826247	0.000000
C	-5.693996	-7.298943	0.000000

N	-5.498541	-5.942004	0.000000
B	-6.578668	-4.983402	0.000000
C	-7.973351	-5.578923	0.000000
H	-9.095519	-7.430155	0.000000
H	-7.092989	-8.910125	0.000000
H	-4.530519	-5.631487	0.000000
H	-4.804972	-7.932313	0.000000
H	-6.285292	-3.817999	0.000000
H	-8.887720	-4.976826	0.000000
C	2.021141	2.211285	0.000000
C	0.882613	3.072392	0.000000
C	-0.390206	2.541747	0.000000
N	-0.582057	1.184348	0.000000
B	0.500834	0.228855	0.000000
C	1.893897	0.828044	0.000000
H	3.010913	2.682558	0.000000
H	1.004139	4.156696	0.000000
H	-1.548949	0.870146	0.000000
H	-1.280959	3.172904	0.000000
H	0.211097	-0.937722	0.000000
H	2.809859	0.228385	0.000000
C	-0.520951	-6.223535	0.000000
C	0.515458	-5.245853	0.000000
C	0.203707	-3.901742	0.000000
N	-1.102025	-3.486464	0.000000
B	-2.225470	-4.394092	0.000000
C	-1.864835	-5.868273	0.000000
H	-0.222790	-7.278199	0.000000
H	1.564227	-5.545897	0.000000
H	-1.237105	-2.476642	0.000000
H	0.969769	-3.125171	0.000000
H	-3.329091	-3.909115	0.000000
H	-2.591490	-6.687825	0.000000
C	-5.552720	1.473521	0.000000
C	-6.592219	0.499272	0.000000
C	-6.284513	-0.845788	0.000000
N	-4.980235	-1.265156	0.000000
B	-3.854075	-0.361233	0.000000
C	-4.210130	1.113859	0.000000
H	-5.847307	2.529092	0.000000
H	-7.640046	0.802419	0.000000
H	-4.848360	-2.275364	0.000000
H	-7.053130	-1.619783	0.000000
H	-2.752485	-0.850288	0.000000
H	-3.480962	1.930977	0.000000

Azaborine Tetramer 2:

48

C	5.503838	0.578263	0.000000
C	5.390289	2.000134	0.000000
C	4.146164	2.597136	0.000000
N	3.007351	1.837644	0.000000
B	3.009024	0.393214	0.000000
C	4.386194	-0.247587	0.000000
H	6.513849	0.152356	0.000000
H	6.280961	2.629994	0.000000
H	2.124766	2.344430	0.000000
H	4.023747	3.682141	0.000000
H	1.935098	-0.148684	0.000000
H	4.565473	-1.329025	0.000000
C	-0.578257	5.503841	0.000000
C	-2.000128	5.390301	0.000000
C	-2.597138	4.146180	0.000000
N	-1.837653	3.007362	0.000000
B	-0.393223	3.009026	0.000000
C	0.247587	4.386192	0.000000
H	-0.152343	6.513850	0.000000
H	-2.629982	6.280977	0.000000
H	-2.344445	2.124780	0.000000
H	-3.682144	4.023769	0.000000
H	0.148669	1.935096	0.000000
H	1.329025	4.565465	0.000000
C	0.578257	-5.503841	0.000000
C	2.000128	-5.390301	0.000000
C	2.597138	-4.146180	0.000000
N	1.837653	-3.007362	0.000000
B	0.393223	-3.009026	0.000000
C	-0.247587	-4.386192	0.000000
H	0.152343	-6.513850	0.000000
H	2.629982	-6.280977	0.000000
H	2.344445	-2.124780	0.000000
H	3.682144	-4.023769	0.000000
H	-0.148669	-1.935096	0.000000
H	-1.329025	-4.565465	0.000000
C	-5.503838	-0.578263	0.000000
C	-5.390289	-2.000134	0.000000
C	-4.146164	-2.597136	0.000000
N	-3.007351	-1.837644	0.000000
B	-3.009024	-0.393214	0.000000
C	-4.386194	0.247587	0.000000
H	-6.513849	-0.152356	0.000000

H	-6.280961	-2.629994	0.000000
H	-2.124766	-2.344430	0.000000
H	-4.023747	-3.682141	0.000000
H	-1.935098	0.148684	0.000000
H	-4.565473	1.329025	0.000000

Azaborine Tetramer 3:

48

C	4.665805	1.590334	0.000000
C	4.554643	3.012409	0.000000
C	3.311506	3.611525	0.000000
N	2.171398	2.853935	0.000000
B	2.170719	1.409501	0.000000
C	3.546761	0.766344	0.000000
H	5.675131	1.162738	0.000000
H	5.446392	3.640810	0.000000
H	1.289648	3.362215	0.000000
H	3.190884	4.696750	0.000000
H	1.095847	0.869347	0.000000
H	3.724096	-0.315437	0.000000
C	-1.408989	6.517097	0.000000
C	-2.830835	6.403674	0.000000
C	-3.427988	5.159684	0.000000
N	-2.668749	4.020829	0.000000
B	-1.224403	4.022512	0.000000
C	-0.583255	5.399396	0.000000
H	-0.982960	7.527009	0.000000
H	-3.460706	7.294241	0.000000
H	-3.175396	3.138165	0.000000
H	-4.512969	5.037526	0.000000
H	-0.682474	2.948474	0.000000
H	0.498173	5.578436	0.000000
C	-0.259109	-4.486890	0.000000
C	1.162971	-4.374739	0.000000
C	1.761260	-3.131178	0.000000
N	1.003103	-1.991450	0.000000
B	-0.441315	-1.991810	0.000000
C	-1.083768	-3.368253	0.000000
H	-0.686029	-5.496539	0.000000
H	1.792105	-5.266003	0.000000
H	1.510841	-1.109355	0.000000
H	2.846449	-3.009982	0.000000
H	-0.982493	-0.917191	0.000000
H	-2.165447	-3.546122	0.000000
C	-6.328493	0.432623	0.000000

C	-6.213848	-0.989198	0.000000
C	-4.969201	-1.585176	0.000000
N	-3.831017	-0.824727	0.000000
B	-3.833851	0.619737	0.000000
C	-5.211493	1.259487	0.000000
H	-7.338905	0.857715	0.000000
H	-7.104021	-1.619793	0.000000
H	-2.948065	-1.330845	0.000000
H	-4.845786	-2.670092	0.000000
H	-2.760081	1.162161	0.000000
H	-5.391481	2.340830	0.000000

Azaborine Tetramer 4:

48

C	4.736380	-1.916734	0.000000
C	5.518899	-0.724668	0.000000
C	4.903465	0.509347	0.000000
N	3.535629	0.612068	0.000000
B	2.655931	-0.534044	0.000000
C	3.347642	-1.882815	0.000000
H	5.271482	-2.873248	0.000000
H	6.608718	-0.772646	0.000000
H	3.174753	1.566295	0.000000
H	5.471318	1.441730	0.000000
H	1.463664	-0.333469	0.000000
H	2.819866	-2.839310	0.000000
C	-0.604335	5.066402	0.000000
C	-1.450586	3.917388	0.000000
C	-0.907739	2.650398	0.000000
N	0.454072	2.473402	0.000000
B	1.394750	3.570748	0.000000
C	0.779984	4.955932	0.000000
H	-1.086979	6.050592	0.000000
H	-2.535309	4.030123	0.000000
H	0.762307	1.502253	0.000000
H	-1.523374	1.751888	0.000000
H	2.575494	3.315834	0.000000
H	1.371294	5.876963	0.000000
C	-0.402084	-5.845726	0.000000
C	0.444429	-4.696910	0.000000
C	-0.098119	-3.429795	0.000000
N	-1.459893	-3.252515	0.000000
B	-2.400820	-4.349642	0.000000
C	-1.786371	-5.734954	0.000000
H	0.080338	-6.830022	0.000000

H	1.529124	-4.809916	0.000000
H	-1.767874	-2.281304	0.000000
H	0.517704	-2.531420	0.000000
H	-3.581503	-4.094473	0.000000
H	-2.377888	-6.655847	0.000000
C	-5.742492	1.137912	0.000000
C	-6.525477	-0.053728	0.000000
C	-5.910619	-1.287909	0.000000
N	-4.542924	-1.391238	0.000000
B	-3.662782	-0.245616	0.000000
C	-4.353873	1.103376	0.000000
H	-6.277137	2.094587	0.000000
H	-7.615195	-0.005291	0.000000
H	-4.182566	-2.345586	0.000000
H	-6.478830	-2.219979	0.000000
H	-2.470694	-0.446755	0.000000
H	-3.825738	2.059565	0.000000