Supporting Information

Revisiting the Electronic Structure of N_2-Bound cAAC-Borylene at the CASSCF Level: A Detailed Bonding Picture of Borylene-N_2 Interaction

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1. Geometrical Parameters

Table S1. Comparison between key geometrical parameters (distances R and angles) calculated at the B3LYP/[def2-TZVP+def2-SVP] level of theory and that reported from the crystal structure of complexes **1**, **2**, and **3**.

	1 (S = 0)		**2** (S = 0)		**3** (S = 1)	
	B3LYP	Experimental	B3LYP	Experimental	B3LYP	Experimental
R_{NN} (Å)	1.22	1.25	1.28	1.30	1.39 Å	1.40
R_{BN}	1.41	1.42	1.48	1.48	1.41	1.42
	1.39	1.40	1.48	1.48	1.42	1.43
∠BNNB (°)	110.7	113.0	177.4	174.1	165.2	168.5

2. Fractional Orbital Density (FOD) Analysis

A proper electronic structure treatment of the non-dynamic or static correlation is the key to determining the electronic structure of highly conjugated π systems. Fractional Orbital Density (FOD)[1,2] plots provide an efficient way to quantify the extent of non-dynamic correlation present in conjugated systems. Here, we have performed FOD analysis of cAAC-

Borylene bound N_2 (**1** and **5**), CO (**4**), and related complexes (**2**, **3**) complexes to determine the extent of multiconfigurational character present in them. All FOD calculations were performed at the B3LYP/def2-TZVP level of theory. FOD plots along with the FOD index (N_{FOD}) are presented in Figure S1. To account for the dependence of FOD and N_{FOD} on the Hartree-Fock (HF) exchange, TPSS density functional with 0% HF exchange and B3LYP density functional having 20% HF exchange were employed. It is to be noted that a large N_{FOD} with delocalized FOD estimated using any density functional with significant HF exchange (e.g., B3LYP, 20% HF exchange) is conclusive of a high order of non-dynamic correlation in the respective system.

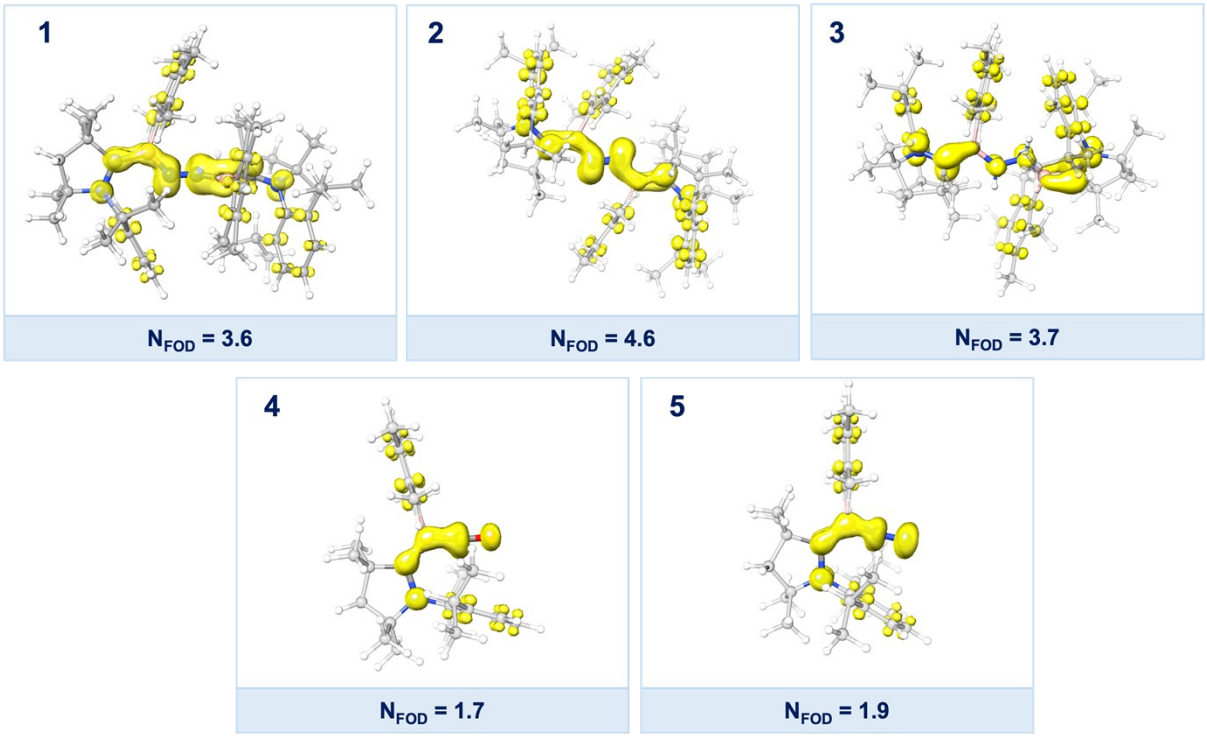

Figure S1. FOD plots and N_{FOD} values calculated at the B3LYP/def2-TZVP level of theory at T_{el} = 9000 K for complexes **1**, **2**, **3**, **4**, and **5** showing strongly correlated electron densities. A contour surface value of σ = 0.005 e Bohr^{-3} is used.

The FOD analysis using B3LYP (20% HF exchange) wavefunction yields a significantly large FOD index N_{FOD} = 3.6 for complex **1** (Figure S1). Most importantly, the FOD plot

reveals that the "strongly correlated" electron density is predominantly delocalized throughout the cAAC–B–N–N–B-cAAC π-orbital framework. This unambiguously suggests that the electronic structure of complex **1** is dominated by strong non-dynamic electron correlation and cannot be accurately described using single-determinant methods, like KS-DFT. Such predominant non-dynamic correlation effect likely stems from a small HOMO-LUMO energy gap, as also explained by Légaré, Rang, Holthausen, Braunschweig and co-workers for cAAC-borylene-(N2)2 systems.[3] In addition to complex **1**, the FOD analysis was also performed for complex **2**, **3**, **4**, and **5**, where a significantly high FOD index N_{FOD} was obtained for all the cases (Figure S1). These results strongly justify the use of the multiconfigurational approach, i.e., the CASSCF method to decode the "true" electronic structure of the cAAC-borylene systems under investigation in this study.

3. Contribution of the Major Configuration in the Ground State

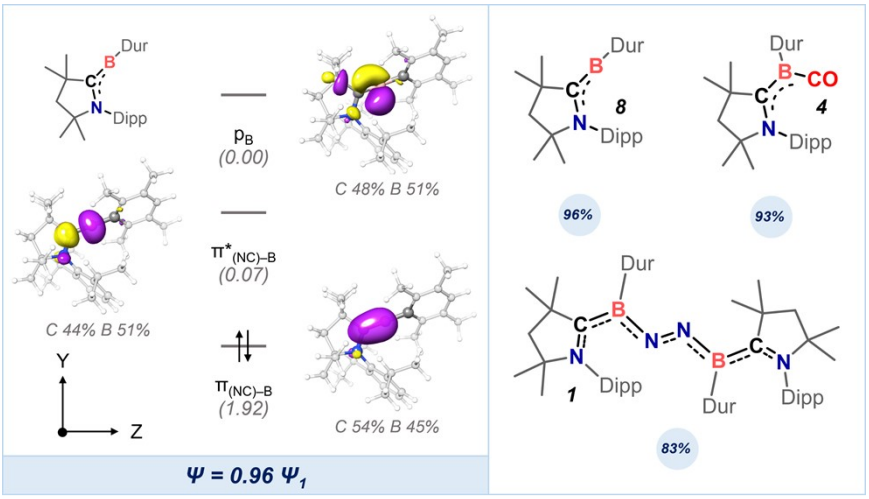

Figure S2. Left panel: Natural orbitals along with their occupation number and atomic orbital contributions obtained from the CASSCF (2,3) calculations for **8**. Right panel: Principal contributions of the predominant electronic configuration in the respective ground state wave functions of complex **1**, **4**, and **8**.

To observe the effect of extended π-conjugation in complex **1** on its ground state wave function, we successively analyzed the CASSCF-derived ground state wavefunction of the building block (**8a**), CO-bound form (**4**), and complex **1** (Figure S2). The contribution of the principal determinant configuration to the ground state wavefunction appears to be 96% in **8a**, which drops to 93% in **4** as **8a** coordinates to CO resulting in enhanced π-conjugation (Figure S2). This value further drops to 83% in **1** due to the extended π-conjugation along the cAAC–B–N–N–B-cAAC moiety (Figure 4, Figure S6), suggesting a high multi-configurational character, where the other determinants contribute >15% in the ground state wavefunction.

4. Natural Bond Orbital (NBO) Analysis

Atomic charges obtained from the Natural Population Analysis (NPA) reveal an increase in negative charge on the NN fragment with simultaneous accumulation of net positive charges on the (NCB)cAAC-Borylene fragments (Figure S3). The NPA analysis along with the presented NBO acceptor-donor interaction suggests the donation of electron density from the cAAC-Borylene fragments to the π^*_{NN} orbitals which finally leads to the activation of the NN bond in complex **1**. The results of this NBO analysis are well in accord with the CASSCF results presented in this work. The NBO calculations were performed using the NBO7.0[4] program interfaced with ORCA 4.1 suit at the B3LYP/6-31G(d,p) level of theory.

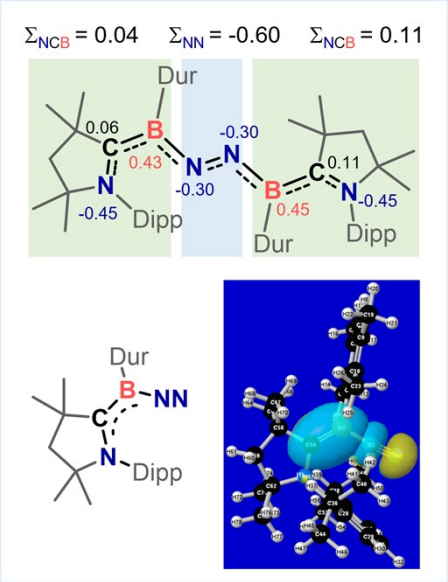

Figure S3. Atomic charges obtained through NPA analysis and NBO plot suggest the interaction of the π_{CB} (donor) and π^*_{NN} (acceptor).

5. Electronic Structure Analysis at the CASSCF Level

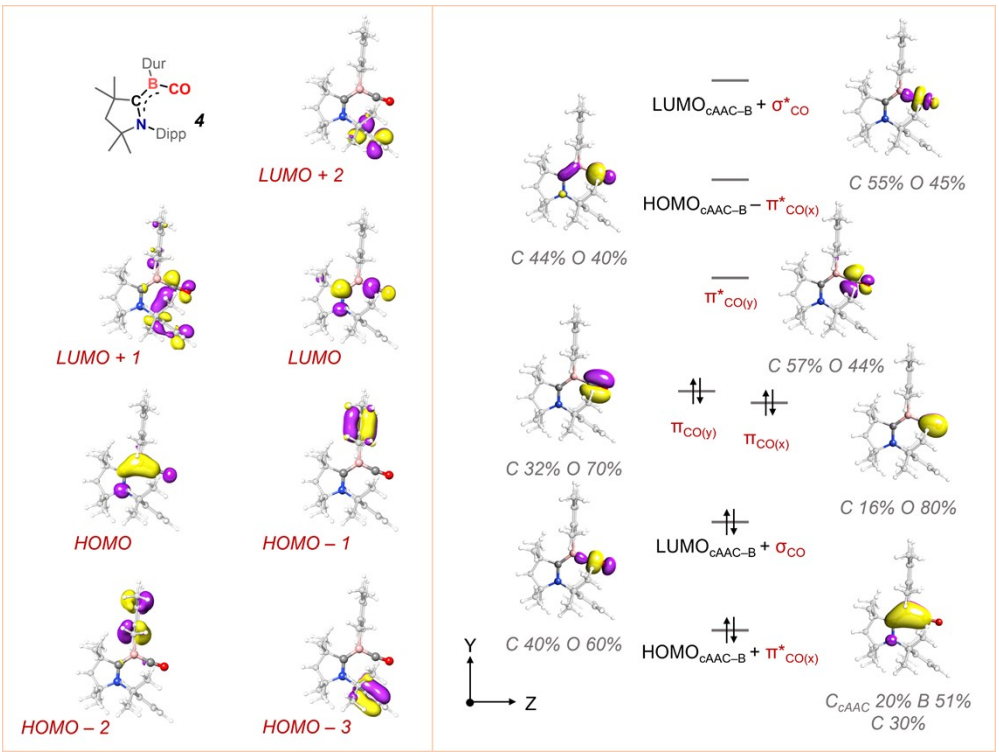

Figure S4. DFT-derived canonical molecular orbitals (left) and natural orbitals obtained from the CASSCF (8,7) calculation (right) for **4**.

The ground-state (S=0) geometry of CO-bound cAAC-Borylene (**4**) was optimized using the hybrid–GGA B3LYP[5,6] density functional with a combination of Ahlrich's triple-ζ def2-TZVP[7] and def2-SVP[8] type basis set. The higher level of basis set was employed to the [(N–C)$_{cAAC}$–B–CO] chain. The DFT-based frontier canonical orbitals of **4** along with the natural orbitals obtained from the CASSCF (8,7) calculation (Figure S4). All the calculations were performed using the ORCA 4.2.1 suite of quantum chemical programs.[9] Although DFT-based frontier orbitals are routinely used to investigate the electronic structure, the presented ones in Figure S4 appear inadequate in providing a complete qualitative picture of the bonding scenario of **4**. Specifically, the DFT-derived frontier orbitals, HOMO and LUMO suggest the presence of π-backdonation interactions. However, a complete picture of the bonding scenario involving all π and σ-type interactions is missing. On the other hand, natural orbitals obtained from the ab initio wave function-based CASSCF method could provide a complete bonding picture with balanced π and σ-type interactions for species **4** (Figure S4, right panel).

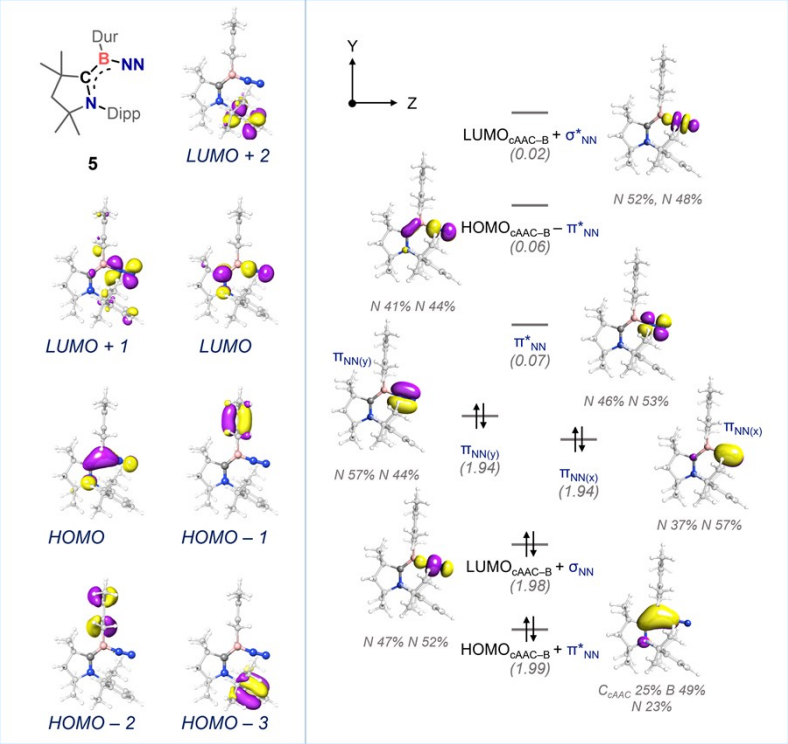

Figure S5. DFT-based canonical molecular orbitals (left) and natural orbitals obtained from the CASSCF (8,7) calculation (right) for **5**.

The ground-state (S=0) geometry of N_2-bound cAAC-Borylene-NN species **5** was optimized using the hybrid–GGA B3LYP[5,6] density functional with a combination of Ahlrich's triple-ζ def2-TZVP[7] and def2-SVP[8] type basis set. The higher level of basis set was employed to the [(N–C)$_{cAAC}$–B–NN] chain. The DFT-derived frontier molecular orbitals for the monomeric N_2-bound cAAC-borylene species **5** also fall short to provide a complete picture of the underlying π and σ-type bonding scenario (Figure S5, left panel). As discussed above, the natural orbitals obtained from the multireference CASSCF method provide a complete bonding picture involving all the crucial π and σ-type bonding and anti-bonding interaction of species **5** (Figure S5).

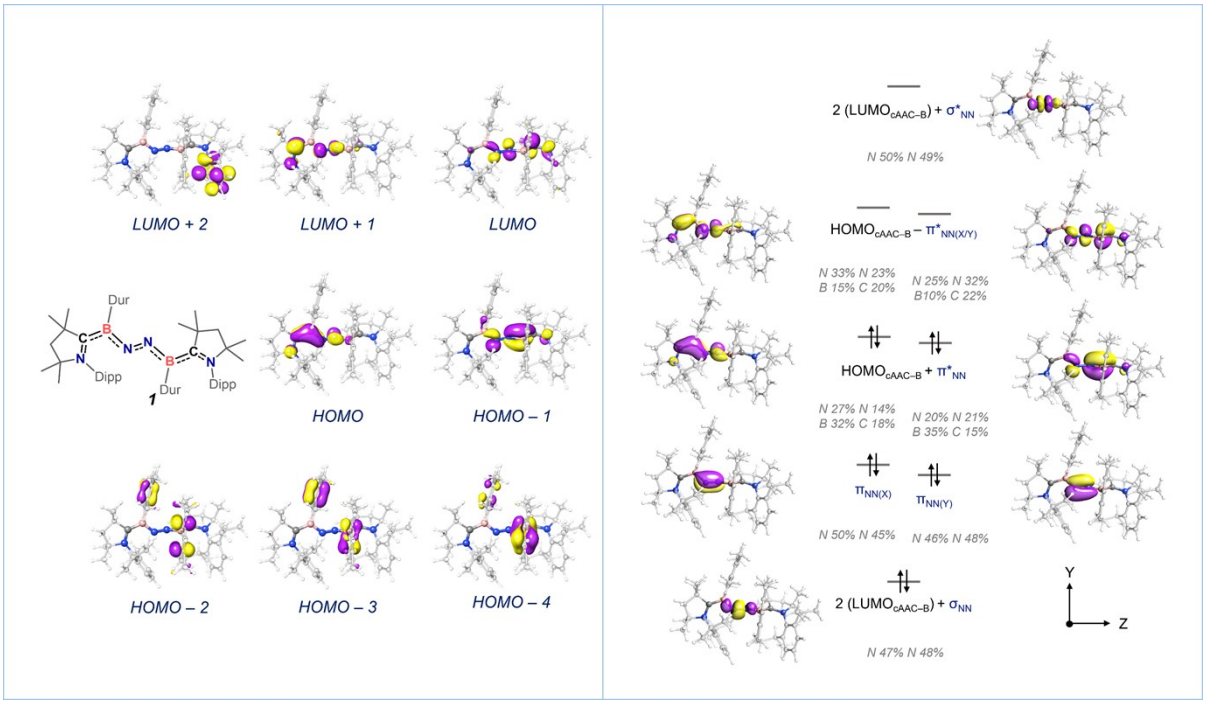

Figure S6. DFT-derived frontier canonical orbitals of **1** (left) and natural orbitals obtained from the CASSCF(10,8) calculation (right).

Analysis of the electronic structure of the highly conjugated N_2-bound cAAC–di-borylene species **1** using DFT-based frontier canonical orbitals could only provide the π-type interactions centered on the B–N–N–B core (Figure S6, left panel), similar to what was observed in the case of species **4** and **5**. However, the remaining crucial π- and σ-type interactions could not be located through the frontier canonical orbitals. A complete qualitative picture of the bonding scenario involving all the crucial π- and σ-type interactions could be obtained through the natural orbitals derived from the CASSCF (10,8) calculation on **1** (Figure S6, right panel).

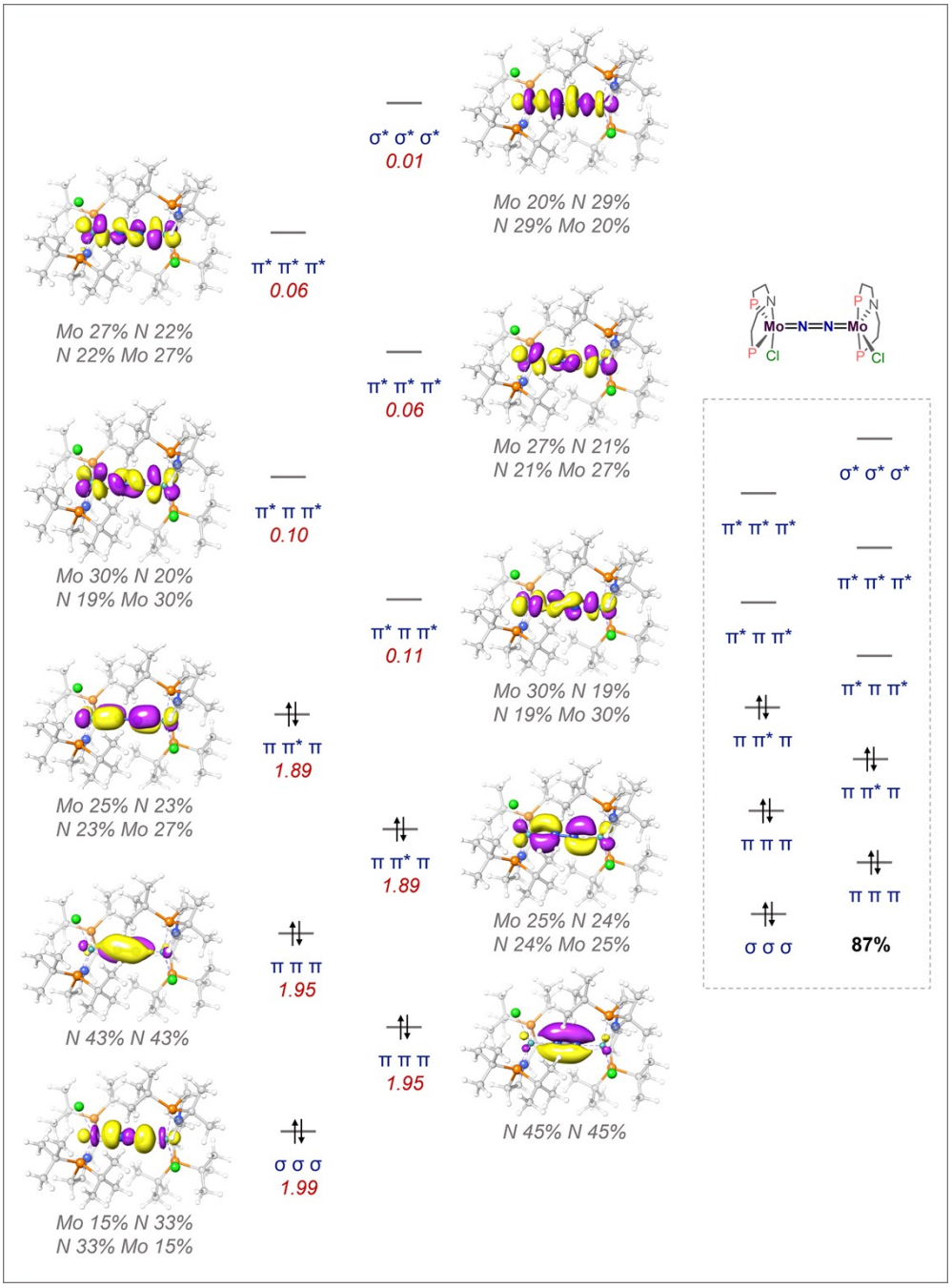

Figure S7. Natural orbitals along with their occupation number and atomic orbital contributions obtained from the CASSCF (10,10) calculations for complex **6**.

The electronic structure of dimeric Mo–N_2 complex (**6**) was investigated at the CASSCF level. A balanced active space consisting of all π-symmetric molecular orbitals along with the lowest energy σ-symmetric orbitals was constructed as presented in Figure S7. The singlet

ground state obtained from the CASSCF(10,10) calculation has a major contribution (87%) from the electronic configuration of$(\sigma\sigma\sigma)^2(\pi\pi\pi)^4,(\pi\pi^*\pi)^4,(\pi^*\pi\pi^*)^0,(\pi^*\pi^*\pi^*)^0(\sigma^*\sigma^*\sigma^*)^0$.

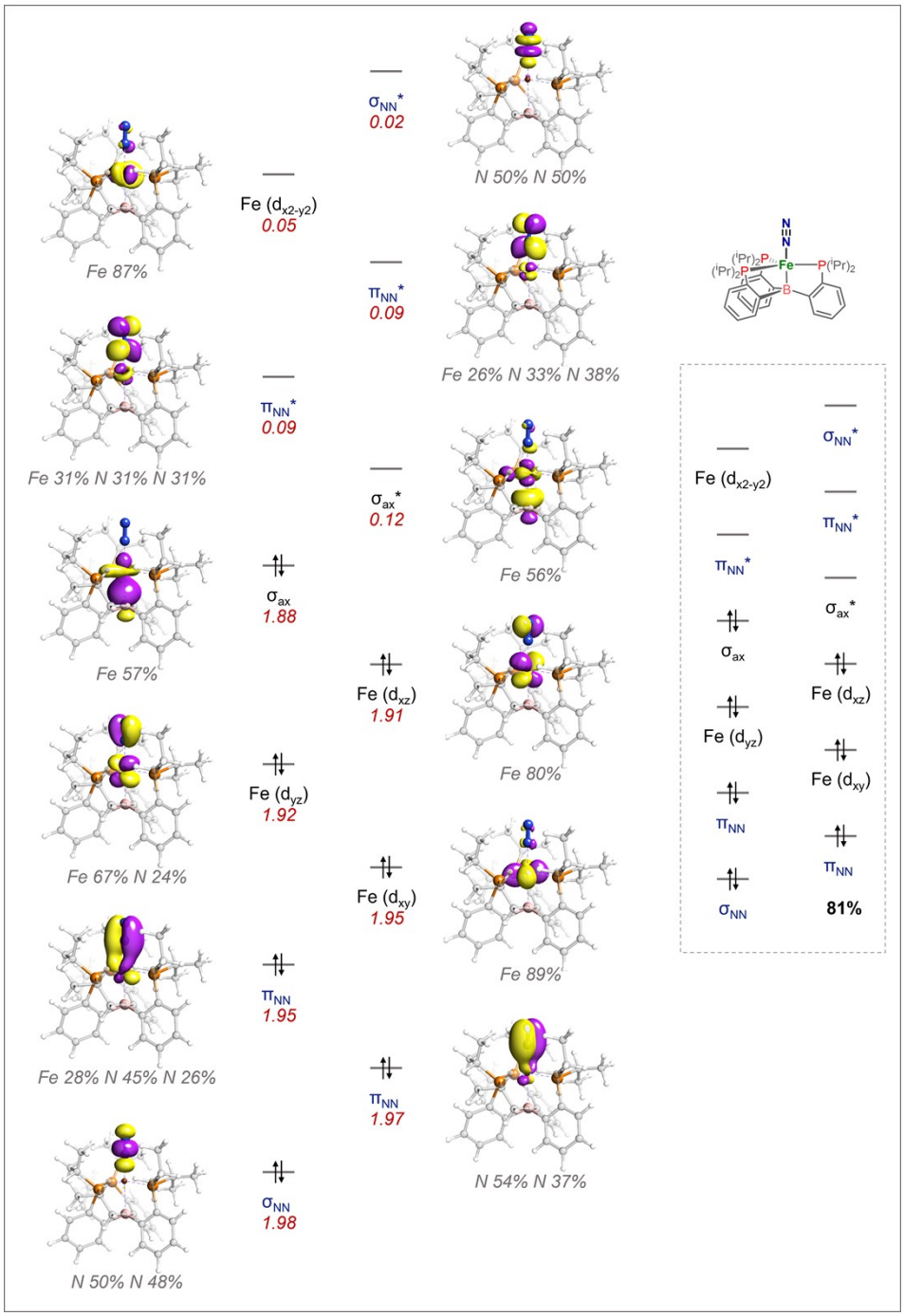

Figure S8. Natural orbitals along with their occupation number and atomic orbital contributions obtained from the CASSCF(14,14) calculations for complex **7**. 4d orbitals are omitted for clarity.

To decipher the electronic structure of the monomeric Fe–N_2 complex **7** a CASSCF(14,14) was undertaken with the active space consisting of Fe-based 3d orbitals, N–N σ- and π-orbitals. The $3d_{xy}$ and $3d_{x2-y2}$ were added as the non-bonding orbitals, and both the σ_{ax} and σ_{ax}* interactions of the d_{z2} orbital with the axial boron orbital were included, along with all possible π-interactions of the d_{xz} and d_{yz} orbitals. In addition to the above-mentioned orbitals, Fe-$4d_{xy}$ and Fe-$4d_{x2-y2}$ orbitals were added to balance the active space. The CASSCF(14,14) calculation suggested a major contribution from the electronic configuration of $(\sigma_{NN})^2(\pi_{NN})^4(\text{Fe-}d_{xy})^2(\text{Fe-}d_{xz})^2(\text{Fe-}d_{yz})^2(\sigma_{ax})^2(\sigma_{ax}^*)^0(\pi_{NN}^*)^0(\text{Fe-}d_{x2-y2})^0(\sigma_{NN}^*)^0$. The ground state (S=0) electronic structure and natural orbitals of Fe–N_2 complex **7**, obtained from CASSCF (14,14), are shown in Figure 8.

6. References

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7. Optimized Cartesian Coordinates of all the Species Involved

Complex 1 [S=0]

7	11.131405000	3.537985000	4.852998000
5	12.060672000	4.532426000	5.144262000
5	9.845391000	2.383960000	3.155560000
7	10.108775000	3.230907000	4.254535000
6	12.079521000	5.857079000	4.246416000
6	11.190469000	6.928366000	4.469965000
6	11.133948000	8.010683000	3.565479000
6	11.927146000	7.972482000	2.417374000
1	11.865697000	8.799914000	1.702582000
6	12.829252000	6.930045000	2.169802000
6	12.925241000	5.881036000	3.107050000
6	10.281501000	6.940580000	5.667028000
1	9.253214000	7.210006000	5.390669000
1	10.620368000	7.672566000	6.416378000
1	10.243414000	5.958824000	6.148487000
6	10.231573000	9.189874000	3.828044000
1	10.330445000	9.953013000	3.041335000
1	10.463979000	9.666103000	4.795948000
1	9.169025000	8.894080000	3.879335000
6	13.693253000	6.987772000	0.931390000
1	13.570760000	6.094300000	0.296149000
1	14.766501000	7.054445000	1.179831000
1	13.438860000	7.866271000	0.319531000

6	13.931036000	4.770555000	2.910380000
1	14.618477000	4.712662000	3.768185000
1	14.542665000	4.905583000	2.010480000
1	13.439070000	3.791049000	2.839329000
6	13.425545000	6.275570000	7.282680000
6	12.441569000	6.284560000	8.307288000
6	11.965844000	7.520703000	8.762823000
1	11.203488000	7.543143000	9.544371000
6	12.445883000	8.719001000	8.240521000
1	12.058502000	9.673446000	8.606264000
6	13.427159000	8.692985000	7.253940000
1	13.809178000	9.633413000	6.852356000
6	13.939196000	7.483394000	6.761910000
6	11.906429000	5.023048000	8.978484000
1	12.530739000	4.181908000	8.660176000
6	15.044199000	7.540352000	5.720726000
1	15.155218000	6.530724000	5.303476000
6	10.464113000	4.693149000	8.562970000
1	9.785885000	5.535762000	8.770801000
1	10.098343000	3.820064000	9.126833000
1	10.396286000	4.452886000	7.494177000
6	12.015243000	5.103791000	10.511042000
1	13.027562000	5.389986000	10.836194000
1	11.776188000	4.125351000	10.958119000
1	11.310305000	5.837784000	10.932018000

6	14.712039000	8.486719000	4.559276000
1	15.435587000	8.347904000	3.739877000
1	14.770917000	9.541996000	4.871981000
1	13.709219000	8.300155000	4.163926000
6	16.375690000	7.970666000	6.364852000
1	17.198142000	7.911691000	5.633008000
1	16.646217000	7.355218000	7.234720000
1	16.309603000	9.014373000	6.712606000
6	13.133985000	4.129475000	6.162128000
7	13.912289000	4.987535000	6.846240000
6	15.134478000	4.340214000	7.457878000
6	14.661707000	2.882297000	7.554290000
1	14.210829000	2.711595000	8.543708000
1	15.496204000	2.175345000	7.448355000
6	13.592905000	2.694115000	6.451875000
6	15.486511000	4.938941000	8.816759000
1	15.743627000	6.004663000	8.737832000
1	16.359676000	4.407219000	9.224615000
1	14.662215000	4.837019000	9.533480000
6	16.339445000	4.454634000	6.509137000
1	16.080026000	4.140067000	5.490056000
1	17.147292000	3.800800000	6.872233000
1	16.732134000	5.474962000	6.463606000
6	12.441713000	1.823431000	6.981587000
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1	11.938909000	2.288603000	7.840002000
1	12.845582000	0.849391000	7.304354000
6	14.162147000	2.014063000	5.191180000
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1	14.510986000	0.999601000	5.443456000
1	15.009908000	2.564073000	4.763351000
6	11.118509000	1.741780000	2.432281000
6	11.688786000	0.553556000	2.952272000
6	12.866024000	0.016768000	2.388031000
6	13.468162000	0.683321000	1.316637000
1	14.382971000	0.269245000	0.879607000
6	12.940240000	1.867360000	0.791914000
6	11.760670000	2.398526000	1.354916000
6	11.071658000	-0.163843000	4.130794000
1	10.189720000	0.368523000	4.506715000
1	11.789365000	-0.258851000	4.961241000
1	10.764860000	-1.191066000	3.868783000
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6	13.633649000	2.569117000	-0.348775000
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1	12.968416000	2.694564000	-1.220133000

6	11.202175000	3.678380000	0.783030000
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6	7.251049000	5.287070000	2.642761000
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6	7.529128000	1.651921000	6.282951000
1	7.550620000	1.017541000	5.389087000
6	8.613712000	5.953462000	2.396862000
1	8.766894000	6.142711000	1.322129000
1	9.436599000	5.329211000	2.763308000
1	8.674040000	6.919108000	2.917619000
6	6.117885000	6.237722000	2.227318000
1	6.187408000	6.464035000	1.150931000
1	6.183241000	7.196536000	2.765956000
1	5.122627000	5.812463000	2.425400000

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6	8.406051000	2.058812000	2.805109000
7	7.280927000	2.474087000	3.428642000
6	7.995916000	1.126720000	1.656020000
6	6.469649000	1.340993000	1.553090000
1	6.263150000	2.106420000	0.789364000
1	5.937114000	0.426796000	1.254398000
6	6.003034000	1.861433000	2.915479000
6	8.359420000	-0.334780000	1.986930000
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1	9.718989000	1.286790000	0.305869000
1	8.499321000	2.566623000	0.087356000
6	5.510894000	0.725023000	3.824230000
1	4.644427000	0.238355000	3.350177000

1	5.184886000	1.110635000	4.797826000
1	6.280914000	-0.038815000	3.991329000
6	4.876910000	2.887282000	2.784016000
1	5.133176000	3.684301000	2.076956000
1	4.627374000	3.342243000	3.753729000
1	3.977012000	2.378240000	2.406112000

Complex 2 [S=0]

7	0.632541000	9.110205000	2.331201000
5	1.517832000	7.928206000	2.360912000
6	0.801231000	6.496470000	2.277602000
6	0.181128000	5.899849000	3.398886000
6	-0.643042000	4.765009000	3.257600000
6	-0.865678000	4.238217000	1.981858000
1	-1.521921000	3.367190000	1.867136000
6	-0.270294000	4.801691000	0.850391000
6	1.208253000	6.520663000	-0.229865000
1	0.445959000	6.921504000	-0.922142000
1	1.793837000	5.772799000	-0.796797000
1	1.873610000	7.344425000	0.056873000
6	-0.527670000	4.207496000	-0.512564000
1	0.403706000	3.847385000	-0.988157000
1	-0.960952000	4.949663000	-1.206221000
1	-1.225017000	3.355728000	-0.451799000
6	-1.318026000	4.153605000	4.459788000

1	-1.902226000	3.261343000	4.180950000
1	-2.006561000	4.870797000	4.941352000
1	-0.587083000	3.856581000	5.232278000
6	0.349824000	6.510079000	4.765558000
1	0.782593000	5.796574000	5.487928000
1	-0.618314000	6.853849000	5.169720000
1	1.014489000	7.376868000	4.708377000
6	0.573735000	5.921698000	1.002955000
6	3.908276000	6.324736000	3.610468000
6	3.893603000	6.806598000	4.954875000
6	3.780483000	5.903329000	6.014868000
1	3.768843000	6.286799000	7.039747000
6	3.711401000	4.524271000	5.798742000
1	3.627545000	3.832058000	6.642503000
6	3.749107000	4.048310000	4.492236000
1	3.682212000	2.971557000	4.312194000
6	3.831210000	4.917813000	3.394108000
6	4.097377000	8.277114000	5.287265000
1	4.305132000	8.784649000	4.343610000
6	3.765755000	4.326160000	1.995133000
1	3.562372000	5.169723000	1.320355000
6	5.320400000	8.483273000	6.198283000
1	5.544918000	9.559499000	6.298879000
1	6.215544000	7.982755000	5.794093000
1	5.149554000	8.085534000	7.213098000

6	2.854626000	8.950869000	5.885450000
1	3.088063000	9.982470000	6.200080000
1	2.480862000	8.404160000	6.767461000
1	2.054751000	9.005396000	5.135195000
6	2.618089000	3.316038000	1.848656000
1	2.449040000	3.075803000	0.785343000
1	1.683146000	3.716915000	2.255404000
1	2.844048000	2.367285000	2.367674000
6	5.089400000	3.661690000	1.579286000
1	5.030339000	3.280616000	0.544082000
1	5.315775000	2.805392000	2.238869000
1	5.941086000	4.354455000	1.637093000
7	3.979249000	7.212609000	2.509284000
6	3.628252000	9.526832000	1.895232000
6	5.137011000	9.168351000	1.898076000
1	5.684515000	9.639470000	1.064397000
1	5.605244000	9.527800000	2.829571000
6	5.240030000	7.619930000	1.858233000
6	3.334461000	10.737651000	2.805583000
1	2.248581000	10.900612000	2.834479000
1	3.692405000	10.579249000	3.832665000
1	3.823655000	11.652344000	2.419574000
6	3.151465000	9.932496000	0.481026000
1	2.067770000	10.114977000	0.518034000
1	3.343792000	9.143155000	-0.260477000

1	3.659027000	10.855208000	0.139202000
6	6.480911000	7.132578000	2.609678000
1	7.391762000	7.494183000	2.103224000
1	6.525491000	6.034902000	2.654818000
1	6.489369000	7.506290000	3.642859000
6	5.289321000	7.122099000	0.398096000
1	6.103158000	7.614539000	-0.163341000
1	4.339068000	7.342338000	-0.105305000
1	5.451676000	6.036379000	0.352002000
6	2.957434000	8.208487000	2.333104000
7	-0.632073000	8.917048000	2.331647000
5	-1.517451000	10.099022000	2.360774000
6	-0.800961000	11.530747000	2.276373000
6	-0.181499000	12.128695000	3.397288000
6	0.642273000	13.263729000	3.255200000
6	0.865299000	13.789255000	1.979008000
1	1.521250000	14.660419000	1.863665000
6	0.270616000	13.224378000	0.847863000
6	-1.206932000	11.503837000	-0.231240000
1	-0.444170000	11.102897000	-0.922929000
1	-1.792830000	12.250841000	-0.798987000
1	-1.871885000	10.679919000	0.055990000
6	0.528509000	13.817120000	-0.515628000
1	-0.402760000	14.176108000	-0.992265000
1	0.962683000	13.074360000	-1.208093000

1	1.225329000	14.669360000	-0.455430000
6	1.316361000	13.876714000	4.457086000
1	1.899656000	14.769412000	4.177748000
1	2.005590000	13.160615000	4.939300000
1	0.584950000	14.173480000	5.229224000
6	-0.350622000	11.519844000	4.764532000
1	-0.786609000	12.233123000	5.485198000
1	0.617775000	11.179364000	5.170805000
1	-1.012851000	10.651162000	4.707429000
6	-0.573133000	12.104281000	1.001225000
6	-3.908425000	11.703071000	3.609352000
6	-3.894084000	11.222189000	4.954106000
6	-3.781543000	12.126245000	6.013493000
1	-3.770227000	11.743520000	7.038655000
6	-3.712618000	13.505158000	5.796398000
1	-3.629209000	14.197993000	6.639694000
6	-3.749932000	13.980171000	4.489534000
1	-3.683178000	15.056808000	4.308743000
6	-3.831548000	13.109868000	3.392010000
6	-4.097691000	9.751877000	5.287445000
1	-4.304687000	9.243586000	4.344033000
6	-3.765911000	13.700547000	1.992633000
1	-3.562405000	12.856521000	1.318475000
6	-5.321185000	9.546048000	6.197891000
1	-5.545511000	8.469840000	6.299105000

1	-6.216212000	10.046071000	5.792839000
1	-5.150998000	9.944548000	7.212519000
6	-2.855088000	9.078986000	5.886880000
1	-3.088287000	8.047468000	6.201954000
1	-2.482139000	9.626373000	6.768817000
1	-2.054703000	9.024392000	5.137172000
6	-2.618248000	14.710582000	1.845604000
1	-2.449197000	14.950226000	0.782159000
1	-1.683310000	14.309919000	2.252565000
1	-2.844188000	15.659619000	2.364111000
6	-5.089515000	14.364689000	1.576148000
1	-5.030317000	14.745036000	0.540685000
1	-5.316023000	15.221445000	2.235094000
1	-5.941182000	13.671935000	1.634318000
7	-3.979018000	10.814432000	2.508784000
6	-3.627622000	8.499935000	1.896003000
6	-5.136420000	8.858227000	1.898497000
1	-5.683809000	8.386482000	1.065095000
1	-5.604708000	8.499379000	2.830199000
6	-5.239567000	10.406603000	1.857602000
6	-3.333668000	7.289693000	2.807082000
1	-2.247755000	7.126904000	2.835919000
1	-3.691536000	7.448707000	3.834093000
1	-3.822765000	6.374693000	2.421673000
6	-3.150749000	8.093517000	0.482045000

1	-2.067052000	7.911067000	0.519154000
1	-3.343102000	8.882441000	-0.259898000
1	-3.658287000	7.170605000	0.140728000
6	-6.480715000	10.894337000	2.608347000
1	-7.391369000	10.532263000	2.101870000
1	-6.525449000	11.992039000	2.652726000
1	-6.489419000	10.521328000	3.641779000
6	-5.288418000	10.903496000	0.397133000
1	-6.101775000	10.410359000	-0.164385000
1	-4.337819000	10.683390000	-0.105684000
1	-5.451245000	11.989111000	0.350306000
6	-2.957023000	9.818620000	2.333259000

Complex 3 [S=1]

7	2.403648000	7.655039000	6.073154000
1	2.619563000	6.174924000	4.742821000
5	3.037061000	8.739686000	5.425667000
5	1.155225000	5.527237000	6.204955000
1	2.112027000	7.714372000	7.033347000
7	2.054257000	6.408757000	5.542099000
6	3.528632000	9.877003000	6.329266000
7	3.735721000	11.178517000	5.885035000
6	4.022258000	9.744496000	7.780771000
6	4.420019000	11.198813000	8.132539000
1	3.598485000	11.684122000	8.681239000

1	5.308535000	11.241418000	8.780006000
6	4.638625000	11.942876000	6.800461000
6	2.947158000	9.253090000	8.776772000
1	1.980874000	9.752237000	8.635188000
1	3.280789000	9.445887000	9.810451000
1	2.778826000	8.170432000	8.705722000
6	5.221925000	8.781130000	7.903475000
1	4.947118000	7.778548000	7.547614000
1	5.537029000	8.692735000	8.956710000
1	6.090104000	9.119215000	7.322818000
6	4.250637000	13.416214000	6.909734000
1	4.327581000	13.932354000	5.943605000
1	4.923805000	13.920181000	7.620298000
1	3.221381000	13.535921000	7.271207000
6	6.104178000	11.816371000	6.344467000
1	6.360032000	10.770871000	6.128709000
1	6.779538000	12.182006000	7.134478000
1	6.299352000	12.403531000	5.440339000
6	0.996105000	4.051597000	5.863530000
7	1.849475000	3.296727000	5.074126000
6	0.126182000	1.822651000	5.590581000
1	-0.134986000	0.925781000	6.171343000
1	-0.503324000	1.824270000	4.687041000
6	-0.114747000	3.130662000	6.385144000
6	-1.515657000	3.679386000	6.059688000

1	-1.594790000	3.962838000	4.999207000
1	-1.746940000	4.560411000	6.671637000
1	-2.282264000	2.913763000	6.269387000
6	-0.043468000	2.884553000	7.906779000
1	0.944936000	2.526695000	8.224821000
1	-0.790418000	2.129293000	8.203001000
1	-0.259871000	3.807710000	8.459340000
6	1.600542000	1.826857000	5.161389000
6	1.821966000	1.118740000	3.824142000
1	1.165560000	1.512889000	3.039182000
1	1.604716000	0.045924000	3.941927000
1	2.863960000	1.218134000	3.485381000
6	2.501253000	1.157270000	6.215699000
1	2.173369000	0.118116000	6.377037000
1	2.461987000	1.680317000	7.179674000
1	3.546146000	1.127369000	5.882148000
6	2.813431000	11.810655000	4.985414000
6	1.479432000	12.047497000	5.415962000
6	0.567992000	12.620610000	4.521303000
1	-0.460207000	12.795730000	4.845877000
6	0.949995000	12.984098000	3.232448000
1	0.224804000	13.428630000	2.545933000
6	2.267264000	12.785170000	2.830533000
1	2.568896000	13.079823000	1.823813000
6	3.215942000	12.204987000	3.685433000

6	1.003646000	11.754367000	6.832512000
1	1.882055000	11.476627000	7.421281000
6	0.388569000	12.996730000	7.498411000
1	1.063860000	13.864721000	7.442684000
1	0.177495000	12.793044000	8.561040000
1	-0.562732000	13.286820000	7.024646000
6	0.027269000	10.572981000	6.894371000
1	-0.866345000	10.765784000	6.279270000
1	-0.306390000	10.394587000	7.928504000
1	0.493804000	9.646578000	6.536413000
6	4.640297000	12.042438000	3.179480000
1	5.137943000	11.326794000	3.848629000
6	5.399420000	13.381316000	3.217020000
1	6.451730000	13.240446000	2.919128000
1	5.387708000	13.849504000	4.210158000
1	4.944267000	14.097979000	2.513891000
6	4.699640000	11.475682000	1.755095000
1	4.391338000	12.226159000	1.008893000
1	4.055805000	10.598533000	1.644001000
1	5.731027000	11.178283000	1.506537000
6	2.795754000	3.844674000	4.156569000
6	4.153498000	4.001053000	4.522357000
6	5.057030000	4.463599000	3.554721000
1	6.111337000	4.575879000	3.817955000
6	4.631068000	4.800648000	2.273596000

1	5.346877000	5.159012000	1.533469000
6	3.281666000	4.703785000	1.944333000
1	2.950404000	5.015268000	0.952448000
6	2.345472000	4.222161000	2.866000000
6	4.652071000	3.760550000	5.939563000
1	3.802809000	3.388549000	6.525184000
6	5.111869000	5.076203000	6.590474000
1	5.990895000	5.495108000	6.075082000
1	5.390827000	4.908554000	7.643347000
1	4.316637000	5.832415000	6.563935000
6	5.773966000	2.712707000	5.994138000
1	5.486216000	1.776722000	5.491672000
1	6.033533000	2.475322000	7.038771000
1	6.688766000	3.081049000	5.502173000
6	0.875927000	4.170590000	2.471662000
1	0.343700000	3.599826000	3.243175000
6	0.283014000	5.586240000	2.462093000
1	0.780555000	6.209274000	1.705284000
1	0.426555000	6.074289000	3.434070000
1	-0.795965000	5.560188000	2.237816000
6	0.644544000	3.477234000	1.121249000
1	1.063056000	4.064251000	0.288310000
1	-0.434972000	3.364407000	0.930513000
1	1.105721000	2.478219000	1.087616000
6	3.267825000	8.622217000	3.857163000

6	2.180340000	8.756154000	2.962817000
6	2.369370000	8.564753000	1.578076000
6	3.639591000	8.214408000	1.110578000
1	3.786457000	8.065267000	0.035854000
6	4.739341000	8.109778000	1.964947000
6	4.551858000	8.319525000	3.346608000
6	0.814054000	9.148710000	3.460686000
1	0.534065000	10.148095000	3.091344000
1	0.777769000	9.181689000	4.553462000
1	0.037614000	8.446575000	3.119552000
6	1.237985000	8.789985000	0.607396000
1	1.538881000	8.547252000	-0.422725000
1	0.909616000	9.843624000	0.624253000
1	0.349299000	8.186545000	0.852843000
6	6.112186000	7.845183000	1.402945000
1	6.064855000	7.599965000	0.331320000
1	6.625631000	7.019369000	1.921146000
1	6.764328000	8.730021000	1.512075000
6	5.747767000	8.216289000	4.258300000
1	6.186202000	7.204674000	4.234864000
1	5.480257000	8.441541000	5.294986000
1	6.547064000	8.914853000	3.957298000
6	0.378460000	6.196997000	7.423319000
6	0.915808000	6.097131000	8.727757000
6	0.285081000	6.749393000	9.807744000

6	-0.882094000	7.479521000	9.565220000
1	-1.378083000	7.978652000	10.403709000
6	-1.434671000	7.595942000	8.286073000
6	-0.787209000	6.964340000	7.204344000
6	2.177857000	5.306605000	8.985475000
1	2.539206000	4.816630000	8.072813000
1	2.017647000	4.522971000	9.744191000
1	2.990313000	5.949086000	9.366449000
6	0.855285000	6.664859000	11.200253000
1	0.903111000	5.622303000	11.558942000
1	0.249241000	7.239482000	11.916096000
1	1.886512000	7.055776000	11.240911000
6	-2.698463000	8.389080000	8.072345000
1	-2.549746000	9.206340000	7.347893000
1	-3.056187000	8.832493000	9.013427000
1	-3.507930000	7.757421000	7.667661000
6	-1.353899000	7.132898000	5.816187000
1	-1.350428000	8.191645000	5.511980000
1	-2.400294000	6.789728000	5.756991000
1	-0.776082000	6.573354000	5.072157000

Complex 4 [S=0]

5	-5.140164000	4.750287000	12.928456000
8	-3.614238000	4.255234000	14.990855000

6	-4.362726000	4.459554000	14.133460000
6	-4.200342000	5.300522000	11.750162000
6	-3.982305000	6.694051000	11.607922000
6	-3.141034000	7.182497000	10.585252000
6	-2.523973000	6.272324000	9.723983000
1	-1.868465000	6.651360000	8.933283000
6	-2.708301000	4.892517000	9.845303000
6	-3.549090000	4.403099000	10.866384000
6	-4.623757000	7.693102000	12.541574000
1	-3.867280000	8.209013000	13.158594000
1	-5.330117000	7.206868000	13.222183000
1	-5.164122000	8.480450000	11.989851000
6	-2.893453000	8.661693000	10.423933000
1	-2.195672000	8.861028000	9.597034000
1	-2.467305000	9.107182000	11.339134000
1	-3.826697000	9.213777000	10.217728000
6	-2.006505000	3.950567000	8.898482000
1	-1.377776000	4.500508000	8.182476000
1	-2.722552000	3.342473000	8.318764000
1	-1.359377000	3.237160000	9.437112000
6	-3.741588000	2.910456000	10.978627000
1	-4.065556000	2.471598000	10.020126000
1	-4.490320000	2.660673000	11.737645000
1	-2.801657000	2.400348000	11.252637000
6	-6.615011000	4.547052000	12.901335000

7	-7.403135000	4.148570000	13.933081000
6	-8.869860000	4.097139000	13.633663000
6	-8.847045000	4.138086000	12.098377000
1	-9.714142000	4.674743000	11.687357000
1	-8.885607000	3.107604000	11.713409000
6	-7.505262000	4.783456000	11.679296000
6	-9.518374000	2.817211000	14.163753000
1	-9.092264000	1.923389000	13.693093000
1	-10.595978000	2.835639000	13.939540000
1	-9.401224000	2.731134000	15.254421000
6	-9.616229000	5.295270000	14.237203000
1	-9.589587000	5.256364000	15.333628000
1	-10.672055000	5.264193000	13.926727000
1	-9.194756000	6.255089000	13.912877000
6	-6.972286000	4.099765000	10.410896000
1	-6.051382000	4.575387000	10.051702000
1	-7.729009000	4.165618000	9.611305000
1	-6.760308000	3.036165000	10.594641000
6	-7.647550000	6.294157000	11.407024000
1	-7.965804000	6.850701000	12.299963000
1	-8.393672000	6.464230000	10.613517000
1	-6.690691000	6.714082000	11.071659000
6	-6.858195000	3.819575000	15.215557000
6	-6.685357000	4.825123000	16.200252000
6	-6.184534000	4.447914000	17.453802000

1	-6.051119000	5.209104000	18.225546000
6	-5.829991000	3.130162000	17.726192000
1	-5.438191000	2.859073000	18.709766000
6	-5.947704000	2.164202000	16.730729000
1	-5.631570000	1.139543000	16.937464000
6	-6.448380000	2.483921000	15.462388000
6	-6.937682000	6.305799000	15.945807000
1	-7.299403000	6.411596000	14.915803000
6	-5.633476000	7.115732000	16.058912000
1	-4.852350000	6.716420000	15.400555000
1	-5.246357000	7.105245000	17.090058000
1	-5.811619000	8.166507000	15.779352000
6	-7.990818000	6.893059000	16.900243000
1	-8.235743000	7.928678000	16.613532000
1	-7.614644000	6.918622000	17.935503000
1	-8.922872000	6.310505000	16.904677000
6	-6.461546000	1.394244000	14.396883000
1	-6.914242000	1.816418000	13.489313000
6	-7.282393000	0.166363000	14.826516000
1	-7.365835000	-0.550889000	13.993731000
1	-8.297690000	0.436741000	15.149705000
1	-6.797755000	-0.359715000	15.664531000
6	-5.029219000	0.962799000	14.034541000
1	-5.045167000	0.241500000	13.201247000
1	-4.532109000	0.477540000	14.889813000

1	-4.417218000	1.821255000	13.731560000

Complex 5 [S=0]

7	11.131405000	3.537985000	4.852998000
5	9.845391000	2.383960000	3.155560000
7	10.108775000	3.230907000	4.254535000
6	11.118509000	1.741780000	2.432281000
6	11.688786000	0.553556000	2.952272000
6	12.866024000	0.016768000	2.388031000
6	13.468162000	0.683321000	1.316637000
1	14.382971000	0.269245000	0.879607000
6	12.940240000	1.867360000	0.791914000
6	11.760670000	2.398526000	1.354916000
6	11.071658000	-0.163843000	4.130794000
1	10.189720000	0.368523000	4.506715000
1	11.789365000	-0.258851000	4.961241000
1	10.764860000	-1.191066000	3.868783000
6	13.484658000	-1.241755000	2.943571000
1	12.773820000	-2.085769000	2.943366000
1	13.799623000	-1.105221000	3.993154000
1	14.369789000	-1.543195000	2.363377000
6	13.633649000	2.569117000	-0.348775000
1	14.525286000	2.014861000	-0.678478000
1	13.954819000	3.584469000	-0.059019000
1	12.968416000	2.694564000	-1.220133000

6	11.202175000	3.678380000	0.783030000
1	11.910181000	4.513901000	0.894793000
1	10.277969000	3.969433000	1.292721000
1	10.987312000	3.582147000	-0.294899000
6	7.248680000	3.464156000	4.468158000
6	7.142687000	4.825145000	4.090627000
6	7.003651000	5.784071000	5.100588000
1	6.906411000	6.836994000	4.828268000
6	7.008748000	5.423388000	6.446902000
1	6.910958000	6.189334000	7.220819000
6	7.163615000	4.086314000	6.801199000
1	7.201354000	3.812544000	7.857960000
6	7.283486000	3.083582000	5.827591000
6	7.251049000	5.287070000	2.642761000
1	7.203224000	4.397430000	2.001387000
6	7.529128000	1.651921000	6.282951000
1	7.550620000	1.017541000	5.389087000
6	8.613712000	5.953462000	2.396862000
1	8.766894000	6.142711000	1.322129000
1	9.436599000	5.329211000	2.763308000
1	8.674040000	6.919108000	2.917619000
6	6.117885000	6.237722000	2.227318000
1	6.187408000	6.464035000	1.150931000
1	6.183241000	7.196536000	2.765956000
1	5.122627000	5.812463000	2.425400000

6	8.904800000	1.528642000	6.953285000
1	9.152101000	0.471413000	7.143384000
1	8.927084000	2.058751000	7.918310000
1	9.681653000	1.962370000	6.316945000
6	6.433328000	1.131699000	7.226206000
1	5.425567000	1.240195000	6.798317000
1	6.444835000	1.676912000	8.183661000
1	6.595840000	0.065118000	7.452332000
6	8.406051000	2.058812000	2.805109000
7	7.280927000	2.474087000	3.428642000
6	7.995916000	1.126720000	1.656020000
6	6.469649000	1.340993000	1.553090000
1	6.263150000	2.106420000	0.789364000
1	5.937114000	0.426796000	1.254398000
6	6.003034000	1.861433000	2.915479000
6	8.359420000	-0.334780000	1.986930000
1	7.923241000	-1.008570000	1.231498000
1	7.991916000	-0.645315000	2.974972000
1	9.448497000	-0.466704000	1.975169000
6	8.643793000	1.499812000	0.313122000
1	8.170057000	0.913094000	-0.491713000
1	9.718989000	1.286790000	0.305869000
1	8.499321000	2.566623000	0.087356000
6	5.510894000	0.725023000	3.824230000
1	4.644427000	0.238355000	3.350177000

1	5.184886000	1.110635000	4.797826000
1	6.280914000	-0.038815000	3.991329000
6	4.876910000	2.887282000	2.784016000
1	5.133176000	3.684301000	2.076956000
1	4.627374000	3.342243000	3.753729000
1	3.977012000	2.378240000	2.406112000

Complex 6 [S=0]

42	0.016275000	2.405298000	0.023490000
6	1.911809000	4.697739000	-2.138218000
15	1.395484000	2.860010000	-1.975774000
7	-1.379939000	3.080707000	-1.258889000
15	-1.817276000	2.912690000	1.649789000
6	-1.585486000	4.239339000	3.003040000
17	1.870423000	3.213166000	1.482769000
6	2.809088000	1.703391000	-2.496721000
6	-2.733561000	1.385952000	2.326508000
7	0.050004000	0.618367000	0.064007000
6	-3.030439000	3.744676000	0.510413000
1	-2.844299000	4.824108000	0.605004000
1	-4.073845000	3.570042000	0.815197000
6	-2.793439000	3.326019000	-0.937450000
1	-3.191725000	4.124885000	-1.594247000
1	-3.386110000	2.421164000	-1.177781000

6	-1.225268000	3.214996000	-2.714929000
1	-2.070995000	2.712569000	-3.223962000
1	-1.304929000	4.283845000	-3.007587000
6	0.077075000	2.625755000	-3.250784000
1	-0.035011000	1.537506000	-3.343629000
1	0.322339000	3.026202000	-4.245522000
6	-0.780053000	3.631777000	4.162058000
1	-0.489003000	4.431730000	4.864218000
1	0.140702000	3.154061000	3.794850000
1	-1.366974000	2.894850000	4.729797000
6	-2.899585000	4.848940000	3.519718000
1	-2.658440000	5.670711000	4.215891000
1	-3.521733000	4.131208000	4.065452000
1	-3.505942000	5.280979000	2.709151000
6	-0.750821000	5.369090000	2.364994000
1	-0.631431000	6.182217000	3.101336000
1	-1.236966000	5.804944000	1.477555000
1	0.249015000	5.016237000	2.082948000
6	0.927619000	5.527410000	-1.288260000
1	1.183866000	6.595984000	-1.388588000
1	1.008179000	5.265963000	-0.224211000
1	-0.117038000	5.399538000	-1.599165000
6	3.317689000	4.918949000	-1.556450000
1	3.512352000	6.003855000	-1.507231000
1	4.104624000	4.475958000	-2.182157000

1	3.394772000	4.514515000	-0.536889000
6	1.852930000	5.196150000	-3.589985000
1	2.209290000	6.239943000	-3.626680000
1	0.826117000	5.190254000	-3.984332000
1	2.484106000	4.606827000	-4.268764000
6	-3.879962000	1.713319000	3.291640000
1	-4.434843000	0.783911000	3.504287000
1	-4.596363000	2.435546000	2.870975000
1	-3.515253000	2.100538000	4.252832000
6	-1.723341000	0.456689000	3.015899000
1	-2.249181000	-0.433218000	3.397434000
1	-1.206397000	0.940245000	3.855311000
1	-0.972938000	0.099713000	2.306349000
6	-3.309540000	0.645070000	1.108963000
1	-3.677419000	-0.339782000	1.435662000
1	-2.544500000	0.468524000	0.344341000
1	-4.150998000	1.185342000	0.649928000
6	2.214912000	0.286950000	-2.605374000
1	3.036047000	-0.423793000	-2.792571000
1	1.509835000	0.194522000	-3.444070000
1	1.702327000	-0.031649000	-1.690088000
6	3.437739000	2.078751000	-3.845920000
1	4.197805000	1.325135000	-4.115083000
1	3.942524000	3.053916000	-3.814321000
1	2.692143000	2.099895000	-4.656533000

6	3.870127000	1.696463000	-1.380362000
1	4.515291000	0.809516000	-1.494508000
1	3.402971000	1.662652000	-0.388129000
1	4.514873000	2.582095000	-1.414558000
42	-0.016150000	-2.405322000	0.023529000
6	-1.912226000	-4.697581000	-2.137953000
15	-1.395391000	-2.859971000	-1.975712000
7	1.380088000	-3.080734000	-1.258830000
15	1.817341000	-2.912793000	1.649866000
6	1.585465000	-4.239542000	3.002990000
17	-1.870329000	-3.213176000	1.482764000
6	-2.808719000	-1.703054000	-2.496711000
6	2.733559000	-1.386139000	2.326870000
7	-0.049852000	-0.618387000	0.064014000
6	3.030598000	-3.744662000	0.510497000
1	2.844577000	-4.824113000	0.605095000
1	4.073978000	-3.569915000	0.815305000
6	2.793584000	-3.326051000	-0.937383000
1	3.191854000	-4.124948000	-1.594155000
1	3.386270000	-2.421218000	-1.177753000
6	1.225365000	-3.215264000	-2.714842000
1	2.071091000	-2.712948000	-3.223985000
1	1.305002000	-4.284163000	-3.007320000
6	-0.076971000	-2.626088000	-3.250782000
1	0.035171000	-1.537864000	-3.343849000

1	-0.322269000	-3.026708000	-4.245440000
6	0.780135000	-3.631983000	4.162083000
1	0.489012000	-4.431959000	4.864187000
1	-0.140575000	-3.154132000	3.794941000
1	1.367160000	-2.895169000	4.729861000
6	2.899520000	-4.849305000	3.519581000
1	2.658319000	-5.671093000	4.215714000
1	3.521756000	-4.131660000	4.065336000
1	3.505807000	-5.281353000	2.708967000
6	0.750645000	-5.369140000	2.364866000
1	0.631240000	-6.182351000	3.101110000
1	1.236670000	-5.804924000	1.477328000
1	-0.249179000	-5.016150000	2.082941000
6	-0.928062000	-5.527479000	-1.288188000
1	-1.184642000	-6.595986000	-1.388381000
1	-1.008287000	-5.265941000	-0.224134000
1	0.116553000	-5.399929000	-1.599352000
6	-3.318024000	-4.918400000	-1.555841000
1	-3.512976000	-6.003251000	-1.506583000
1	-4.104995000	-4.475186000	-2.181348000
1	-3.394741000	-4.513950000	-0.536258000
6	-1.853849000	-5.196043000	-3.589720000
1	-2.210516000	-6.239735000	-3.626303000
1	-0.827136000	-5.190447000	-3.984324000
1	-2.485030000	-4.606553000	-4.268355000

6	3.879713000	-1.713678000	3.292240000
1	4.434620000	-0.784333000	3.505090000
1	4.596152000	-2.435929000	2.871680000
1	3.514751000	-2.100949000	4.253317000
6	1.723241000	-0.456894000	3.016139000
1	2.249053000	0.432916000	3.397935000
1	1.206047000	-0.940535000	3.855351000
1	0.973048000	-0.099760000	2.306452000
6	3.309887000	-0.645174000	1.109546000
1	3.677766000	0.339607000	1.436459000
1	2.545067000	-0.468446000	0.344754000
1	4.151410000	-1.185471000	0.650666000
6	-2.214227000	-0.286741000	-2.605400000
1	-3.035205000	0.424186000	-2.792594000
1	-1.509139000	-0.194480000	-3.444110000
1	-1.701548000	0.031756000	-1.690132000
6	-3.437440000	-2.078337000	-3.845897000
1	-4.197352000	-1.324578000	-4.115094000
1	-3.942424000	-3.053399000	-3.814256000
1	-2.691846000	-2.099673000	-4.656507000
6	-3.869749000	-1.695872000	-1.380349000
1	-4.514949000	-0.808980000	-1.494730000
1	-3.402566000	-1.661801000	-0.388136000
1	-4.514460000	-2.581542000	-1.414269000

Complex 7 [S=0]

26	3.025831000	13.176592000	13.828813000
15	2.593737000	12.857012000	16.037804000
6	3.231807000	13.821673000	17.511078000
1	3.030040000	13.160051000	18.365534000
6	2.529179000	15.144128000	17.815720000
1	1.440141000	15.033574000	17.892574000
1	2.899418000	15.534010000	18.778747000
1	2.744632000	15.904755000	17.055813000
6	4.746763000	14.020024000	17.400331000
1	5.287002000	13.085212000	17.192125000
1	4.990960000	14.726130000	16.593516000
1	5.146102000	14.434792000	18.340491000
6	3.295840000	11.148403000	16.440164000
1	4.347686000	11.209459000	16.114361000
6	3.269784000	10.749362000	17.919671000
1	3.913469000	11.374630000	18.553235000
1	2.245885000	10.779622000	18.323434000
1	3.626861000	9.711248000	18.021034000
6	2.596311000	10.070410000	15.611657000
1	2.648636000	10.261324000	14.536508000
1	3.060689000	9.089522000	15.802587000
1	1.530585000	10.002062000	15.872763000
15	2.338121000	15.193331000	13.303124000

6	3.516214000	16.221503000	12.275665000
1	2.937185000	17.111395000	11.986955000
6	4.732893000	16.680426000	13.088657000
1	4.459318000	17.149679000	14.044413000
1	5.401805000	15.839987000	13.313728000
1	5.314827000	17.419367000	12.512905000
6	3.953937000	15.526783000	10.990607000
1	3.092329000	15.228727000	10.379720000
1	4.579231000	16.204536000	10.385701000
1	4.551427000	14.631612000	11.210369000
6	1.830516000	16.480517000	14.580171000
1	2.657177000	16.469625000	15.307381000
6	1.677323000	17.913655000	14.050883000
1	2.607393000	18.345971000	13.659656000
1	0.909723000	17.966953000	13.263796000
1	1.339253000	18.564144000	14.874474000
6	0.535147000	16.081509000	15.288575000
1	0.579215000	15.082120000	15.722909000
1	0.314061000	16.796238000	16.097238000
1	-0.309862000	16.091050000	14.584605000
15	3.171041000	12.077901000	11.762021000
7	4.817612000	13.420311000	14.093530000
7	5.898394000	13.614473000	14.284832000
6	0.149867000	13.839389000	12.574875000
6	-1.052114000	13.608623000	11.882205000

1	-1.584793000	12.665227000	12.032953000
6	1.906462000	10.847633000	12.194481000
5	0.814795000	12.813996000	13.631978000
6	2.883304000	12.433879000	9.928446000
1	3.599888000	13.232674000	9.689264000
6	0.882950000	11.292541000	13.072979000
6	4.757351000	11.086266000	11.658643000
1	4.583068000	10.311642000	10.898399000
6	-0.074802000	10.325550000	13.457726000
1	-0.869153000	10.615437000	14.147216000
6	5.913765000	11.967586000	11.170674000
1	5.720198000	12.391104000	10.173970000
1	6.109510000	12.802236000	11.857419000
1	6.840488000	11.374120000	11.102147000
6	-1.558145000	14.537783000	10.968230000
1	-2.486757000	14.326126000	10.430399000
6	-0.034863000	9.010504000	13.000159000
1	-0.801838000	8.299021000	13.319643000
6	5.096589000	10.351765000	12.958455000
1	5.240961000	11.035981000	13.804197000
1	4.311002000	9.636314000	13.233424000
1	6.035336000	9.787653000	12.830780000
6	1.960657000	9.512537000	11.750377000
1	2.776304000	9.179561000	11.106377000
6	0.994249000	8.591882000	12.146577000

1	1.044473000	7.556338000	11.800773000
6	0.324573000	15.990636000	11.396806000
1	0.872661000	16.911580000	11.185596000
6	-0.869838000	15.731434000	10.719839000
1	-1.256095000	16.450539000	9.992854000
6	0.804768000	12.728474000	16.279264000
6	0.063952000	12.828105000	15.078279000
6	0.823587000	15.049726000	12.309209000
6	1.467912000	12.951337000	9.672498000
1	1.329931000	13.134810000	8.594541000
1	0.715833000	12.214286000	9.988485000
1	1.257464000	13.882382000	10.204425000
6	-1.337095000	12.890621000	15.211254000
1	-1.952246000	13.007524000	14.316422000
6	3.165760000	11.249791000	8.993757000
1	2.954579000	11.557915000	7.956565000
1	4.207945000	10.904508000	9.020353000
1	2.508895000	10.395734000	9.215348000
6	0.179029000	12.650224000	17.534327000
1	0.775031000	12.585382000	18.447685000
6	-1.968107000	12.827299000	16.456175000
1	-3.058866000	12.887141000	16.517161000
6	-1.212183000	12.693569000	17.626672000
1	-1.702366000	12.643913000	18.602253000