

Electronic Supplementary Information

Title: B-H_b... π Interaction in Benzene-borazine Sandwich and Multidecker Complexes: A DFT Study

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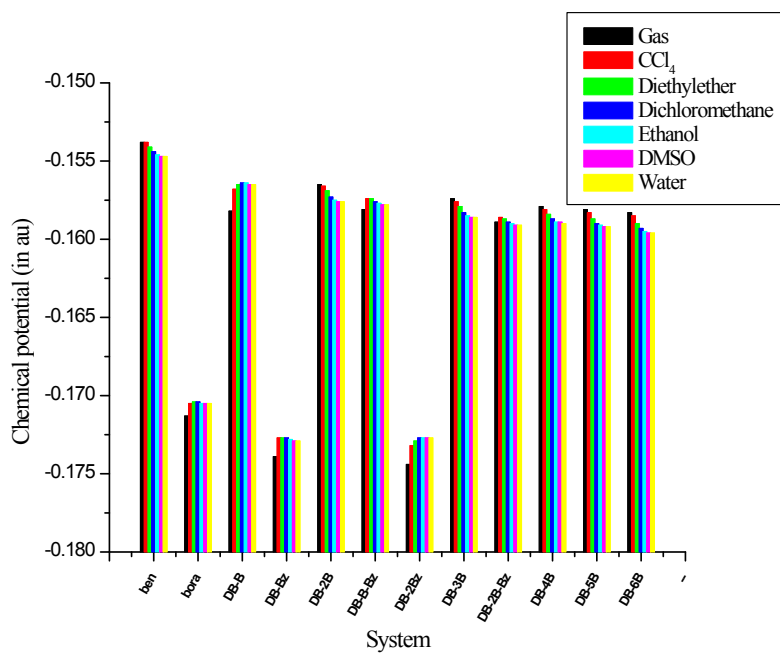
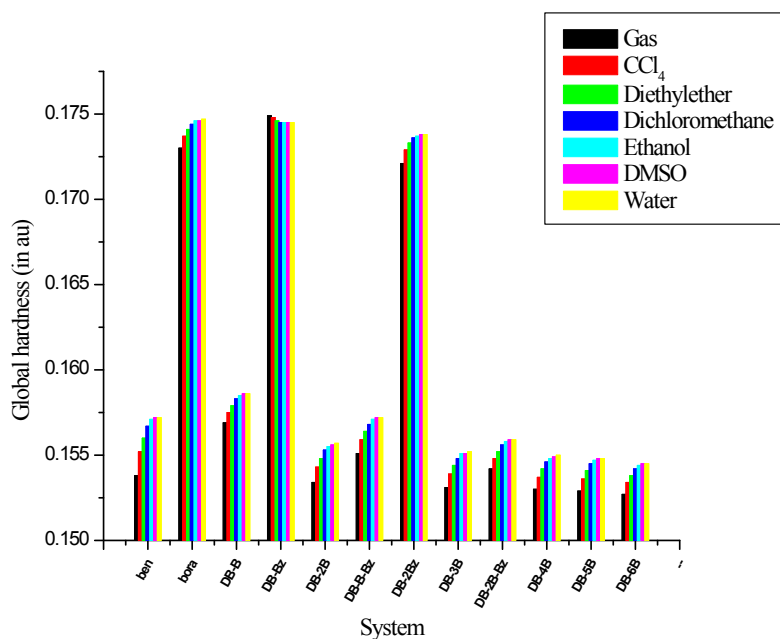
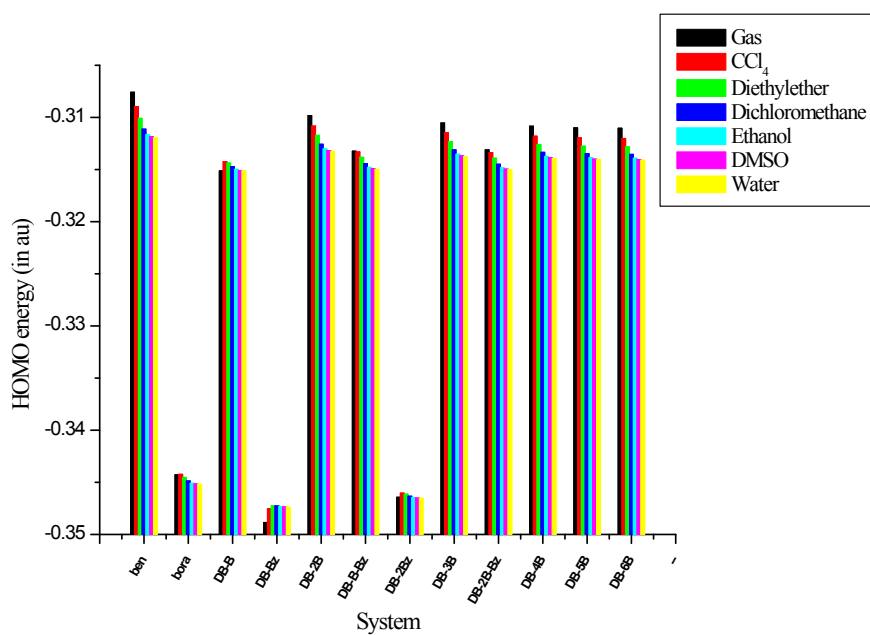
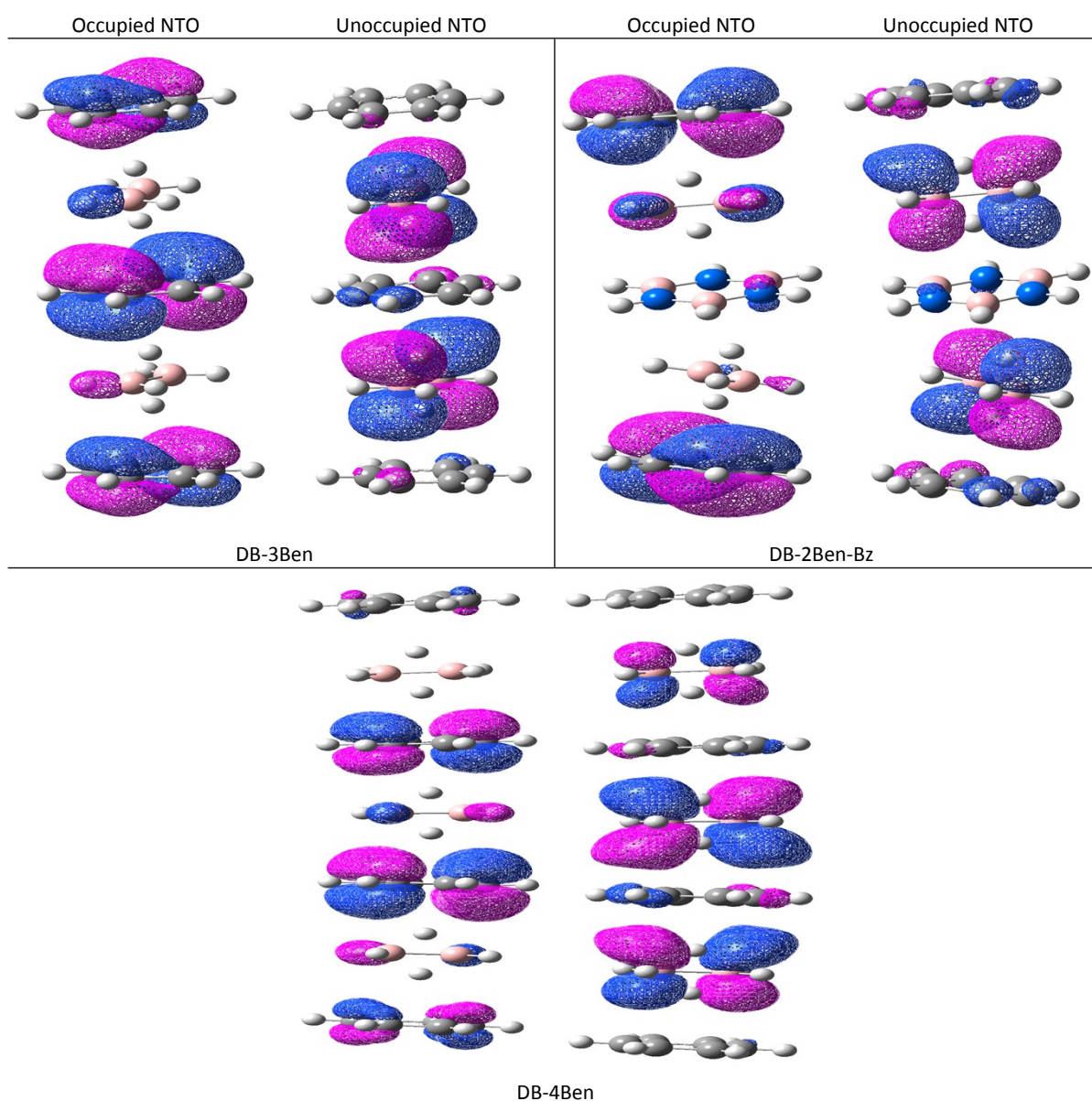


Figure S1 contd...



Supplement Figure S1: Solvent phase homo energy, global hardness and chemical potential of the complexes obtained at M06-2X/6-31++G(d,p) level of theory.



Supplement Figure S2: Shapes of the highest occupied and lowest unoccupied natural transition orbitals (NTO)s of the complexes obtained at M06-2X/6-31++G(d,p) level of theory.

Supplement Table S1:

Cartesian coordinates of optimized DB-B complex:

H,-2.2275334928,-1.7595873001,0.2747552083
B,-2.2231535828,-0.7717322383,-0.3868996634
H,-3.1989852784,0.0123586814,0.018232212
B,-2.2130290249,0.7880779181,0.4146116549
H,-2.2147168514,1.7758790123,-0.2471244255
H,-2.2111280642,0.8255246208,1.6030924766
H,-2.2318858156,-0.8090346205,-1.5753343798
H,-1.2441799845,0.003878154,0.0099439719
C,1.1784894873,1.190408623,0.7084072159
C,1.1830425614,-0.0302273193,1.3841100401
C,1.1723132514,-1.2251706132,0.6653348373
C,1.1584828306,-1.1996833241,-0.7298615713
C,1.1607658164,0.0209351379,-1.4056238437
C,1.1700005991,1.2158464714,-0.6868513028
H,1.1776288681,2.1205672718,1.2683511995
H,1.1848098567,-0.0491468661,2.4694959133
H,1.1658714535,-2.1749892142,1.1910237839
H,1.1420937647,-2.1297932775,-1.2896636409
H,1.14504918,0.0398941044,-2.4909000862
H,1.1616506593,2.1657129855,-1.2124256404

Cartesian coordinates of optimized DB-Bz complex:

H,-2.78448221,-1.4835592358,0.9165264003
B,-2.4536644356,-0.8766062844,-0.0504514433
H,-3.383783538,0.0094231808,-0.3323890234
B,-2.45284402,0.8781092459,-0.0020385229
H,-2.1179328543,1.4764011284,-0.9738249187
H,-2.7834306877,1.4310521168,0.9969531122
H,-2.1182932176,-1.4204025254,-1.0535502658
H,-1.5320707928,-0.0081458429,0.2870163644
H,0.9050783405,2.1133125267,1.1865368808
H,0.9428651553,0.0394294224,2.6551341234
H,0.9100242841,-2.0772660479,1.2508469439
H,0.9107153481,-2.3118322453,-1.2783291228
H,0.8983467767,-0.0377864235,-2.4095519308

H,0.9038446523,2.2697147494,-1.3487091081
B,0.9262146801,0.0217678377,1.4630364528
B,0.9092700866,-1.2695952962,-0.6991100106
B,0.905817228,1.2461011303,-0.7378858156
N,0.9033255542,1.2308369877,0.6960162106
N,0.9054582574,-1.2101971398,0.7335452656
N,0.9094943928,-0.0220712849,-1.4002725921

Cartesian coordinates of optimized DB-2B complex:

C,3.4088133468,-1.264004199,-0.5866891936
C,3.4087443312,-0.1231781349,-1.3895284987
C,3.4027857671,1.1417079204,-0.8023474571
C,3.4014839839,1.265990567,0.587391381
C,3.4070040986,0.1251548904,1.3901051991
C,3.4084205208,-1.1396391225,0.8030174093
H,3.4018051344,-2.2490548,-1.043115802
H,3.4016727639,-0.2202389996,-2.4706815917
H,3.3908672067,2.0299919343,-1.4262336879
H,3.3883066801,2.2509586661,1.043848494
H,3.3990114584,0.2223111764,2.4712401549
H,3.4012018414,-2.0280322193,1.4268278675
H,0.0062573002,1.4496014865,1.039915036
B,0.0002584669,0.870735687,-0.0004456756
H,0.9795335537,-0.0033799899,-0.0063622615
B,-0.000339142,-0.8765843702,-0.0003714532
H,-0.0064163833,-1.4550382212,-1.0409627839
H,0.0053827278,-1.455310248,1.0400740718
H,-0.0053820908,1.4491065419,-1.0410869087
H,-0.9795901757,-0.0027036696,0.0060286763
C,-3.4086136807,-1.2637498748,0.587480566
C,-3.4083875816,-0.1228077419,1.3901477688
C,-3.4027434897,1.1419852368,0.8027831234
C,-3.4019136252,1.2660706681,-0.5869640646
C,-3.4075885589,0.1251264929,-1.3895236454
C,-3.4086910821,-1.1395867697,-0.802248953
H,-3.4013315844,-2.2487350866,1.0440442476
H,-3.4009297081,-0.2197287409,2.4713111145
H,-3.3906748505,2.0303594349,1.4265399201
H,-3.3889717127,2.2509772575,-1.0435635708

H,-3.3999427541,0.2221235262,-2.4706751023
H,-3.401569762,-2.0280702982,-1.4259313801

Cartesian coordinates of optimized DB-B-Bz complex:

C,3.2093036766,1.2990325934,0.6822273837
C,3.1238394102,0.159593973,1.482298526
C,3.2652241176,-1.1051330532,0.9116652969
C,3.4965645814,-1.2299330865,-0.4589512228
C,3.587776773,-0.0902935351,-1.2579757966
C,3.442519977,1.1743423832,-0.6879261819
H,3.0873287087,2.2829309455,1.1246500145
H,2.9365834293,0.2575863147,2.5471213585
H,3.1899204911,-1.9927486693,1.5322044335
H,3.6006954937,-2.2145644693,-0.904269632
H,3.7616976725,-0.1885744503,-2.3250258355
H,3.5011896659,2.061333767,-1.3110856387
H,0.1684165727,-1.4956198371,-1.497470445
B,0.0129121256,-0.9425384496,-0.4554807919
H,0.9708750647,-0.0619555391,-0.2945789871
B,-0.007578266,0.8061264249,-0.4126500231
H,-0.1710928107,1.3544378826,0.631377748
H,0.1337571209,1.4143173016,-1.4256158699
H,-0.1387358941,-1.5453184387,0.5599939681
H,-0.9657913636,-0.0772298366,-0.5779410624
H,-3.4301286693,2.205413964,-0.9258820015
H,-3.8299959034,0.2528481662,-2.502019106
H,-3.6660158581,-1.9640807836,-1.2732312262
H,-3.2369537141,-2.3912016454,1.1931046856
H,-2.9096252961,-0.2121737783,2.4568544597
H,-2.9849042231,2.1680128644,1.5754020133
B,-3.6086323375,0.1439346744,-1.3350832865
B,-3.2843271223,-1.3082176686,0.6959530532
B,-3.1443569954,1.1948641046,0.9050784476
N,-3.3934920488,1.2891121668,-0.5036406475
N,-3.5307198006,-1.1399120525,-0.7061478019
N,-3.0987495777,-0.1191712331,1.4697521677

Cartesian coordinates of optimized DB-2Bz complex:

H,-2.9914321974,-2.4325933653,1.2255160406
H,-2.630040654,-0.2441864121,2.4642841033
H,-2.8550690379,2.1323466425,1.5987289722
H,-3.51071213,2.156151901,-0.8561402615
H,-3.9784114426,0.1912714643,-2.39888013
H,-3.6379894145,-2.0186862556,-1.1951887129
H,-0.0673511501,1.4679550551,-1.7518406149
B,-0.0359490335,0.8818451305,-0.7172334512
H,-0.9767261654,-0.0318243735,-0.7175273648
B,0.0346761497,-0.868217585,-0.724017724
H,0.0627926428,-1.4426254801,0.3187828757
H,0.0489273791,-1.4469780515,-1.7631584834
H,-0.04764166,1.4486630125,0.3300654358
H,0.9757675115,0.0456980043,-0.734474332
H,3.5012014669,-2.1627792996,-0.8537246255
H,3.98087097,-0.201855416,-2.3977094455
H,3.6513324058,2.0109007735,-1.1964123627
H,3.0038825958,2.4305913805,1.2232011606
H,2.6288861787,0.2451694575,2.4634127151
H,2.8421169827,-2.133205252,1.600088718
B,3.6573911795,-0.097733863,-1.2545831577
B,3.1217186288,1.3487358735,0.7363405927
B,3.0318887184,-1.157346924,0.9420868923
N,3.4021381936,-1.247018276,-0.4401820911
N,3.4893706224,1.1845305929,-0.6394390172
N,2.9012703463,0.1559604279,1.495573946
N,-2.9015209942,-0.1572589593,1.4959735776
N,-3.481200156,-1.1908580304,-0.6389081171
N,-3.4075933053,1.2413274587,-0.441490558
B,-3.038828295,1.1549105406,0.9413289064
B,-3.114607545,-1.3518904025,0.7374729755
B,-3.6554877911,0.0899112307,-1.2554024622

Cartesian coordinates of optimized DB-3B complex:

C,-6.7462099629,1.2239173684,-0.8790561273
C,-6.804383269,-0.048348708,-1.4464624535
C,-6.8711237128,-1.1752154278,-0.6266987872

C,-6.8850774075,-1.0290264676,0.7610252435
C,-6.8275983611,0.2433274051,1.3284463649
C,-6.7553287572,1.3699207446,0.5087158661
H,-6.6817434889,2.1005400791,-1.5162015584
H,-6.7875486556,-0.1628950462,-2.5258050762
H,-6.9066996777,-2.1664304668,-1.0682583031
H,-6.9320158771,-1.9065748873,1.3984605557
H,-6.82843967,0.3570412849,2.4080105362
H,-6.6991201145,2.3601283925,0.9504806482
H,-3.4559463068,-1.7617951661,0.4882221363
B,-3.433098935,-0.8746649436,-0.3050588534
H,-4.3917823395,-0.0252693894,-0.0203841869
B,-3.3921673786,0.7768159409,0.2662981669
H,-3.3680241468,1.6626535971,-0.5283041407
H,-3.3885957654,0.9845585764,1.4383781271
H,-3.4353107155,-1.0802023366,-1.4775378663
H,-2.4333716754,-0.074980995,-0.0169118553
C,0.0041820676,1.074305156,0.7846902682
C,0.0006900118,-0.1852860755,1.3865877695
C,0.0024854685,-1.334700831,0.5970985553
C,0.0113450673,-1.2256146598,-0.7946555076
C,0.016154773,0.0340158661,-1.3965242528
C,0.0107726341,1.1833429184,-0.6070380797
H,0.0013221909,1.9691910603,1.3993089176
H,-0.0041265932,-0.2692713301,2.4688423289
H,-0.0014525405,-2.3145732086,1.0639849387
H,0.0143948744,-2.1204992766,-1.4092691381
H,0.0230264848,0.1180967426,-2.4787516105
H,0.0131091816,2.1632402045,-1.0738759236
H,3.4615927298,-1.837735931,-0.1426746184
B,3.4430909269,-0.7206800826,-0.5539252079
H,2.4494147185,-0.0768050038,0.0120724942
B,3.4145131437,0.60522723,0.5846235004
H,3.3940232878,1.7214134695,0.1712439346
H,3.413688344,0.3678999283,1.7509555555
H,3.4425725226,-0.4809809449,-1.7197642673
H,4.4081319175,-0.0407696654,0.0195229706
C,6.7719457226,1.2014447217,-0.8218533684
C,6.8264181803,-0.0706778863,-1.3901021496
C,6.8847358159,-1.198903225,-0.571020911

C,6.891344308,-1.0541566937,0.8165429338
C,6.8340602639,0.21791746,1.3848740732
C,6.7728672373,1.3459413936,0.5657497811
H,6.7159605552,2.0788493264,-1.4586986109
H,6.8147220759,-0.1841017934,-2.4696537454
H,6.9190495839,-2.1897336618,-1.0134817141
H,6.9316146908,-1.9323346178,1.4535410674
H,6.8279521154,0.3304688905,2.4645678848
H,6.718277227,2.3358391446,1.0083287748

Cartesian coordinates of optimized DB-2B-Bz complex:

C,-6.8112561968,-0.5879955023,1.2858011931
C,-6.9538151644,0.7374018365,0.8770249941
C,-6.8277292565,1.0679181716,-0.4723619053
C,-6.5650420406,0.0718191706,-1.4137438828
C,-6.424152009,-1.2539198125,-1.0051004081
C,-6.544438151,-1.5836264024,0.3450320582
H,-6.8981619706,-0.8447598614,2.3370232865
H,-7.1503698565,1.5138547359,1.6097705047
H,-6.9278002387,2.1013586986,-0.7897736824
H,-6.4616420908,0.3309507531,-2.4628917924
H,-6.212555483,-2.028270779,-1.7359574416
H,-6.4251872917,-2.6142944705,0.6648293752
H,-3.2671662139,1.069253251,-1.2139080622
B,-3.42791607,1.0222147894,-0.0350469708
H,-4.3157107409,0.0966441976,0.2425463303
B,-3.2877175324,-0.5220381005,0.7753690518
H,-3.435821547,-0.5751289595,1.9548238035
H,-3.0355187824,-1.489167787,0.128676839
H,-3.6694543107,1.9950562685,0.6057951464
H,-2.4013240539,0.4073166407,0.5038004671
H,-0.0251064093,-2.3441118509,-0.1625422199
H,-0.2831873021,-0.8015757331,-2.1654701043
H,-0.3073924201,1.7384196882,-2.2301564932
H,0.0216378516,2.7149357442,0.0923093063
H,0.3283048829,1.5032462174,2.3047575559
H,0.2580953926,-1.0161226149,1.9837104778
H,3.7071693061,1.9985434504,-0.5313685502
B,3.4217545139,1.0014219134,0.0517966456

H,2.4153143695,0.4259470375,-0.5640165166
B,3.3026958281,-0.5034039575,-0.8327602521
H,3.0057600087,-1.4940083579,-0.2428152746
H,3.5099122557,-0.5070539497,-2.0043769122
H,3.2035933795,0.9978377786,1.2222803233
H,4.3102718528,0.0756667051,-0.223745284
C,6.4388607201,-0.7678827766,1.3803703971
C,6.6552781417,0.5990568516,1.2063692526
C,6.9039414076,1.1094719569,-0.0684353616
C,6.9339302788,0.253265015,-1.1689441644
C,6.7118178593,-1.1128150485,-0.9956853035
C,6.4652359788,-1.6237704217,0.279271445
H,6.2414573625,-1.1644767413,2.3715195749
H,6.6254227072,1.2665716248,2.0619891763
H,7.0655149445,2.1743599635,-0.2045551923
H,7.1180712222,0.6518668769,-2.1617970326
H,6.7238500197,-1.7775688667,-1.8538535353
H,6.2871492731,-2.6862991152,0.4131594366
B,-0.168651943,1.0889859836,-1.2401432901
B,0.1804565398,0.959985091,1.2542286038
B,-0.0144474756,-1.1539361051,-0.103132023
N,0.0123655314,1.7064673949,0.0412958314
N,-0.1568906327,-0.3417699861,-1.275443929
N,0.1419085555,-0.4664596061,1.1447665079

Cartesian coordinates of optimized DB-4B complex:

C,-6.9025813015,-1.4112367438,0.0818404017
C,-6.7882549509,-0.8396984462,-1.1861304006
C,-6.7019740656,0.5453181261,-1.3211724456
C,-6.72759739,1.3594757907,-0.1885066303
C,-6.8457894673,0.7883099743,1.0792220301
C,-6.934418919,-0.5967927036,1.2140821188
H,-6.9609975831,-2.4901993222,0.1879765621
H,-6.7569658839,-1.4743298938,-2.0662768966
H,-6.6025776853,0.9899204972,-2.3065325359
H,-6.648584989,2.4372502609,-0.2934770345
H,-6.8593951498,1.4218436935,1.9606009623
H,-7.0183892979,-1.042223387,2.200511474
H,-3.3329788706,1.3669938383,-0.7124307953

B,-3.3881332306,0.6659288656,0.2478714637
H,-4.4011468015,-0.158991831,0.1176421983
B,-3.4571702639,-1.0666127683,0.0275090548
H,-3.5106084479,-1.7726400106,0.9844298145
H,-3.4481925096,-1.5073880722,-1.0783061067
H,-3.3947328036,1.112354819,1.351561324
H,-2.4444105547,-0.2434853213,0.1662899775
C,0.0348804838,-0.6578651741,1.4208859872
C,0.0535009786,0.6882771781,1.0559405406
C,0.0147477333,1.0458371857,-0.2933696439
C,-0.0424705768,0.0575016876,-1.2764745889
C,-0.061075729,-1.2883967546,-0.911670194
C,-0.0228051621,-1.6461692368,0.4378249393
H,0.0654435598,-0.9365239269,2.4695463338
H,0.1006658465,1.4582650551,1.8196997735
H,0.0289643837,2.093491869,-0.5776372279
H,-0.0731593638,0.3363599748,-2.3250693362
H,-0.1084134275,-2.0583340908,-1.6754561707
H,-0.037547141,-2.693823168,0.7220730711
H,3.3690349119,1.2673875839,-0.8394718231
B,3.3988794269,0.5360205241,0.099002236
H,2.4349243908,-0.3485987518,-0.021301398
B,3.4289305078,-1.1913236078,-0.1698667382
H,3.4590468909,-1.9212101571,0.7697995226
H,3.4191676501,-1.6037009791,-1.2864565121
H,3.4084696571,0.9473272296,1.2159289716
H,4.3928375452,-0.3094771713,-0.05263558
C,6.8481308874,-0.5202284842,1.2960254679
C,6.7689202735,0.8225546934,0.928108302
C,6.7525765314,1.1758118193,-0.422692507
C,6.8115189487,0.1859168318,-1.4044474586
C,6.8874573432,-1.1571516495,-1.0365862769
C,6.9075857338,-1.5101311791,0.3143145983
H,6.862588279,-0.7958361714,2.3458363055
H,6.7207523441,1.5937964919,1.6905578848
H,6.6931730178,2.2212338748,-0.709489725
H,6.7986117699,0.4617602125,-2.4542276652
H,6.934566132,-1.9284121995,-1.7990905075
H,6.9682153577,-2.5554521641,0.6011987723
H,10.1565998161,1.2501554103,-1.3937559592

B,10.1766556848,0.910043067,-0.2533126384
H,9.2683322136,-0.0208337255,-0.0720302321
B,10.3126660875,-0.7906648435,0.1258548117
H,10.3310815251,-1.1291316221,1.2667639572
H,10.3829156256,-1.5789251271,-0.7635986907
H,10.1046172587,1.6969548253,0.6370641061
H,11.2210414052,0.1385797542,-0.0579078624
C,13.619647627,0.0147271706,1.3710459839
C,13.5041405893,1.3547879499,1.0041294827
C,13.517153893,1.711809206,-0.3446404358
C,13.6504505198,0.7289107662,-1.3258824667
C,13.765369503,-0.6114009471,-0.9589180329
C,13.7473801705,-0.9688947753,0.3897237352
H,13.5991554729,-0.2648519957,2.4198459248
H,13.3922780583,2.1194888915,1.7664579116
H,13.4175880687,2.7542407696,-0.6314079674
H,13.6544684932,1.0069499502,-2.3752948881
H,13.860168017,-1.3777446728,-1.7219806188
H,13.8265019518,-2.0132537627,0.6758059897

Cartesian coordinates of optimized DB-5B complex:

C,13.6091662562,0.0715110946,1.3620598786
C,13.5407401117,-1.2701716476,0.9893089969
C,13.5718373216,-1.6209199949,-0.3608032349
C,13.6759817892,-0.630060906,-1.3374894615
C,13.7437359725,0.7119106217,-0.9646519012
C,13.7078122833,1.0629289738,0.3852903121
H,13.5747775414,0.3460063628,2.4118450811
H,13.4512514964,-2.0413404911,1.7480870305
H,13.5089105556,-2.664970925,-0.6520431595
H,13.6938977054,-0.9035206254,-2.3879562413
H,13.8159188165,1.484196889,-1.7242138564
H,13.7502883659,2.1082011464,0.6758392607
H,10.1902191234,-1.2884288173,-1.4088204452
B,10.2026386172,-0.9387787071,-0.2711553661
H,11.2221810628,-0.1327798165,-0.0860675647
B,10.2849703377,0.7681810746,0.0954164828
H,10.2959673801,1.114101193,1.2341487131
H,10.3269548182,1.5526326088,-0.799169646

H,10.1587551449,-1.7200828793,0.6259390636
H,9.265306812,-0.0364784325,-0.0951792545
C,6.8915545717,1.4462267794,0.1573283725
C,6.8148148721,0.8747216994,-1.1141474556
C,6.7535691053,-0.5114653179,-1.2528973672
C,6.7652504696,-1.3270692649,-0.1200134655
C,6.8396880616,-0.7555205774,1.151569933
C,6.904323599,0.6304602964,1.2901777209
H,6.9414931413,2.5253501022,0.2654726783
H,6.8042954354,1.5099443515,-1.994201055
H,6.6936585379,-0.9566278175,-2.241084458
H,6.7156731267,-2.4062072571,-0.2280770356
H,6.8490586539,-1.3907324777,2.0316570718
H,6.9661683128,1.0755515138,2.2782760449
H,3.368204048,-1.4156104283,-0.6687340861
B,3.390493965,-0.6801933036,0.2668256383
H,4.3952973243,0.1534076643,0.1293950225
B,3.4422516631,1.044694132,-0.0138001004
H,3.4646954013,1.7835682926,0.9191440944
H,3.4539014119,1.4462010491,-1.1341881897
H,3.3780554001,-1.0858940898,1.3857846998
H,2.4376103938,0.2121753538,0.1292919559
C,-0.0445004424,0.6230747365,1.3716752923
C,-0.0628909639,-0.7215461425,1.0010324021
C,-0.0172757536,-1.0736034133,-0.3495286356
C,0.0470319876,-0.081328732,-1.3281087659
C,0.065519389,1.2631609571,-0.9575550627
C,0.0199938494,1.6153351462,0.3931372979
H,-0.0802414798,0.8974503839,2.4212968329
H,-0.1153884958,-1.4945368902,1.7614376829
H,-0.032176671,-2.1200676098,-0.6381142782
H,0.0828576324,-0.3558416917,-2.3776871879
H,0.1182238186,2.0361221697,-1.7179671864
H,0.035042118,2.6617963597,0.6817231693
H,-3.3733496698,-1.3017545049,-0.887660523
B,-3.4026271511,-0.559630029,0.0424640247
H,-2.4384031095,0.3232017077,-0.0888204168
B,-3.4320851951,1.1647498034,-0.2451412788
H,-3.4613798134,1.9042823415,0.6870676774
H,-3.4229057488,1.5654573866,-1.3658912727

H,-3.4115802029,-0.9579194728,1.1640000923
H,-4.3963098968,0.2845354197,-0.1185045074
C,-6.8307070219,0.4922528501,1.2671241241
C,-6.7577292783,-0.8493499749,0.8936417275
C,-6.7614395262,-1.1981915037,-0.4583684661
C,-6.8342749703,-0.2049662344,-1.4359386001
C,-6.903969352,1.1369142529,-1.0625614198
C,-6.9041583787,1.4854369725,0.2896380879
H,-6.8295237369,0.7644816366,2.3179162089
H,-6.6979117504,-1.6229281102,1.6528376505
H,-6.7067961886,-2.2426999118,-0.7493854632
H,-6.8370089177,-0.4774684199,-2.4866723824
H,-6.9625782325,1.9105377291,-1.8218186118
H,-6.9600943177,2.5298479442,0.5807446183
H,-10.178769366,-1.270498592,-1.3713015539
B,-10.1859626072,-0.9237053372,-0.2327198127
H,-9.269724782,0.0020119737,-0.0652876449
B,-10.3071134878,0.7800879446,0.1373577177
H,-10.3126868382,1.1255939692,1.2762774848
H,-10.3807319058,1.5632360392,-0.7562882547
H,-10.1105401125,-1.7057412054,0.6616247821
H,-11.2233368641,-0.144385154,-0.032133873
C,-13.6012032812,-0.0022378548,1.4331084548
C,-13.504855059,-1.3417279814,1.0586843012
C,-13.5387661319,-1.6923438505,-0.2913830444
C,-13.6736333516,-0.7034646866,-1.2664331292
C,-13.7691935578,0.6363054262,-0.891973268
C,-13.7304506571,0.9872985113,0.457895263
H,-13.5647380081,0.2722976673,2.4828042206
H,-13.3921600421,-2.1111028154,1.8161411458
H,-13.4542305791,-2.7344832568,-0.5839681041
H,-13.693586097,-0.9766228885,-2.3169465192
H,-13.8648789174,1.4071235962,-1.650366123
H,-13.7945098909,2.0311429162,0.7495694196

Cartesian coordinates of optimized DB-6B complex:

C,-16.9444641856,1.0623292916,-1.2330651824
C,-17.0528208742,-0.3218844166,-1.1065638267
C,-17.1378860844,-0.9018844054,0.1594311374

C,-17.1205077047,-0.0964942382,1.2988592987
C,-17.013070381,1.2879802977,1.1723050872
C,-16.9221828929,1.8675181791,-0.0935448959
H,-16.8653116937,1.5134130836,-2.2173459136
H,-17.0594361347,-0.949337991,-1.9923518514
H,-17.2119738337,-1.9805653544,0.2585271376
H,-17.1823656874,-0.5488826669,2.2838002472
H,-16.9906212491,1.9142476673,2.0586973289
H,-16.8276227686,2.9446587033,-0.19213844
H,-13.7107235712,-1.0066506365,1.3951095685
B,-13.6953227911,-0.6218730136,0.2688091232
H,-14.6143967021,0.3040417549,0.124237303
B,-13.5790640114,1.0938262562,-0.0440579892
H,-13.5622486473,1.4747757971,-1.1715184546
H,-13.5164592774,1.8483764607,0.8745901989
H,-13.7559515969,-1.3733908387,-0.65234987
H,-12.6598068437,0.1681087826,0.1062476291
C,-10.1542957891,1.3359379314,-0.3957469798
C,-10.1076369768,0.9753061155,0.9522703109
C,-10.1861231718,-0.3684880766,1.3171551567
C,-10.3084102581,-1.3520229795,0.3347153989
C,-10.3515986307,-0.9916703472,-1.0136759951
C,-10.2761412765,0.3522121483,-1.3783050756
H,-10.0950843972,2.3820931959,-0.6798582986
H,-10.0097513611,1.7411060808,1.7152923255
H,-10.1515396719,-0.650001814,2.3649270532
H,-10.3683393921,-2.3981347121,0.6188218794
H,-10.4483614897,-1.7575640196,-1.7767507319
H,-10.3124222265,0.6340305546,-2.4259437328
H,-6.906931031,-1.8405016388,0.5947353025
B,-6.871194498,-1.0872384431,-0.3262360304
H,-7.8029759466,-0.177159939,-0.1673275475
B,-6.7786597507,0.6299414736,-0.0118150008
H,-6.7428524688,1.386953684,-0.9297693945
H,-6.7530206014,1.0086523294,1.1161836828
H,-6.8967503748,-1.4701720933,-1.4529348229
H,-5.8469640291,-0.2808317409,-0.177280699
C,-3.3422648102,0.204480889,-1.3460210728
C,-3.4019619432,-1.1835733732,-1.2189079598
C,-3.4762282985,-1.7665178569,0.0476975016

C,-3.4841044365,-0.9610668549,1.1870678063
C,-3.4216640462,0.4266481814,1.0599902474
C,-3.3540479143,1.0098768954,-0.2069538148
H,-3.2845965062,0.6573657398,-2.330819955
H,-3.3930562026,-1.8106831269,-2.1049238166
H,-3.525850819,-2.8465215109,0.1457276702
H,-3.5409840793,-1.4140572261,2.17186393
H,-3.4287485251,1.0538364261,1.9459622825
H,-3.3064175421,2.0899683532,-0.3049623325
H,0.0077327882,-2.2373617851,-0.2685444672
B,0.009564909,-1.0912766753,-0.5895592568
H,-0.9797551765,-0.4795931423,0.0181417602
B,-0.0105919507,0.1401175515,0.651019777
H,-0.0087832193,1.2853340973,0.3272392624
H,-0.0255780062,-0.1890172478,1.7947030689
H,0.0247198083,-0.7590383381,-1.732297424
H,0.978587986,-0.475244972,0.0450980981
C,3.4070426636,0.4210645268,-1.0542799451
C,3.4561708544,-0.9673995832,-1.1808045927
C,3.4679430731,-1.7720961771,-0.0403044942
C,3.4244964697,-1.1877621247,1.2263931016
C,3.3652988255,0.200368873,1.3527039074
C,3.3597327434,1.0052657757,0.2122091414
H,3.4028674664,1.046792412,-1.9412165493
H,3.4910417895,-1.4217558889,-2.1660945559
H,3.5112580053,-2.8522815043,-0.1387837775
H,3.4323511092,-1.8133353374,2.1134254832
H,3.3258032788,0.6546415913,2.3378611284
H,3.3169702191,2.0854661594,0.3107248456
H,6.8826937358,-1.0185614371,1.7244687248
B,6.8664223271,-1.0077749167,0.5343311338
H,5.8468206452,-0.2875050891,0.1309716219
B0,6.7835156934,0.5248553808,-0.3022734598
H,6.7673316458,0.5331197174,-1.4923717448
H,6.7448735856,1.5306946086,0.3330062456
H,6.9049160274,-2.0120343536,-0.1034618005
H,7.8032265191,-0.1957889516,0.1050125707
C,10.1914527729,-0.3906539564,-1.3657374869
C,10.3106384375,-1.3737732178,-0.3832646114
C,10.3495844805,-1.0126909369,0.9651886579

C,10.2734016649,0.3316446728,1.3296214698
C,10.1565324234,1.3149496307,0.3469581903
C,10.1137908454,0.9538200637,-1.0011830514
H,10.1583763606,-0.671660514,-2.4136998239
H,10.3707743383,-2.4200345468,-0.6664530233
H,10.4435318233,-1.778184907,1.7291272258
H,10.3058150504,0.6127295645,2.3775719444
H,10.0974602793,2.3612655353,0.630141465
H,10.0187220037,1.7192184507,-1.7651019907
H,13.7209363552,-1.0357712163,1.1313733289
B,13.7053700936,-0.6398996112,0.0089899299
H,12.6638461058,0.1428812525,-0.1518831795
B,13.5754320048,1.0792595356,-0.2787221788
H,13.5575601099,1.4816040946,-1.3988878372
H,13.5044382637,1.8150931499,0.6541894757
H,13.7750820192,-1.3813991302,-0.9196974188
H,14.6170317864,0.2951163662,-0.1263882164
C,16.9342209097,1.8470980901,-0.3387912492
C,17.0803920707,0.8659600761,-1.3199692815
C,17.1724890537,-0.4767352369,-0.9548868609
C,17.1193450443,-0.8382105096,0.3916671025
C,16.9789308759,0.1436243767,1.3730849081
C,16.8856107025,1.4858933499,1.0080366348
H,16.8524182203,2.8915450024,-0.6238631938
H,17.1118981409,1.1475091843,-2.3679845653
H,17.2768147283,-1.2415270429,-1.7182157504
H,17.1807865204,-1.8843233392,0.6757409511
H,16.9311872628,-0.1393394285,2.4201000184
H,16.7642618318,2.2492220701,1.7702606901

Supplement Table S2: BSSE corrected energies (in kcal/mol) of the chosen complexes at different levels of theory.

System	M06-2X/6-31++G(d,p)	ω B97X-D/6-31++G(d,p)	M06-2X/6-311++G(d,p)	ω B97X-D/6-311++G(d,p)
DB-B	0.37	0.36	0.46	0.40
DB-Bz	0.31	0.30	0.18	0.18
DB-2B	0.85	0.83	0.98	0.84
DB-B-Bz	0.77	0.74	0.71	0.63
DB-2Bz	0.68	0.65	0.43	0.41
DB-3B	1.73	1.70	1.89	1.63
DB-2B-Bz	1.63	1.58	1.47	1.33
DB-4B	2.57	2.57	2.75	2.41
DB-5B	3.45	3.44	3.66	3.20
DB-6B	4.37	4.33	4.63	4.03