N/O→B dative bond supplemented by N-HN/HC Hydrogen Bonds make BN-cages an attractive candidate for DNA-nucleobases adsorption – An MP2 prediction

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Supplementary Documents

S1. MP2 (SP) and DFT (M06-2X) adsorption energies (E_{ads})

Electron-correlation methods (such as MP2) to optimize geometries for larger systems, such as in the present study, demand extensive computational resources, limiting the inclusion of a wide range of larger systems. It may be noted that the use of a method, such as CCSD(T), to optimize geometry is not even feasible for such large systems. One common approach is to consider single-point energy and property calculations at the MP2 level using lower-level optimized geometries. In the present investigation, M06-2X optimized geometries were used for MP2 single-point (SP) calculations to verify the reliability of such an approach. Adsorption energies are compared in Table S1, where MP2(OPT) E_{ads} (without BSSE correction) are shown in the first columns, followed by MP2(SP) values. Although the same basis function is used, BSSE correction energy may differ in MP2 and M06-2X methods. We used non-BSSE corrected adsorption energies for all MP2 calculations, but BSSE corrected adsorption energies for M06-2X are given in the same table.

Results are very encouraging as MP2(SP) E_{ads} values are close to the corresponding MP2(OPT) values. Compared to the reference MP2(OPT) adsorption energies, both overestimation and underestimation are recorded for the cost-effective MP2(SP) method. The largest difference is only +1.4 kcal/mol (overestimation), while less than half of that value (-0.6 kcal/mol) is underestimated by MP2(SP). Interestingly, MP2(SP) adsorption energies show the opposite trend for B-N and B-O linked structures, except in the C1 case. MP2(SP) values are underestimated for B-N connected structures, while B-O linked systems are overestimated. Whatever the circumstances, MP2(SP) E_{ads} values are within 99% to 104% of the MP2(OPT) values, indicating results of the former method can be used with confidence. However, such a conclusion is only valid for the interaction of DNA nucleobases or similar molecules with BN-cage. For other systems, such as BN-tube or sheet type structures, one needs to verify the reliability of MP2(SP) method.

Next, we compare adsorption energies from the computationally more efficient M06-2X (OPT)/6-311+G** method, also collected in Table S1, with MP2(OPT)/6-311+G** values. Although adsorption energies from this DFT variant are noticeably underestimated (by 5 to 8 kcal/mol, except for T3 structure), the trend of stability predicted by MP2(OPT) method is preserved. For example, E_{ads} values of three complexes of BN-cage-adenine are in the range of -35.4 to -38.2 kcal/mol where the A3 structure is the most stable one. The stability order of guanine cases is also maintained, where G3 is the least stable among the three structures. It is also true that

thymine binding with $B_{12}N_{12}$ according to the M06-2X method is weaker in the series. Albeit adsorption energies are underestimated compared to the MP2 method, stability trends according to M06-2X of the entire series of structures are reliable. It is worth mentioning that E_{ads} values may depend on method-to-method and the concern of the present investigation is not to judge the reliability of different DFT methods.

The other factor of the computational cost for larger systems is the basis function. Smaller basis sets are efficient, but results may not always be reliable. To verify the effect of the basis set on adsorption energies, we compare the results of split-valence double-ξ basis set (6-31+G*), summarized in the last two columns of Table S1, with the split-valence triple-ξ 6-311+G** set. It is obvious that a smaller basis set will show higher BSSE energies than an extended basis set. The range is 2.5 to 3.4 kcal/mol for 6-31+G*, compared to 1.9 to 2.5 kcal/mol in the case of 6-311+G**. Mixed results were observed for the smaller basis set compared to the larger one: for adenine and guanine complexes, E_{ads} (BSSE corrected) values are comparable (within 1.2 kcal/mol) to those of the extended basis set. However, the smaller basis set underestimated cytosine and thymine adsorption energies by 9.0 to 17.0 kcal/mol. Thus widely employed 6-31+G* basis set should be used with caution for similar systems.

Table S1

Comparison of Adsorption Energies (kcal/mol) of DNA nucleobases adsorbed at the surface of $B_{12}N_{12}$ nanocage at different level of calculations[a]

	MP2 (OPT) 6-311+G**	MP2 (SP) 6-311+G**	M06-2X (OPT) 6-311+G**		M06-2X (OPT) 6-31+G*	
	Without BSSE	Without BSSE	Without BSSE	With BSSE	Without BSSE	With BSSE
A1	-43.4	-43.0	-35.4	-33.4	-37.1	-34.2
A2	-43.1	-42.7	-36.0	-33.9	-37.4	-34.5
A3	-45.3	-45.0	-38.2	-36.3	-39.7	-37.0
G1	-43.3	-42.8	-35.0	-32.8	-36.6	-33.2
G2	-41.9	-41.3	-33.8	-31.6	-35.3	-32.4
G3	-37.1	-38.5	-31.9	-29.9	-33.8	-31.1
C1	-43.4	-44.2	-36.4	-33.9	-20.1	-17.1
C2	-41.3	-42.5	-35.0	-32.7	-19.9	-16.7
T1	-19.2	-18.9	-7.9	-5.3	-13.2	-9.6
T2	-31.3	-32.5	-25.7	-23.8	-9.7	-7.1
T3	-29.3	-30.6	-26.6	-24.7	-17.9	-15.4

[a] OPT stands for full optimization and SP corresponds to MP2 single-point energies at the M06-2X/6-311+G** optimized geometry.

S2. Changes in enthalpy (ΔH) and free energy (ΔG) at the DFT level

Enthalpy and free energies were calculated at the DFT levels in both gas and water phases, and changes upon complexations are given in Table S2. It can be seen that trends in the stability of individual nucleobases, predicted from E_{ads}, are preserved. Only T1 case is the odd member in the list where the corresponding ΔG value of about +6.0 kcal/mol, which does not support the thermodynamic stability of **T1** structure.

Table S2. Changes in enthalpy (ΔH) and free energy (ΔG) of DNA nucleobases adsorbed at the surface of $B_{12}N_{12}$ nanocage in gas and water phases.

Name of the system	M06-2X/6-311+G** (OPT) (Gas phase) Kcal/mol		M06-2X /6-31+G* OPT (Gas phase) Kcal/mol		M06-2X /6-31+G* OPT (Water phase) Kcal/mol	
	ΔH	ΔG	ΔH	ΔG	ΔH	ΔG
A1	-33.68	-19.61	-35.29	-21.07	-35.40	-22.30
A2	-34.28	-20.98	-35.63	-22.05	-36.11	-21.53
A3	-36.50	-22.79	-37.91	-23.99	-36.98	-24.37
G1	-33.71	-21.45	-35.20	-21.90	-33.22	-19.71
G2	-32.18	-19.37	-33.63	-20.79	-37.17	-24.36
G3	-31.08	-18.15	-32.93	-20.03	-51.92	-39.41
C1	-34.61	-21.86	-35.81	-23.07	-41.07	-27.77
C2	-33.35	-20.13	-35.68	-22.47	-53.25	-40.17
T1	-6.46	6.36	-12.30	0.46	-7.17	5.60
T2	-23.04	-10.37	-8.05	-4.84	-43.83	-30.84
T3	-24.58	-11.74	-16.62	-3.79	-42.78	-30.12

Fig S1. M06-2X/6-311+G** optimized structure of B12N12 dimer. Bond distances are in Angstrom (Å). Color scheme: Boron –Yellow and Nitrogen-Blue. Dimerization energy (bold number) in kcal/mol
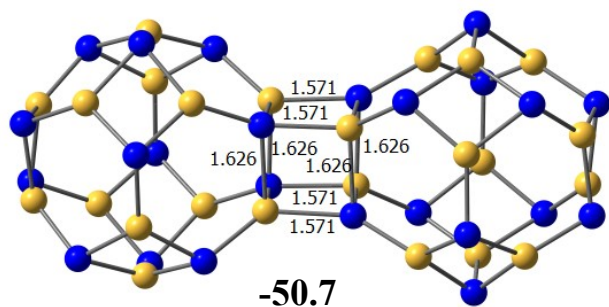
S3. Comparison of geometric parameters

The N/O→B dative bond, where one of the boron atoms of the BN-cage accepts electron pair from N or O atom of DNA-nucleobases, is the primary interaction force holding two units in addition to N-HN and N-HC hydrogen bonds. In both types of hydrogen bonds, the N atom of the BN-cage, adjacent to the boron atom participating in the dative bond, is the proton acceptor. To understand the influence of different methods and basis sets on key geometric parameters, three sets of data are collected in Table S3; fully optimized structures at MP2/6-311+G**, M06-2X/6-311+G**, and M06-2X/6-31+G*. The BN bond is more sensitive than BO-bond to methods: DFT predicts slightly longer (9.0 to 16.0 mÅ) BN distances than the reference MP2 distances. However, the difference between MP2 and DFT BO-bond lengths is negligible (+/- 3.0 mÅ). Expansion of basis set from 6-31+G* to 6-311+G** at the DFT level has a negligible effect on the BN bond lengths; only 1.0 mÅ stretched at a more extensive basis set, except for **C1** structure, where the change is +2.0 mÅ. However, the BO bond is slightly more affected due to the expansion of basis set: mostly elongated by about 3.0 to 5.0 mÅ, except for **T2** where a reverse trend within the same range is found. As expected, H-bonds are more affected by methods; electron-correlation MP2 predicted N-HN bond lengths are shorter than the DFT method, whereas DFT predicts shorter N-HC bond lengths than MP2 values.

Table S3. Comparison of B-N/O and Hydrogen Bond distances (in Å) optimized at MP2 and DFT methods. N-HC Hydrogen bonds distances are in Italic.

	MP2 6-311+G**		M06-2X 6-311+G**		M06-2X 6-31+G*		MP2 6-311+G**	M06-2X 6-311+G**	M06-2X 6-31+G*
	B-N	B-O	B-N	B-O	B-N	B-O	N-HN/HC	N-HN/HC	N-HN/HC
A1	1.594		1.603		1.602		1.950 *2.426*	1.961 *2.420*	1.967 *2.421*
A2	1.609		1.620		1.619		1.861 *2.440*	1.893 *2.421*	1.907 *2.421*
A3	1.590		1.599		1.598		2.050 *2.556*	2.101 *2.513*	2.106 *2.517*
G1	1.604		1.620		1.619		1.903 1.952	1.900 1.989	1.935 1.995
G2	1.590		1.599		1.598		*2.554*	*2.550*	*2.557*
G3		1.528		1.528		1.525	1.688	1.712	1.748
C1	1.596		1.606		1.604		*2.321*	*2.329*	*2.330*
C2		1.520		1.521		1.518	1.868	2.019	2.028
T2		1.556		1.553		1.557	1.830	1.818	1.892
T3		1.551		1.554		1.549	1.767	1.792	1.845

S4. Interaction of DNA-nucleobases with BH_3 – the simplest model

Since the adsorption property of BN-nanocages is almost independent of their size, the natural question arises what could be the strength of the BN/BO dative bonds, the main force of interaction between BN-nanocage with DNA-nucleobases, in the absence of the BN network. To explore that, BN cage is replaced by a BH_3 molecule, and geometries of BH_3-**A/G/C/T** structures were fully optimized at the MP2 and DFT levels. MP2/6-311+G** optimized structures of simplest models are depicted in Fig. S2, where the same naming scheme is used as in BN-cage complexes, and **M** stands for the BH_3-DNA models. For example, structure **A1-M** is the BH_3 model of $B_{12}N_{12}$-A-1 (**A1**) (Fig. 2 main text). Binding energies (BE) between BH_3 and nucleobases, summarized in Table S4, are differences in energy between BH_3-DNA and the sum of BH_3 and DNA energies. Interestingly, binding energies are almost independent of the method and extension of the basis set. The maximum difference in MP2(OPT) and M06-2X(OPT) BE values is only 1.6 kcal/mol (in **G2-M**), underestimated by the DFT method. Compared to the more extended basis set, E_{ads} is overestimated by the smaller basis set, and the maximum difference is 1.6 kcal/mol in **G3-M**. Such difference in the case of the chemisorption process is not alarming.

In the absence of proton acceptor nitrogen atoms of the cage, no hydrogen bond (as typical in BN-cage-DNA structures) is possible in these simplest BH_3-DNA models. Thus, these models are representative cases of stand-alone BN/BO dative bonds where nucleobases share electron pairs to the boron atom of BH_3. The BN bond length of BH3-**A/G/C** (Fig. S2) is longer than the corresponding BN-cage-DNA structures. In the case of adenine complexes, such distance is in the range of 1.613 to 1.619Å, i.e., longer by 10.0 to 24.0 mÅ. Even longer BN distance is found in **G2-M** (36.0 mÅ) and in **C1-M** (27.0 mÅ). The MP2/6-311+G** BN bond length in ammonia-borane ($H_3N \rightarrow BH_3$), a textbook example of a BN dative bond, is 1.656 Å, which is the longest among all structures considered in this study. The difference in BO bond lengths in BH_3-models and BN-cages is significantly longer than the corresponding distances in BN-cage-DNA. MP2 optimized BO distances in the BH_3 models are in the range 1.592Å to 1.638Å, whereas such distances in BN cage cases are 1.520 Å to 1.556 Å; i.e., a difference of 71.0 to 82.0 mÅ. Such contraction of BN and BO bonds in BN-fullerene-DNA systems is partly due to hydrogen bonds in cage structures and the effect of an extended BN cage network.

Since the separation between two units in BH_3-nucleobases is wider than in BN-cage-nucleobases structures, it is expected that interaction strength will be less in simple models. Indeed,

MP2(OPT) binding energies, given in the first column of Table S4, clearly support weaker attraction between BH_3 and all four nucleobases than the corresponding BN-cage-nucleobase. For the sake of comparison, both MP2 binding energies of the BH3-model and BN-cage (in parenthesis) are included in Fig. S2. In the case of adenine complexes, such energy difference is within 6.7 to 9.8 kcal/mol, where both H-bonds seem responsible for extra stability in addition to shorter B-N distances. The binding between guanine and BH_3 is weaker by almost the same range (6.5 to 10.2 kcal/mol) as found in adenine cases. Such energy differences are slightly more in cytosine and thymine systems. Out of four DNA-nucleobases considered in this study, thymine adsorption/binding is the weakest. In general, structural and energy difference between BH_3 model and BN-cage complexes is more prominent in B-O linked structures than B-N linked cases. Electron-correlation seems to play an important role for BN-cages in complexation, as DFT binding energies are closer to their corresponding MP2 values in BH_3-models, but a wide difference is found when BN-cage replaces BH_3 molecule.

Table S4
Binding energies (kcal/mol) between DNA nucleobases and BH_3[a].

	MP2 (OPT) 6-311+G**	MP2 (SP) 6-311+G**	M06-2X (OPT) 6-311+G**	M06-2X (OPT) 6-31+G*
A1-M	-35.3	-35.0	-35.4	-36.5
A2-M	-36.4	-36.0	-36.8	-37.7
A3-M	-35.5	-35.5	-36.0	-37.1
G1-M	-36.8	-36.2	-35.8	-36.8
G2-M	-32.3	-32.0	-30.7	-31.9
G3-M	-26.9	-26.5	-26.6	-28.2
C1-M	-31.1	-32.4	-32.5	-33.3
C2-M	-28.1	-28.7	-29.2	-30.7
T2-M	-19.9	-19.9	-20.7	-22.0
T3-M	-22.0	-22.0	-22.6	-24.0

[a] OPT stands for full optimization and SP corresponds to MP2 single-point energies at the M06-2X/6-311+G** optimized geometry.

Fig. S2. MP2/6-311+G** optimized geometries of BH$_3$-A/G/C/T models. Bond distances are in Angstrom (Å). MP2 Binding energies (without BSSE) are in bold. Corresponding adsorption energies of BN-cage are given in parenthesis. Energies are in kcal/mol. Color scheme: Boron-Yellow, Nitrogen-Blue, Carbon-Gray, Oxygen-Red and Hydrogen-Silver.

A1-M **-35.3 (-43.4)**

A2-M **-36.4 (-43.1)**

A3-M **-35.5 (-45.3)**

G1-M **-36.8 (-43.3**

G2-M **-32.2 (-41.9)**

G3-M **-26.9 (-37.1)**

C1-M **-31.1 (-43.4)**

C2-M **-28.1 (-41.3)**

T2-M **-19.9 (-31.3)**

T3-M **-22.0 (-29.3)**
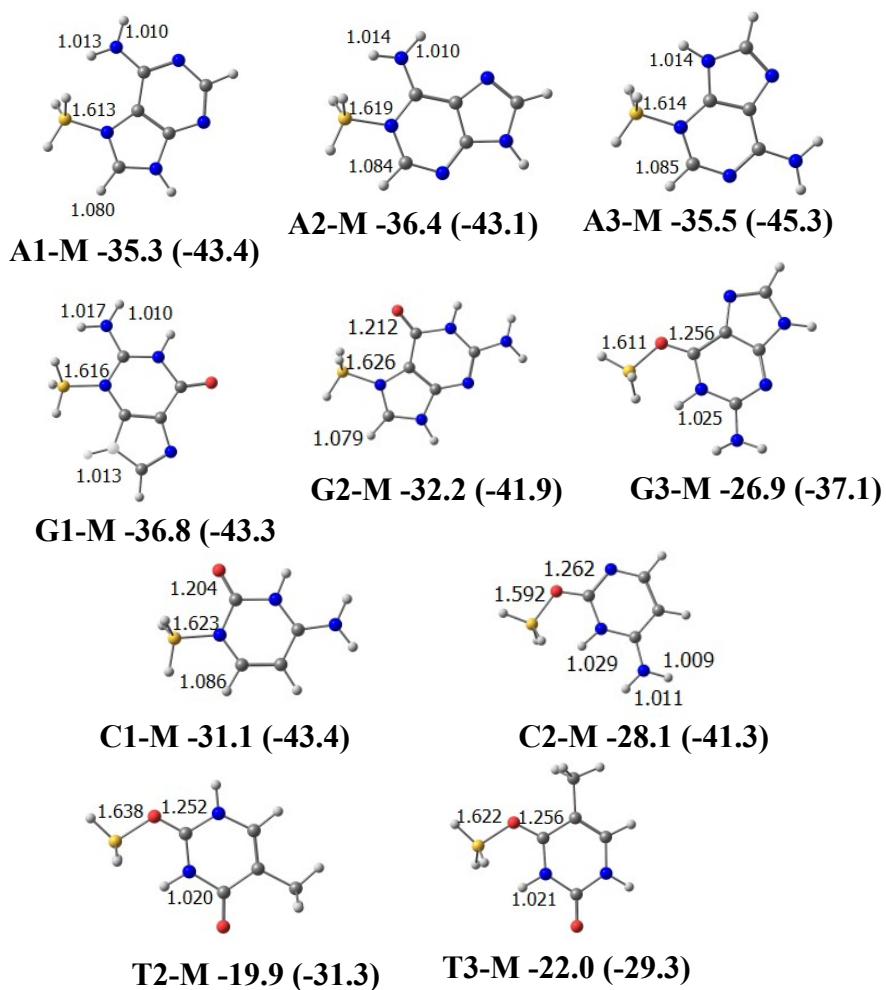
S5. Charge redistribution upon complexation

Since different schemes of partitioning electron density to one atom or another typically lead to discrepant atomic charges, maps of total electron density in space are considered to understand charge redistribution upon BN-cage-DNA complex formation. In addition, such a map of total density is independent primarily on methods and basis sets, whereas atomic charges estimation by various schemes strongly depends on the method of calculations. Redistributions of electron density upon $B_{12}N_{12}$-**A/G/C/T** complex formation are illustrated in Fig. S3. Electron densities of BN-cage and nucleobases were subtracted from the density of the total system at the MP2/6-311+G** level. As two units approach and form a complex structure, new bonds form between them, and some bonds may break, fully or partially. In the case of a new bond formation, electron density build-up along that particular bond, whereas depletion of electron density results in the region where bond breaking or weakening takes place upon complexation. The gain (loss) of electron density in BN-cage-DNA structure formation is shown in purple (yellow) color.

The purple and yellow color zones in all cases are localized in the union region of BN-cage and **A/G/C/T**. That indicates the electron density of the BN-cage outside of adsorption sites is not perturbed upon complex formation, which is also reflected in bond distances. As new BN or BO dative bond formed, electron density build-up along those bonds. However, loss of electron density (encircled yellow contours) is found outside those bonds' regions. There is a slight charge accumulation at the electron pair donating N and O atoms. Yellow contours near those atoms inside the pentagon or hexagon of nucleobases indicate loss of density in C-N-C area. Yellow contours in B-O linked four cases are spread over C=O bond region, supporting the weakening of those bonds in **G3**, **C2**, **T2** and **T3** complexes.

In the cases of H-bonds, the accepted notation [1] is the loss of density around the bridging hydrogen, and the lost density is shifted around the proton-accepting atoms. Charge accumulation in the area of the H-X (X = N, O, C) bond of the proton-donating molecule is also a common phenomenon of hydrogen bonding. In present cases, all three features of electron density shift of hydrogen bonding are exhibited: yellow contour on bridging H-atoms, and purple regions around proton-acceptor, as well as proton-acceptor donor atoms. Therefore, these changes in electron density upon complex formation between BN-cage and DNA nucleobases confirm the presence of N-HN and N-HC hydrogen bonds. Although the size of purple and yellow contours along hydrogen bond regions are slightly different from each other, the energetic contribution of H-bond strength

cannot be estimated from such a difference. In general, the strength of N-HN bonds varies in the range of 3 to 6 kcal/mol, whereas N-HC bond may contribute around 1-3 kcal/mol. [2-5].

Fig. S3. MP2/6-311+G** density redistribution (isosurface = 0.003au) upon complex formation. Purple and yellow zones represent density gain and loss, respectively.
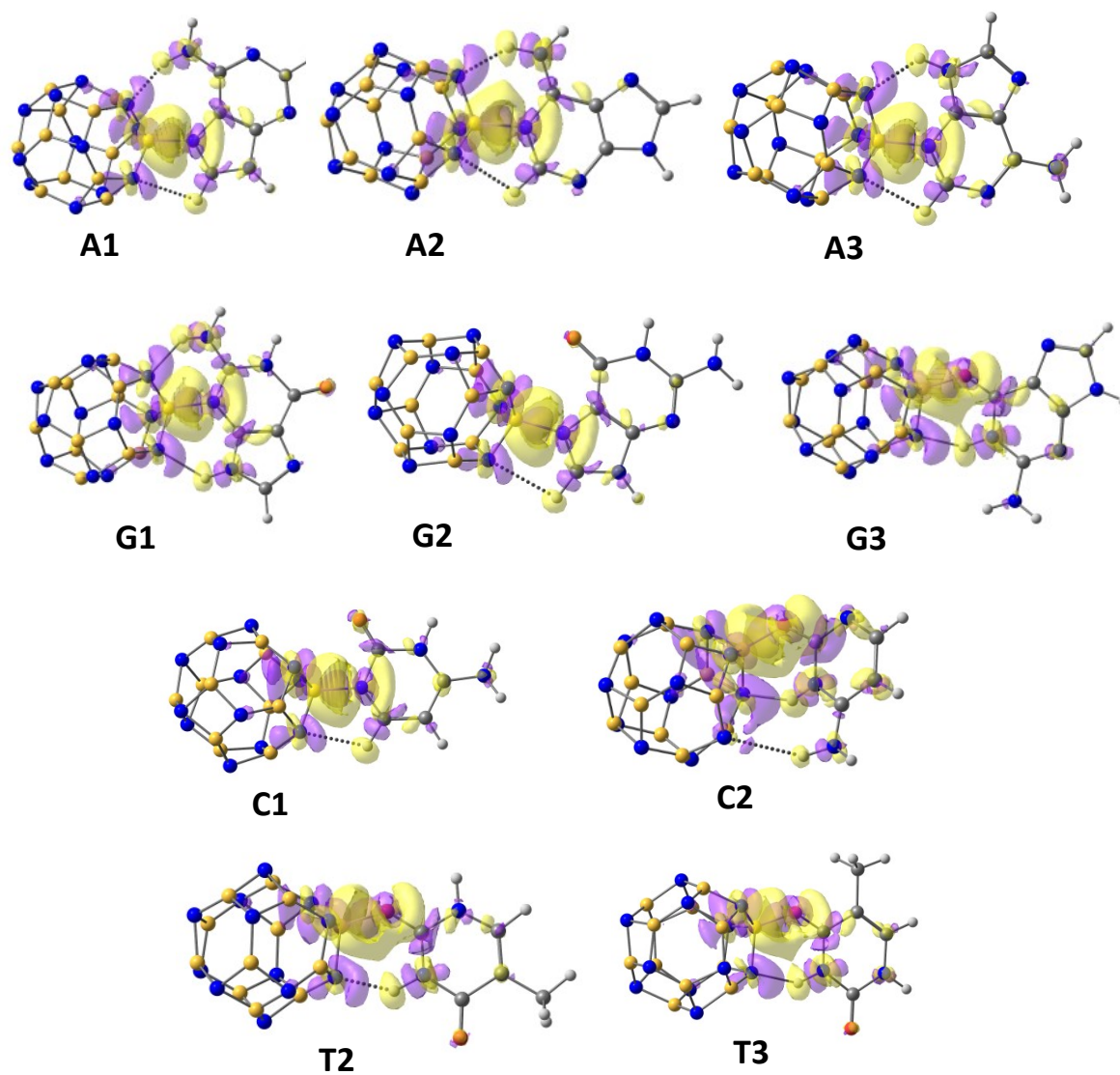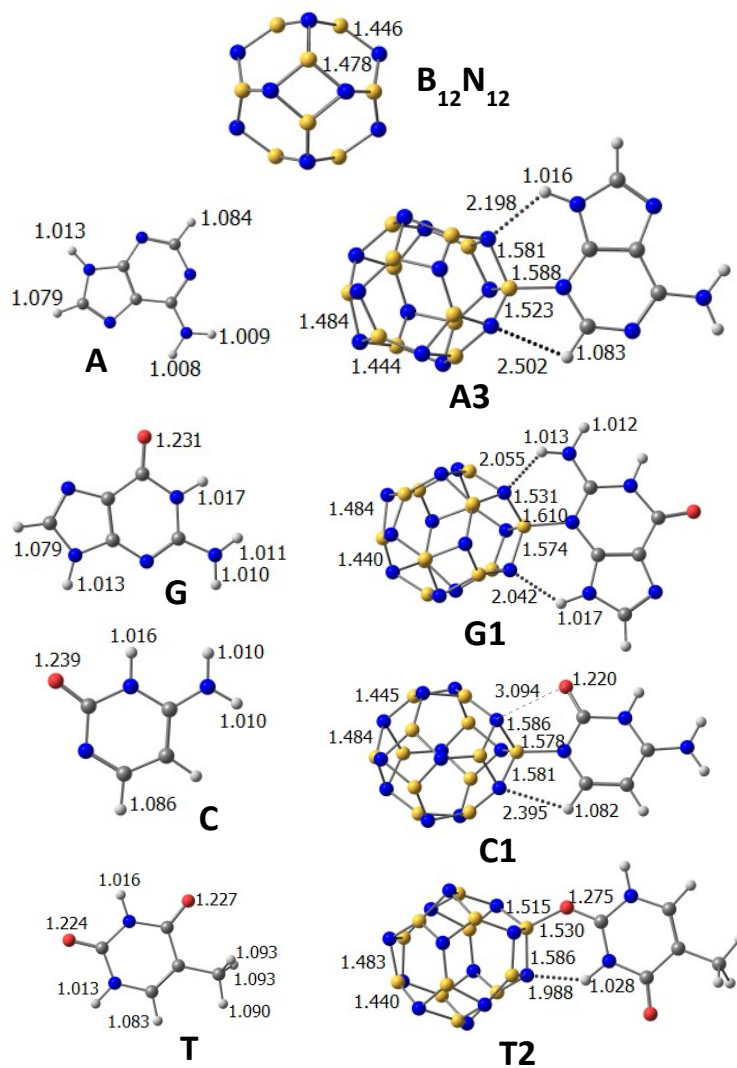
Fig. S4. M06-2X/6-311+G** optimized geometries of adenine (**A**), guanine (**G**), cytosine (**C**), thymine (**T**) and $B_{12}N_{12}$-**A/G/C/T** in aqueous media. Bond distances are in Angstrom (Å). Color scheme: Boron –Yellow, Nitrogen-Blue, Carbon-Grey, Oxygen- Red and Hydrogen-Silver.

S6. Assessment of BSSE correction at MP2 and DFT levels

BSSE correction to interaction/binding energy not only depends on the used method and basis set but also on the interaction types, non-covalent (H-bond, van der Waal, $\pi-\pi$ interaction) and covalent interaction. Since, in the present cases, the N$\rightarrow$B dative bond (covalent interaction) is the main force of interaction holding nucleobases at the surface of BN-cages, ammonia-borane (NH$_3$BH$_3$) seems to be a simplest model (without any environmental effect) to assess interaction energy and BSSE correction energy at different computational methods and basis sets. Binding energy, given in Table S5, is the difference in energy of ammonia borane and the sum of NH$_3$ and BH$_3$ energies. A negative value of BE is in support of favorable interaction.

As recommended in literature [6-8], energies from CCSD(T) method with aug-cc-pv6z basis set, which is close to the complete basis set limit (CBS), is considered as reference. CCSD(T) energies were also obtained using aug-cc-pvTz and 6-311+G** basis set, where later basis set is used for all calculations in this investigation. Number of basis functions of NH$_3$-BH$_3$ is 80 (6-311+G**), 230 (aug-cc-pvTz), 1140 (aug-cc-pv6z). MP2/6-311+G** optimized geometries were used for all CCSD(T) calculations.

Binding energies from aug-cc-pvTz and 6-311+G** are slightly lower (weaker interaction) than the reference value of -31.57 kcal/mol at CCSD(T)/aug-cc-pv6z.. Interestingly, CCSD(T)/6-311+G** predicted binding energy of -31.38 kcal/mol is closer to the reference value, than the corresponding estimate of -31.14 kcal/mol at the CCSD(T)/aug-cc-pvTz. However, the BSSE correction energy of 4.67 kcal/mol at 6-311+G** is significantly larger compared to the reference value of 0.07 kcal/mol. Hence the BSSE corrected BE value of ammonia-borane at the 6-311+G** is highly underestimated compared to that of aug-cc-pvTz basis set. Thus, the uncorrected CCSD(T) BE energies at lower basis sets are more reliable than the corrected values.

In the case of MP2 method, optimized geometries were used at each basis set considered here to obtain binding energies. Compared to the reference value of -31.57 kcal/mol, MP2 binding energies overestimated by 0.27 to 0.62 kcal/mol, where maximum deviation from reference BE is from aug-cc-pv6z basis set. MP2 BSSE energy of larger basis sets (aug-cc-pv6Z and aug-cc-pvTz) is slightly higher than the reference value of 0.07 kcal/mol, while corresponding 6-311+G** value is lower by 0.29 kcal/mol. Thus the BSSE correction to binding energy varies in a wider range than the uncorrected values. Similar to the MP2 method, estimated binding energies of ammonia-borane at the M06-2X method (-31.93 to -32.24 kcal/mol) is slightly higher than the reference value. Interestingly. BSSE correction energy at the 6-311+G** basis set is almost one-third than corresponding values at MP2 and CCSD(T).

In summary, BSSE correction to binding energy of ammonia-borane depends on both basis set and method. Non-corrected BE values at both MP2 and DFT levels are reasonably accurate, even at the 6-311+G** basis set.

Table S5. Comparison of binding energies (BE in kcal/mol) with and without BSSE correction of NH_3-BH_3 model.

Method/basis set[a] //Geometry (method/basis set)	BE	BSSE energy	BE-BSSE corrected
CCSD(T) SP/aug-cc-pv6z //MP2/6-311+G**	-31.57	0.07	-31.51
CCSD(T) SP/aug-cc-pvTz //MP2/6-311+G**	-31.14	0.92	-30.22
CCSD(T) SP/6311+G** //MP2/6-311+G**	-31.38	4.67	-26.70
MP2 OPT/aug-cc-pv6z	-32.19	0.14	-32.05
MP2 OPT/aug-cc-pvTz	-31.84	1.06	-30.78
MP2 OPT/6-311+G**	-31.98	4.38	-27.60
M06-2X OPT/aug-cc-pv6z	-31.93	0.11	-31.82
M06-2X OPT/aug-cc-pvTz	-31.59	0.15	-31.44
M06-2X OPT/6-311+G**	-32.24	1.34	-30.90

[a] Number of basis functions of NH_3-BH_3: 80 (6-311+G**), 230 (aug-cc-pvTz), 1140 (aug-cc-pv6z)

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Optimized Coordinates

B12N12-A/G/C/T complexes

B12N12 MP2/6-311+G** in gas-phase

7	-2.243256000	-0.898652000	-0.000300000
5	-2.084761000	0.456315000	0.469843000
5	-1.423573000	-1.113990000	-1.227863000
5	-1.163504000	-1.763812000	0.557194000
7	-1.427721000	0.877749000	1.741030000
7	-1.033947000	-0.103847000	-2.181757000
7	-0.571122000	-2.231997000	-0.729287000
7	-0.454441000	-1.551776000	1.795898000
5	-0.443146000	-0.099752000	2.137496000
5	-0.821745000	1.861269000	0.797259000
5	-0.975858000	1.231242000	-1.518947000
5	0.443143000	0.099772000	-2.137468000
5	0.821733000	-1.861243000	-0.797282000
5	0.975825000	-1.231229000	1.518933000
7	1.033940000	0.103855000	2.181752000
7	0.571111000	2.231990000	0.729292000
7	0.454428000	1.551792000	-1.795896000
7	1.427723000	-0.877736000	-1.741031000
7	1.734140000	-1.643455000	0.362578000
5	1.423577000	1.114007000	1.227872000
5	1.163493000	1.763811000	-0.557197000
5	2.084765000	-0.456319000	-0.469795000
7	2.243260000	0.898667000	0.000302000
7	-1.734145000	1.643449000	-0.362571000

A1 - MP2/6-311+G** in gas-phase

7	-1.567902000	0.157692000	-2.368486000
5	-1.360762000	1.350466000	-1.578656000
5	-0.930102000	-0.997439000	-1.675006000
5	-2.785843000	-0.558964000	-1.892033000
7	-2.431078000	2.149042000	-0.898395000
7	0.210250000	-0.968944000	-0.809573000
7	-2.150549000	-1.858029000	-1.532318000
7	-3.936421000	0.035562000	-1.250717000
5	-3.527525000	1.287610000	-0.545290000
5	-1.376969000	2.071702000	0.162331000
5	0.569580000	0.429648000	-0.165070000
5	-0.249724000	-1.294835000	0.566971000
5	-2.377367000	-2.144629000	-0.137660000
5	-4.021948000	-0.423619000	0.166883000
7	-3.948559000	0.907041000	0.836555000
7	-1.593969000	1.799788000	1.563845000
7	0.189478000	-0.090860000	1.274575000

7	-1.335042000	-2.191297000	0.923665000
7	-3.526275000	-1.673147000	0.692031000
5	-2.808151000	0.949901000	1.725475000
5	-0.948748000	0.494809000	1.904726000
5	-2.390326000	-1.409777000	1.627488000
7	-2.176557000	-0.214908000	2.402932000
7	-0.242797000	1.615555000	-0.659727000
7	4.871230000	-1.665691000	0.199350000
6	3.588739000	-1.334265000	-0.034044000
6	3.267171000	0.052451000	-0.059248000
6	4.355365000	0.932603000	0.037717000
7	5.639422000	0.625125000	0.234755000
6	5.800364000	-0.700880000	0.326622000
7	3.824024000	2.200733000	-0.111223000
6	2.491718000	2.087776000	-0.278837000
7	2.115706000	0.804608000	-0.257137000
7	2.685532000	-2.322316000	-0.190649000
1	6.812505000	-1.049217000	0.514206000
1	1.797095000	2.904564000	-0.409217000
1	3.067282000	-3.254596000	-0.276988000
1	1.787738000	-2.099233000	-0.621623000
1	4.353245000	3.063786000	-0.089653000

A2 - MP2/6-311+G** in gas-phase

7	1.561427000	0.801795000	-2.219875000
5	1.214966000	-0.573823000	-1.929656000
5	1.136799000	1.650499000	-1.073946000
5	2.892121000	1.122792000	-1.627989000
7	2.189256000	-1.695234000	-1.723370000
7	0.042603000	1.418881000	-0.177147000
7	2.471667000	2.239192000	-0.733130000
7	3.971201000	0.193997000	-1.383567000
5	3.414037000	-1.178342000	-1.177839000
5	1.207668000	-1.918859000	-0.613840000
5	-0.499024000	-0.071904000	-0.084065000
5	0.602007000	1.121373000	1.167834000
5	2.800672000	1.922923000	0.634659000
5	4.187380000	0.042254000	0.085335000
7	3.951455000	-1.425796000	0.194725000
7	1.528426000	-2.251953000	0.756104000
7	0.031833000	-0.207597000	1.396984000
7	1.826297000	1.667795000	1.729823000
7	3.905650000	1.031871000	1.098245000
5	2.860109000	-1.683681000	1.108532000
5	1.100617000	-1.121706000	1.635365000
5	2.787840000	0.554479000	1.968452000
7	2.440302000	-0.815638000	2.243272000

7	0.119414000	-1.043083000	-1.072743000
7	-2.102732000	-0.194996000	-0.121896000
6	-2.978708000	0.847181000	-0.087994000
6	-4.347225000	0.493437000	-0.014862000
6	-4.669652000	-0.862366000	0.031885000
7	-3.807704000	-1.900401000	0.012094000
6	-2.558274000	-1.493874000	-0.065620000
7	-6.039695000	-0.887738000	0.100529000
6	-6.462326000	0.418794000	0.092219000
7	-5.464416000	1.292118000	0.022653000
7	-2.584822000	2.120429000	-0.119444000
1	-1.772614000	-2.239869000	-0.101455000
1	-7.511212000	0.679753000	0.139074000
1	-1.583554000	2.323061000	-0.188182000
1	-3.299995000	2.833914000	-0.112132000
1	-6.616601000	-1.718136000	0.149022000

A3 - MP2/6-311+G** in gas-phase

7	1.459342000	0.387031000	-2.315143000
5	1.222311000	-0.950297000	-1.813018000
5	0.948593000	1.375468000	-1.325660000
5	2.750703000	0.907597000	-1.782455000
7	2.281350000	-1.938531000	-1.425619000
7	-0.139964000	1.205708000	-0.408489000
7	2.228895000	2.116848000	-1.082191000
7	3.897454000	0.122175000	-1.389490000
5	3.451015000	-1.240951000	-0.966882000
5	1.302773000	-2.064642000	-0.297742000
5	-0.547370000	-0.302065000	-0.085300000
5	0.427984000	1.164632000	0.965179000
5	2.560859000	2.050514000	0.319456000
5	4.102820000	0.226076000	0.084936000
7	3.984805000	-1.219479000	0.429039000
7	1.628509000	-2.142117000	1.108309000
7	-0.039360000	-0.151435000	1.402175000
7	1.592034000	1.895069000	1.438965000
7	3.725505000	1.338717000	0.924392000
5	2.903073000	-1.416760000	1.368971000
5	1.094573000	-0.925947000	1.791407000
5	2.636176000	0.916414000	1.856972000
7	2.394666000	-0.415411000	2.347349000
7	0.153260000	-1.369608000	-0.897153000
7	-3.988572000	-1.989369000	-0.001529000
6	-4.870501000	-0.967156000	0.071475000
6	-4.392107000	0.359486000	0.018343000
6	-3.008348000	0.532166000	-0.089168000
7	-2.124834000	-0.490905000	-0.148372000
6	-2.690615000	-1.716292000	-0.102099000

7	-2.806733000	1.879511000	-0.136964000
6	-4.052285000	2.454374000	-0.063267000
7	-5.040876000	1.572664000	0.036969000
7	-6.177723000	-1.251123000	0.184351000
1	-1.994210000	-2.546222000	-0.164630000
1	-4.181198000	3.528313000	-0.084540000
1	-6.471645000	-2.215553000	0.210057000
1	-6.854408000	-0.505151000	0.235465000
1	-1.877943000	2.284799000	-0.276962000

G1 - MP2/6-311+G** in gas-phase

7	1.653153000	2.149855000	0.986481000
5	1.384440000	1.977090000	-0.417020000
5	1.093599000	0.974374000	1.724515000
5	2.920512000	1.441605000	1.333152000
7	2.385704000	1.792759000	-1.504990000
7	-0.027966000	0.180573000	1.344536000
7	2.376872000	0.500275000	2.347180000
7	4.031083000	1.192827000	0.440150000
5	3.547132000	1.128681000	-0.970367000
5	1.341968000	0.786997000	-1.879129000
5	-0.505109000	0.230899000	-0.161052000
5	0.458027000	-1.157730000	1.000475000
5	2.635588000	-0.858588000	1.945545000
5	4.162033000	-0.271296000	0.185494000
7	4.005427000	-0.251952000	-1.300073000
7	1.597691000	-0.571319000	-2.293901000
7	-0.055393000	-1.271219000	-0.389611000
7	1.605380000	-1.858571000	1.549650000
7	3.754645000	-1.331675000	1.074303000
5	2.872309000	-1.060056000	-1.686698000
5	1.055959000	-1.497450000	-1.261860000
5	2.609809000	-2.078054000	0.473659000
7	2.324267000	-2.221960000	-0.933106000
7	0.235560000	1.260610000	-1.021125000
6	-3.825311000	-2.704570000	-0.058633000
7	-2.650096000	-2.012212000	-0.225343000
1	-1.691673000	-2.334793000	-0.375951000
6	-2.964074000	-0.690411000	-0.135949000
6	-4.343670000	-0.647553000	0.069195000
7	-4.872285000	-1.913031000	0.123184000
6	-5.007270000	0.622917000	0.203042000
8	-6.163731000	0.911340000	0.419435000
7	-4.042865000	1.678812000	-0.005330000
1	-4.444873000	2.607590000	0.077402000
6	-2.700481000	1.581512000	-0.177580000
7	-2.098079000	0.387950000	-0.262159000
7	-1.970035000	2.719239000	-0.221335000

1	-3.854150000	-3.785280000	-0.080147000
1	-2.467256000	3.583683000	-0.382211000
1	-1.063862000	2.609158000	-0.682331000

G2 - MP2/6-311+G** in gas-phase

7	1.001397000	-2.196258000	-0.169839000
5	0.816866000	-1.456860000	1.057868000
5	0.872747000	-1.258722000	-1.322249000
5	2.421371000	-2.133897000	-0.599494000
7	1.867074000	-1.241831000	2.113388000
7	0.119113000	-0.048266000	-1.371130000
7	2.226407000	-1.505277000	-1.936969000
7	3.573393000	-1.974777000	0.263034000
5	3.168626000	-1.245283000	1.503992000
5	1.260898000	0.124461000	1.985320000
5	-0.271177000	0.598430000	0.004482000
5	1.046789000	1.088320000	-1.459792000
5	2.953995000	-0.264659000	-2.000506000
5	4.215424000	-0.654593000	0.007089000
7	4.099753000	-0.079881000	1.379719000
7	1.991420000	1.374978000	1.931502000
7	0.643929000	1.856754000	-0.259477000
7	2.359402000	1.098181000	-2.092842000
7	4.192861000	0.081596000	-1.235104000
5	3.336305000	1.146619000	1.333457000
5	1.785030000	1.993108000	0.587718000
5	3.401687000	1.336620000	-1.058394000
7	3.224911000	2.071380000	0.169769000
7	0.045708000	-0.218036000	1.237768000
6	-2.196088000	2.336614000	-0.002738000
7	-3.554105000	2.386450000	0.004417000
1	-4.119665000	3.226123000	0.007992000
6	-4.039152000	1.098669000	0.014089000
6	-2.915201000	0.278681000	0.010485000
7	-1.790754000	1.067931000	0.002694000
6	-3.067423000	-1.158778000	-0.021149000
8	-2.230342000	-2.035416000	-0.062881000
7	-4.464689000	-1.458048000	0.011821000
1	-4.667817000	-2.450912000	0.077292000
6	-5.504006000	-0.560202000	0.010473000
7	-5.348685000	0.744714000	0.001321000
7	-6.768400000	-1.092248000	0.095922000
1	-1.525116000	3.182907000	-0.015765000
1	-6.925594000	-1.975906000	-0.368731000
1	-7.494882000	-0.408632000	-0.070697000

G3 - MP2/6-311+G** in gas-phase

7	1.796026000	0.553112000	-2.300934000
5	1.709318000	-0.853080000	-1.950327000
5	1.106202000	1.351565000	-1.257608000
5	2.974857000	1.169541000	-1.630020000
7	2.870045000	-1.736537000	-1.598027000
7	-0.005017000	0.944958000	-0.437455000
7	2.256178000	2.219893000	-0.846699000
7	4.191390000	0.498036000	-1.240205000
5	3.906124000	-0.951386000	-0.991363000
5	1.850932000	-2.111614000	-0.559054000
5	-0.230031000	-0.656736000	-0.286677000
5	0.494308000	0.817626000	0.964189000
5	2.516714000	2.038913000	0.559803000
5	4.298969000	0.462721000	0.247052000
7	4.355925000	-1.013157000	0.433815000
7	2.111837000	-2.296049000	0.853096000
7	0.179947000	-0.579478000	1.230616000
7	1.516069000	1.639370000	1.587995000
7	3.729794000	1.420208000	1.168384000
5	3.260118000	-1.449741000	1.271699000
5	1.383461000	-1.246149000	1.619962000
5	2.659400000	0.760832000	1.977013000
7	2.570955000	-0.634502000	2.313140000
7	0.662748000	-1.495903000	-1.157502000
6	-5.808916000	-2.000491000	0.155265000
7	-6.173047000	-0.674910000	0.276763000
1	-7.100420000	-0.304996000	0.441723000
6	-5.033815000	0.065726000	0.127126000
6	-4.020879000	-0.888486000	-0.074747000
7	-4.515886000	-2.172412000	-0.056358000
6	-2.713133000	-0.389698000	-0.253692000
8	-1.678837000	-1.110996000	-0.460283000
7	-2.629553000	0.976755000	-0.215030000
1	-1.648834000	1.326376000	-0.385212000
6	-3.688386000	1.819732000	0.009642000
7	-4.926564000	1.409988000	0.192826000
7	-3.403060000	3.160641000	-0.042346000
1	-6.536340000	-2.797685000	0.232259000
1	-2.467653000	3.442121000	0.219127000
1	-4.138779000	3.747303000	0.327007000

C1 - MP2/6-311+G** in gas-phase
7	1.233706000	1.470665000	-1.888495000
5	0.817098000	0.086620000	-1.994834000
5	0.863488000	1.974217000	-0.532195000
5	2.583416000	1.540624000	-1.262788000
7	1.727361000	-1.096529000	-2.148812000
7	-0.228437000	1.544817000	0.281786000

7	2.237772000	2.372814000	-0.075618000
7	3.613019000	0.527627000	-1.325573000
5	2.981734000	-0.817568000	-1.507330000
5	0.737489000	-1.583235000	-1.125204000
5	-0.825793000	0.118152000	-0.037038000
5	0.324311000	0.854134000	1.469690000
5	2.561788000	1.658606000	1.134196000
5	3.835503000	-0.051284000	0.031766000
7	3.522894000	-1.475265000	-0.278371000
7	1.064571000	-2.303898000	0.085511000
7	-0.309133000	-0.461638000	1.330127000
7	1.587219000	1.149416000	2.135261000
7	3.621776000	0.617270000	1.293672000
5	2.425490000	-1.928116000	0.550476000
5	0.705094000	-1.460003000	1.263483000
5	2.485277000	-0.033687000	2.017729000
7	2.069082000	-1.407105000	1.900221000
7	-0.295221000	-0.552862000	-1.286522000
6	-4.460034000	1.460988000	-0.028807000
6	-3.075196000	1.349309000	-0.037383000
7	-2.420108000	0.187266000	-0.047366000
6	-3.099528000	-1.030600000	-0.027744000
8	-2.586312000	-2.123789000	-0.012858000
7	-4.512279000	-0.889329000	-0.028771000
1	-5.000195000	-1.779858000	-0.048399000
6	-5.197065000	0.277525000	-0.019607000
7	-6.553367000	0.226244000	-0.068298000
1	-4.945063000	2.427687000	-0.018439000
1	-2.426452000	2.222208000	-0.026450000
1	-7.025193000	-0.618424000	0.221002000
1	-7.051723000	1.083171000	0.120826000

C2 - MP2/6-311+G** in gas-phase

7	-1.615406000	-1.655010000	-1.737652000
5	-0.615014000	-0.628642000	-1.904261000
5	-1.609683000	-2.109684000	-0.311927000
5	-2.891784000	-1.048565000	-1.274992000
7	-0.878376000	0.814681000	-2.248651000
7	-0.509528000	-2.090894000	0.593759000
7	-3.046490000	-1.795130000	0.002529000
7	-3.343746000	0.303949000	-1.534714000
5	-2.168137000	1.197588000	-1.745166000
5	0.132105000	0.922559000	-1.153103000
5	0.696972000	-1.194272000	0.226458000
5	-0.772485000	-1.113609000	1.652666000
5	-3.104967000	-0.875346000	1.105876000
5	-3.385358000	1.078984000	-0.264155000

7	-2.435671000	2.173748000	-0.643017000
7	0.113383000	1.875055000	-0.045308000
7	0.403379000	-0.218555000	1.493662000
7	-2.077545000	-0.722292000	2.173069000
7	-3.592541000	0.541512000	1.058683000
5	-1.323296000	2.198967000	0.272890000
5	-0.090178000	1.089192000	1.223479000
5	-2.348505000	0.702914000	1.862281000
7	-1.348299000	1.732519000	1.684475000
7	0.607441000	-0.458542000	-1.107771000
6	5.075665000	0.616220000	-0.367136000
6	5.193364000	-0.766428000	-0.517408000
7	4.225255000	-1.665445000	-0.281290000
6	3.076807000	-1.174020000	0.178731000
8	2.032531000	-1.909936000	0.350749000
7	2.961863000	0.154905000	0.502956000
1	2.105397000	0.390785000	1.025165000
6	3.874532000	1.091759000	0.162629000
7	3.548308000	2.384953000	0.424885000
1	5.871853000	1.291062000	-0.656416000
1	6.128710000	-1.179996000	-0.889112000
1	2.559086000	2.621044000	0.399383000
1	4.166652000	3.091710000	0.053712000

T1 - MP2/6-311+G** in gas-phase

7	-0.549621000	-2.242304000	-0.352575000
5	-0.749603000	-1.383123000	-1.497386000
5	-0.020647000	-1.427528000	0.782930000
5	-1.757973000	-2.199429000	0.524254000
7	-2.062599000	-1.038969000	-2.124338000
7	0.774963000	-0.244394000	0.691086000
7	-1.109368000	-1.708298000	1.771558000
7	-3.112989000	-1.927594000	0.103089000
5	-3.100994000	-1.082232000	-1.127774000
5	-1.386734000	0.295429000	-2.087625000
5	0.687954000	0.521316000	-0.656837000
5	-0.019427000	0.903363000	1.184183000
5	-1.713866000	-0.466076000	2.187033000
5	-3.572395000	-0.627228000	0.674868000
7	-3.874508000	0.081481000	-0.602708000
7	-1.986732000	1.543810000	-1.682426000
7	0.017288000	1.762916000	-0.016648000
7	-1.051305000	0.867572000	2.202984000
7	-3.110088000	-0.020950000	1.899573000
5	-3.077515000	1.283905000	-0.699549000
5	-1.325441000	2.024560000	-0.431338000
5	-2.358370000	1.232993000	1.589648000

7	-2.544705000	2.081010000	0.439454000
7	-0.003239000	-0.148224000	-1.814602000
6	4.091497000	-2.416274000	-0.503838000
6	3.566295000	-1.015836000	-0.421132000
6	2.890718000	-0.416122000	-1.417122000
7	2.273804000	0.872158000	-1.201196000
1	2.135828000	1.383176000	-2.078325000
6	2.957590000	1.785928000	-0.280183000
8	2.929427000	2.976205000	-0.457729000
7	3.526150000	1.116828000	0.768741000
1	3.900177000	1.690213000	1.519651000
6	3.823558000	-0.262115000	0.829484000
8	4.334376000	-0.738736000	1.822505000
1	5.168892000	-2.432996000	-0.317671000
1	3.616692000	-3.031761000	0.266144000
1	3.884117000	-2.849610000	-1.484897000
1	2.629846000	-0.888527000	-2.357475000

T2 - MP2/6-311+G** in gas-phase

7	1.913659000	2.261602000	0.853055000
5	1.533883000	2.072518000	-0.530274000
5	1.221409000	1.237728000	1.688588000
5	3.067889000	1.382808000	1.185547000
7	2.450549000	1.658779000	-1.644709000
7	-0.030484000	0.607344000	1.409759000
7	2.442396000	0.598046000	2.287392000
7	4.077405000	0.907181000	0.265445000
5	3.510815000	0.846352000	-1.116707000
5	1.241352000	0.807256000	-1.893450000
5	-0.540851000	0.667981000	-0.069569000
5	0.211777000	-0.809365000	1.134049000
5	2.459599000	-0.803634000	1.959763000
5	3.960521000	-0.569312000	0.100070000
7	3.730247000	-0.611390000	-1.373507000
7	1.255054000	-0.601319000	-2.235557000
7	-0.392888000	-0.917372000	-0.224192000
7	1.264270000	-1.648465000	1.675978000
7	3.441157000	-1.500814000	1.074063000
5	2.465903000	-1.249288000	-1.655119000
5	0.629760000	-1.371088000	-1.127822000
5	2.162788000	-2.088638000	0.574359000
7	1.783417000	-2.267935000	-0.804945000
7	0.279052000	1.490898000	-1.024369000
6	-4.357541000	2.674897000	0.127706000
6	-4.336162000	1.177019000	0.049249000
6	-5.448386000	0.388385000	0.085089000
7	-5.375518000	-0.977532000	0.014350000
1	-6.216365000	-1.540892000	0.039758000

6	-4.190294000	-1.694636000	-0.106492000
8	-4.131171000	-2.902006000	-0.179344000
7	-3.069342000	-0.860481000	-0.134998000
1	-2.120074000	-1.290074000	-0.225179000
6	-3.076221000	0.492486000	-0.067379000
8	-2.005141000	1.177464000	-0.113515000
1	-3.793449000	3.020255000	0.998535000
1	-3.890473000	3.111240000	-0.759459000
1	-5.385143000	3.038981000	0.203275000
1	-6.447813000	0.803089000	0.175146000

T3 - MP2/6-311+G** in gas-phase

7	1.488112000	1.059898000	-2.239266000
5	1.592742000	-0.384462000	-2.187063000
5	0.679252000	1.528214000	-1.081862000
5	2.561606000	1.673849000	-1.407594000
7	2.856459000	-1.163790000	-1.972394000
7	-0.367541000	0.809988000	-0.407922000
7	1.697046000	2.433024000	-0.457959000
7	3.854518000	1.100976000	-1.113658000
5	3.768568000	-0.391351000	-1.176201000
5	1.886730000	-1.875118000	-1.074525000
5	-0.356615000	-0.775542000	-0.591598000
5	0.116435000	0.476111000	0.960022000
5	1.961331000	2.004810000	0.892697000
5	3.947098000	0.774307000	0.338880000
7	4.203844000	-0.689347000	0.222892000
7	2.149692000	-2.314147000	0.279260000
7	-0.005609000	-0.983295000	0.924401000
7	1.014336000	1.270649000	1.775892000
7	3.241509000	1.436471000	1.411075000
5	3.167355000	-1.428792000	0.908664000
5	1.276035000	-1.547975000	1.214806000
5	2.260017000	0.490345000	2.023218000
7	2.359540000	-0.945431000	2.064242000
7	0.630833000	-1.313237000	-1.585934000
6	-6.733964000	0.593545000	0.674456000
6	-5.400645000	0.058729000	0.249278000
6	-5.190419000	-1.234271000	-0.104270000
7	-3.938027000	-1.690841000	-0.487106000
1	-3.775941000	-2.662282000	-0.722142000
6	-2.859076000	-0.878421000	-0.536005000
8	-1.754082000	-1.376245000	-0.920923000
7	-3.043656000	0.408125000	-0.202086000
1	-2.183066000	0.990024000	-0.264691000
6	-4.268344000	0.991290000	0.219722000
8	-4.317396000	2.171450000	0.508305000
1	-6.669853000	1.001981000	1.686846000

1	-7.040324000	1.409857000	0.014498000
1	-7.494631000	-0.190440000	0.652120000
1	-5.976350000	-1.982090000	-0.107300000

b12n12 MP2/6-311+G** water phase

7	-0.009719000	0.008251000	-0.013738000
5	-0.005802000	0.005352000	1.430456000
5	1.391786000	0.011855000	-0.526297000
5	0.081403000	-1.391007000	-0.528056000
7	-0.475436000	-1.103878000	2.312400000
7	1.069391000	0.547313000	2.312028000
7	2.551728000	0.543153000	0.152211000
7	1.336772000	-1.248897000	-1.322944000
7	-0.370914000	-2.582738000	0.151811000
5	-0.345458000	-2.370114000	1.629959000
5	0.807098000	-0.755120000	2.991288000
5	2.341873000	0.501963000	1.629104000
5	3.485145000	-0.563953000	0.516507000
5	2.332589000	-2.178946000	-0.844822000
5	0.797814000	-3.436030000	0.517362000
7	0.587959000	-3.477220000	1.994255000
7	1.802915000	-1.685170000	3.469410000
7	3.510601000	-0.351329000	1.994655000
7	3.615123000	-1.830189000	-0.165934000
7	2.070296000	-3.481379000	-0.165562000
5	1.747901000	-2.945922000	2.672763000
5	3.058284000	-1.543060000	2.674522000
5	3.145489000	-2.939419000	0.716010000
7	3.149406000	-2.942317000	2.160204000

A3 - MP2/6-311+G** water phase

7	1.485551000	0.451187000	-2.309068000
5	1.232129000	-0.896198000	-1.837737000
5	0.965658000	1.410883000	-1.288658000
5	2.772576000	0.949587000	-1.747538000
7	2.285683000	-1.909317000	-1.478979000
7	-0.114575000	1.209087000	-0.381999000
7	2.255409000	2.139752000	-1.016013000
7	3.914776000	0.142567000	-1.368753000
5	3.451389000	-1.227287000	-0.986434000
5	1.292724000	-2.057593000	-0.360760000
5	-0.558561000	-0.289106000	-0.106867000
5	0.428069000	1.136453000	0.987647000
5	2.576042000	2.028006000	0.386438000
5	4.111297000	0.201602000	0.110107000
7	3.982210000	-1.254146000	0.411658000
7	1.613791000	-2.181082000	1.046781000

7	-0.049316000	-0.189741000	1.397650000
7	1.600152000	1.846762000	1.494994000
7	3.736587000	1.292919000	0.979792000
5	2.888864000	-1.469457000	1.338005000
5	1.078044000	-0.979892000	1.760611000
5	2.632901000	0.850472000	1.889655000
7	2.382215000	-0.495278000	2.343934000
7	0.156869000	-1.338166000	-0.946542000
7	-3.975138000	-1.979063000	-0.042929000
6	-4.874540000	-0.963724000	0.035277000
6	-4.402027000	0.365298000	-0.015348000
6	-3.019993000	0.557959000	-0.109858000
7	-2.126909000	-0.461362000	-0.183073000
6	-2.681992000	-1.690843000	-0.136683000
7	-2.834173000	1.907059000	-0.136159000
6	-4.078812000	2.469196000	-0.052986000
7	-5.060405000	1.575200000	0.025479000
7	-6.178280000	-1.268252000	0.094210000
1	-1.981888000	-2.517940000	-0.185867000
1	-4.211270000	3.542321000	-0.054266000
1	-6.435986000	-2.228514000	0.286040000
1	-6.840627000	-0.542716000	0.336353000
1	-1.929689000	2.368359000	-0.227030000

G1 - MP2/6-311+G** water phase

7	1.683590000	2.236273000	0.795822000
5	1.373628000	1.940690000	-0.584766000
5	1.134866000	1.131821000	1.643879000
5	2.953468000	1.555360000	1.174308000
7	2.360164000	1.660776000	-1.676455000
7	0.002040000	0.312427000	1.372519000
7	2.434283000	0.709614000	2.283723000
7	4.046896000	1.224217000	0.282585000
5	3.526386000	1.037520000	-1.107419000
5	1.300621000	0.624098000	-1.925177000
5	-0.508255000	0.225870000	-0.131942000
5	0.472570000	-1.057565000	1.127805000
5	2.678102000	-0.681970000	1.992700000
5	4.166761000	-0.258137000	0.155891000
7	3.978463000	-0.370569000	-1.322017000
7	1.548098000	-0.769723000	-2.230972000
7	-0.058205000	-1.283693000	-0.231123000
7	1.638748000	-1.710817000	1.715417000
7	3.780298000	-1.236206000	1.145889000
5	2.831366000	-1.206266000	-1.608652000
5	1.023065000	-1.596983000	-1.105245000
5	2.617191000	-2.029083000	0.639266000
7	2.302204000	-2.297629000	-0.743285000

7	0.223476000	1.171885000	-1.088161000
6	-3.859246000	-2.697988000	-0.346860000
7	-2.673190000	-2.018707000	-0.419753000
1	-1.724915000	-2.384541000	-0.515385000
6	-2.960426000	-0.704250000	-0.217796000
6	-4.340531000	-0.646149000	-0.048316000
7	-4.899488000	-1.901219000	-0.125555000
6	-4.974862000	0.614107000	0.187562000
8	-6.163595000	0.856788000	0.384766000
7	-4.032135000	1.661681000	0.148266000
1	-4.418053000	2.597330000	0.272661000
6	-2.687279000	1.563678000	-0.022434000
7	-2.093625000	0.372743000	-0.214850000
7	-1.956770000	2.688319000	0.059931000
1	-3.902190000	-3.771455000	-0.464680000
1	-2.461059000	3.568593000	0.036045000
1	-1.059483000	2.670186000	-0.416692000

C1 - MP2/6-311+G** water phase

7	-0.002782000	0.001613000	0.006372000
5	-0.002303000	-0.004621000	1.456519000
5	1.420679000	0.003573000	-0.456958000
5	0.100701000	-1.393109000	-0.501434000
7	-0.532721000	-1.112434000	2.329359000
7	1.025113000	0.536719000	2.343704000
7	2.548427000	0.545818000	0.216413000
7	1.364483000	-1.260494000	-1.278755000
7	-0.372274000	-2.589609000	0.167126000
5	-0.370677000	-2.367499000	1.648013000
5	0.763173000	-0.740470000	3.004792000
5	2.421273000	0.808924000	1.776813000
5	3.423013000	-0.561791000	0.630633000
5	2.346932000	-2.189491000	-0.777517000
5	0.790289000	-3.440367000	0.558050000
7	0.554496000	-3.480118000	2.031396000
7	1.743359000	-1.676062000	3.520256000
7	3.478031000	-0.344077000	2.080405000
7	2.948634000	2.236865000	2.154237000
7	3.608199000	-1.833747000	-0.073885000
7	2.071127000	-3.500472000	-0.107758000
5	1.704178000	-2.934129000	2.726796000
5	3.004933000	-1.516367000	2.729157000
5	3.124863000	-2.939923000	0.795710000
7	3.110648000	-2.940769000	2.237646000
6	3.123423000	3.208183000	1.218059000
6	3.540914000	4.476726000	1.512173000
6	3.809005000	4.780952000	2.865726000
1	3.667444000	5.227349000	0.743197000

1	2.903911000	2.905984000	0.199819000
6	3.190667000	2.495377000	3.483374000
8	3.042729000	1.671717000	4.384345000
7	3.627988000	3.788801000	3.770338000
1	3.805468000	3.970392000	4.758188000
7	4.186725000	5.981800000	3.287731000
1	4.472139000	6.126633000	4.249274000
1	4.421956000	6.686771000	2.600709000

T2 - MP2/6-311+G** water phase

7	1.623989000	0.320650000	-2.354489000
5	1.684421000	-1.030055000	-1.830976000
5	0.768433000	1.141840000	-1.446772000
5	2.671310000	1.160241000	-1.707878000
7	2.921411000	-1.713675000	-1.314187000
7	-0.314120000	0.688767000	-0.632099000
7	1.786520000	2.194373000	-1.099855000
7	3.937505000	0.699177000	-1.177872000
5	3.812779000	-0.731617000	-0.759634000
5	1.888367000	-2.081360000	-0.285228000
5	-0.366681000	-0.870427000	-0.301800000
5	0.087363000	0.811229000	0.786131000
5	1.977063000	2.221281000	0.330157000
5	3.954647000	0.857571000	0.306214000
7	4.179830000	-0.568853000	0.681406000
7	2.080684000	-2.067740000	1.151105000
7	-0.070895000	-0.578729000	1.227145000
7	0.973665000	1.821829000	1.353210000
7	3.221487000	1.840796000	1.070351000
5	3.090180000	-1.036519000	1.514145000
5	1.180481000	-1.028562000	1.741115000
5	2.185739000	1.151579000	1.901279000
7	2.245851000	-0.196796000	2.409935000
7	0.674423000	-1.709597000	-1.015652000
6	-6.751520000	0.725194000	0.400854000
6	-5.400492000	0.122056000	0.175832000
6	-5.163100000	-1.213825000	0.257226000
7	-3.903023000	-1.740355000	0.045199000
1	-3.740942000	-2.742014000	0.124614000
6	-2.857237000	-0.970991000	-0.270825000
8	-1.723596000	-1.533376000	-0.507078000
7	-3.063194000	0.352528000	-0.363038000
1	-2.234805000	0.915919000	-0.609639000
6	-4.291499000	1.003743000	-0.146351000
8	-4.353899000	2.227180000	-0.249403000
1	-6.716042000	1.432427000	1.234886000
1	-7.072842000	1.273205000	-0.489871000
1	-7.483247000	-0.054157000	0.624156000

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1      -5.930390000    -1.941904000     0.494347000

B16N16 - M06-2X/6-311+G** gas-phase
5      0.654523000     2.358362000     0.654523000
7      1.464273000     1.464273000     1.464273000
5      1.493908000    -1.493908000     1.493908000
7      0.794011000    -2.563000000     0.794011000
5     -0.654523000    -2.358362000     0.654523000
5      0.654523000     0.654523000     2.358362000
5      2.358362000     0.654523000     0.654523000
5      0.654523000    -0.654523000    -2.358362000
5     -2.358362000     0.654523000    -0.654523000
5     -0.654523000     2.358362000    -0.654523000
5      0.654523000    -2.358362000    -0.654523000
5     -0.654523000     0.654523000    -2.358362000
5     -0.654523000    -0.654523000     2.358362000
5      2.358362000    -0.654523000    -0.654523000
5     -2.358362000    -0.654523000     0.654523000
7     -1.464273000    -1.464273000     1.464273000
7      1.464273000    -1.464273000    -1.464273000
7     -1.464273000     1.464273000    -1.464273000
5     -1.493908000     1.493908000     1.493908000
5      1.493908000     1.493908000    -1.493908000
5     -1.493908000    -1.493908000    -1.493908000
7     -0.794011000     2.563000000     0.794011000
7      0.794011000     0.794011000    -2.563000000
7     -2.563000000     0.794011000     0.794011000
7      0.794011000    -0.794011000     2.563000000
7      2.563000000     0.794011000    -0.794011000
7     -0.794011000    -2.563000000    -0.794011000
7      0.794011000     2.563000000    -0.794011000
7     -0.794011000     0.794011000     2.563000000
7     -0.794011000    -0.794011000    -2.563000000
7     -2.563000000    -0.794011000    -0.794011000
7      2.563000000    -0.794011000     0.794011000

B16N16 - A1 M06-2X/6-311+G** gas-phase
5     -3.483470000     1.616164000     0.623648000
7     -2.562295000     2.354153000    -0.225544000
5     -0.057317000     1.389158000    -1.483128000
7      0.727829000     0.186437000    -1.535914000
5      1.162694000    -0.549306000    -0.234300000
5     -1.246550000     2.484789000     0.380416000
5     -2.489285000     1.790882000    -1.563983000
5     -2.333098000    -1.893749000    -1.488376000
5     -1.850333000    -1.339824000     2.131786000
5     -3.748458000    -0.049572000     1.386579000
5     -0.098199000    -1.002224000    -1.686608000
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5	-3.096545000	-2.034300000	0.189318000
5	0.190655000	1.462027000	0.960274000
5	-1.993312000	0.263544000	-2.478750000
5	-0.133698000	-0.658711000	1.930518000
7	0.704012000	0.130810000	1.070369000
7	-1.443786000	-1.057743000	-2.267519000
7	-3.153281000	-1.371056000	1.481566000
5	-1.803070000	1.107169000	2.344419000
5	-3.973468000	-0.107634000	-1.066567000
5	-0.651881000	-2.352755000	0.239123000
7	-3.218309000	1.176557000	2.001119000
7	-3.697325000	-1.537414000	-1.058054000
7	-1.248511000	-0.166276000	2.771039000
7	0.041811000	2.242437000	-0.293089000
7	-3.341531000	0.714380000	-2.089823000
7	0.394935000	-1.847375000	-0.610929000
7	-4.369482000	0.528189000	0.184701000
7	-0.897310000	2.074963000	1.742262000
7	-1.931974000	-2.738638000	-0.357238000
7	-0.635735000	-2.019460000	1.660624000
7	-1.255480000	1.520680000	-2.310021000
7	5.373643000	1.726655000	0.070274000
6	4.102313000	1.328289000	-0.074274000
6	3.852476000	-0.066502000	-0.068340000
6	4.973568000	-0.880886000	0.037678000
7	6.239033000	-0.503058000	0.165795000
6	6.344763000	0.821721000	0.183673000
7	4.499444000	-2.176429000	-0.017212000
6	3.159723000	-2.126735000	-0.145285000
7	2.730766000	-0.884500000	-0.175245000
7	3.163107000	2.271615000	-0.205131000
1	7.346805000	1.221071000	0.298274000
1	2.503845000	-2.979374000	-0.219113000
1	3.476116000	3.230053000	-0.220288000
1	2.197267000	2.079059000	-0.426083000
1	5.068660000	-3.008900000	0.030439000

B16N16 - G1 M06-2X/6-311+G** gas-phase

5	-3.780780000	0.603281000	1.414057000
7	-2.873100000	1.732910000	1.517677000
5	-0.215074000	2.064663000	0.265025000
7	0.683034000	1.331853000	-0.605878000
5	1.104315000	-0.128118000	-0.248364000
5	-1.616266000	1.368921000	2.156784000
5	-2.659082000	2.375624000	0.232437000
5	-2.185793000	-0.092937000	-2.471267000
5	-1.997710000	-2.465587000	0.358196000

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5    -3.945233000    -1.066627000     0.631471000
5    -0.026932000     0.648124000    -1.685222000
5    -3.044509000    -1.458095000    -1.567406000
5    -0.125376000     0.282329000     1.930886000
5    -1.966027000     2.066869000    -1.454343000
5    -0.349386000    -1.838112000     0.935125000
7     0.477887000    -0.677382000     1.051021000
7    -1.318784000     1.045431000    -2.249894000
7    -3.242581000    -2.001228000    -0.233815000
5    -2.181185000    -1.014952000     2.342036000
5    -3.999759000     0.746624000    -1.035958000
5    -0.593996000    -1.678614000    -1.504567000
7    -3.569941000    -0.723973000     2.010399000
7    -3.600379000    -0.194755000    -2.073463000
7    -1.549468000    -2.171044000     1.720324000
7    -0.272279000     1.727532000     1.678919000
7    -3.371389000     2.060645000    -1.014765000
7     0.466506000    -0.708489000    -1.550415000
7    -4.532958000     0.214110000     0.211630000
7    -1.322450000     0.074040000     2.775548000
7    -1.787650000    -1.497635000    -2.323463000
7    -0.691373000    -2.545441000    -0.324984000
7    -1.355304000     2.767351000    -0.318809000
6     4.550387000     2.686597000    -0.090137000
7     3.343956000     2.037943000    -0.231591000
1     2.418445000     2.399351000    -0.444122000
6     3.610115000     0.715275000    -0.128823000
6     4.973820000     0.621178000     0.073970000
7     5.544100000     1.868572000     0.096363000
6     5.589114000    -0.673416000     0.181692000
8     6.728404000    -1.004870000     0.353637000
7     4.586092000    -1.695866000     0.021688000
1     4.968359000    -2.633303000     0.045617000
6     3.253867000    -1.539801000    -0.160821000
7     2.706674000    -0.326338000    -0.214159000
7     2.501164000    -2.642275000    -0.264367000
1     4.618653000     3.762356000    -0.133963000
1     2.929855000    -3.551740000    -0.230403000
1     1.535322000    -2.595389000    -0.561706000

B16N16 - C1 M06-2X/6-311+G** gas-phase
5    -3.552477000     0.251381000     1.350673000
7    -2.784821000     1.462800000     1.584250000
5    -0.132570000     2.192502000     0.475609000
7     0.859493000     1.630629000    -0.406341000
5     1.407571000     0.194168000    -0.151450000
5    -1.515585000     1.184307000     2.244531000
5    -2.598662000     2.229571000     0.363989000
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5	-1.756829000	0.060788000	-2.501305000
5	-1.403383000	-2.498878000	0.133499000
5	-3.504424000	-1.353470000	0.430784000
5	0.269792000	0.966679000	-1.565041000
5	-2.486004000	-1.458873000	-1.748508000
5	0.088784000	0.286969000	1.993059000
5	-1.820287000	2.142854000	-1.309674000
5	0.161028000	-1.770048000	0.820138000
7	0.825757000	-0.523077000	1.074528000
7	-1.038237000	1.270458000	-2.157163000
7	-2.677249000	-2.129773000	-0.473361000
5	-1.810115000	-1.257727000	2.211822000
5	-3.702849000	0.575399000	-1.086372000
5	-0.017635000	-1.427063000	-1.595964000
7	-3.215839000	-1.089509000	1.848148000
7	-3.167530000	-0.225495000	-2.178058000
7	-1.034818000	-2.283278000	1.537073000
7	-0.206886000	1.728583000	1.858046000
7	-3.232238000	1.946592000	-0.933494000
7	0.909758000	-0.329726000	-1.524680000
7	-4.220026000	-0.112714000	0.091124000
7	-1.102439000	-0.117385000	2.774273000
7	-1.208903000	-1.297707000	-2.450001000
7	-0.087497000	-2.382137000	-0.495784000
7	-1.332814000	2.811100000	-0.096638000
6	5.075329000	1.457200000	-0.008602000
6	3.697263000	1.366456000	-0.056508000
7	3.019638000	0.223353000	-0.064573000
6	3.676635000	-0.994743000	-0.038372000
8	3.156402000	-2.072431000	-0.052603000
7	5.088985000	-0.891016000	0.010758000
1	5.552751000	-1.791648000	0.028627000
6	5.791006000	0.261731000	0.024728000
7	7.131088000	0.195539000	0.069467000
1	5.577972000	2.411402000	-0.002750000
1	3.067915000	2.249606000	-0.099449000
1	7.626190000	-0.680707000	0.087246000
1	7.672801000	1.043468000	0.077691000

B16N16 - T2 M06-2X/6-311+G** gas-phase

5	3.513074000	1.590312000	0.918645000
7	2.824379000	1.025749000	2.066106000
5	0.581147000	-0.924214000	2.090253000
7	-0.212916000	-1.635235000	1.132641000
5	-0.939249000	-0.908057000	-0.012274000
5	1.420293000	1.397900000	2.099462000
5	2.999942000	-0.417065000	2.149834000

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5      2.658281000     -2.029859000     -1.151924000
5      1.466989000      1.321722000     -2.151351000
5      3.533718000      1.557327000     -0.932610000
5      0.563197000     -2.171820000      0.027725000
5      3.046751000     -0.493278000     -2.101434000
5     -0.152454000      1.209548000      1.146362000
5      2.631878000     -1.986909000      1.247392000
5     -0.127598000      1.167659000     -1.228002000
7     -0.767110000      0.640733000     -0.037525000
7      1.994758000     -2.487834000      0.049209000
7      2.869960000      0.951517000     -2.073680000
5      1.490147000      2.598013000     -0.047923000
5      4.256997000     -0.588049000      0.040074000
5      0.627218000     -0.998773000     -2.077566000
7      2.945645000      2.560789000     -0.031027000
7      3.918615000     -1.265165000     -1.203615000
7      0.798835000      2.314270000     -1.296424000
7      0.291065000      0.490858000      2.343644000
7      3.890999000     -1.220250000      1.299582000
7     -0.187555000     -1.675291000     -1.112553000
7      4.415920000      0.863312000      0.015729000
7      0.771661000      2.358702000      1.194641000
7      1.988334000     -1.478592000     -2.336557000
7      0.343223000      0.406120000     -2.387892000
7      1.936003000     -1.393768000      2.396392000
6     -7.257221000      1.508473000      0.012865000
6     -5.943787000      0.793789000      0.002471000
6     -4.747071000      1.401476000     -0.010625000
7     -3.552500000      0.699252000     -0.019617000
1     -2.633059000      1.151146000     -0.032545000
6     -3.512990000     -0.641938000     -0.015121000
8     -2.461153000     -1.326258000     -0.024666000
7     -4.701942000     -1.282468000     -0.001508000
1     -4.673706000     -2.296959000      0.002616000
6     -5.977934000     -0.673225000      0.007413000
8     -6.969948000     -1.352877000      0.018399000
1     -7.849367000      1.222171000     -0.858446000
1     -7.832680000      1.227161000      0.896891000
1     -7.113891000      2.588619000      0.008470000
1     -4.637755000      2.478313000     -0.015013000


B24N24 -  M06-2X/6-311+G** gas-phase
5      0.273383000      0.872750000      3.451119000
7      1.062872000     -0.359483000      3.667826000
7      1.719441000     -1.604622000      1.548502000
5      1.970580000     -0.563470000      2.558211000
7      0.621441000      1.933772000      2.539687000
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5	-0.377197000	2.230688000	1.499949000
5	1.973362000	1.781879000	2.047749000
7	2.808133000	0.576663000	2.227045000
7	0.359483000	1.062872000	-3.667826000
5	0.872750000	-0.273383000	-3.451119000
5	0.563470000	1.970580000	-2.558211000
7	1.604622000	1.719441000	-1.548502000
5	2.230688000	0.377197000	-1.499949000
7	1.933772000	-0.621441000	-2.539687000
7	-0.576663000	2.808133000	-2.227045000
5	1.781879000	-1.973362000	-2.047749000
7	2.227947000	-2.474418000	-0.750013000
5	2.382648000	-1.444603000	0.230416000
7	2.822210000	-0.113521000	-0.238874000
5	1.444603000	2.382648000	-0.230416000
5	-0.844946000	2.948881000	-0.802159000
7	0.113521000	2.822210000	0.238874000
7	2.474418000	2.227947000	0.750013000
5	2.948881000	0.844946000	0.802159000
5	-0.273383000	-0.872750000	3.451119000
7	-1.062872000	0.359483000	3.667826000
7	-1.719441000	1.604622000	1.548502000
5	-1.970580000	0.563470000	2.558211000
7	-0.621441000	-1.933772000	2.539687000
5	0.377197000	-2.230688000	1.499949000
5	-1.973362000	-1.781879000	2.047749000
7	-2.808133000	-0.576663000	2.227045000
7	-0.359483000	-1.062872000	-3.667826000
5	-0.872750000	0.273383000	-3.451119000
5	-0.563470000	-1.970580000	-2.558211000
7	-1.604622000	-1.719441000	-1.548502000
5	-2.230688000	-0.377197000	-1.499949000
7	-1.933772000	0.621441000	-2.539687000
7	0.576663000	-2.808133000	-2.227045000
5	-1.781879000	1.973362000	-2.047749000
7	-2.227947000	2.474418000	-0.750013000
5	-2.382648000	1.444603000	0.230416000
7	-2.822210000	0.113521000	-0.238874000
5	-1.444603000	-2.382648000	-0.230416000
5	0.844946000	-2.948881000	-0.802159000
7	-0.113521000	-2.822210000	0.238874000
7	-2.474418000	-2.227947000	0.750013000
5	-2.948881000	-0.844946000	0.802159000

B24N24 - A1 M06-2X/6-311+G** gas-phase

5	-4.785124000	-0.266198000	1.090615000
7	-4.784217000	-1.664961000	0.608895000

7	-2.518548000	-2.544832000	-0.140626000
5	-3.511728000	-2.287319000	0.913057000
7	-3.882226000	0.276602000	2.074024000
5	-3.067449000	1.418969000	1.626575000
5	-3.132030000	-0.769381000	2.735021000
7	-3.085640000	-2.179340000	2.298133000
7	2.225106000	1.093296000	0.782098000
5	2.463558000	-0.247647000	0.081237000
5	1.109422000	1.269076000	1.674954000
7	0.327327000	0.137434000	2.193775000
5	0.477801000	-1.160674000	1.492096000
7	1.502473000	-1.364452000	0.478795000
7	0.516962000	2.604931000	1.685798000
5	1.033668000	-2.127975000	-0.639715000
7	-0.118094000	-3.036999000	-0.685368000
5	-1.107768000	-2.709183000	0.290775000
7	-0.633204000	-2.146417000	1.567515000
5	-1.028512000	0.421115000	2.717058000
5	-0.937878000	2.639007000	1.742056000
7	-1.770607000	1.630569000	2.298452000
7	-1.788875000	-0.646565000	3.295509000
5	-1.674352000	-1.858939000	2.484590000
5	-4.795885000	-0.904194000	-0.623623000
7	-5.225873000	0.414721000	-0.108904000
7	-3.341580000	2.068865000	0.323500000
5	-4.321895000	1.444563000	-0.579731000
7	-3.911639000	-1.113230000	-1.742432000
5	-2.685126000	-1.875368000	-1.451629000
5	-3.692766000	0.114514000	-2.475667000
7	-4.097374000	1.458953000	-2.015042000
7	2.184791000	0.352372000	-1.344936000
5	1.761360000	1.465348000	-0.569784000
5	1.112953000	-0.237991000	-2.086213000
7	-0.103571000	0.523127000	-2.461004000
5	-0.347276000	1.809176000	-1.775637000
7	0.669115000	2.364879000	-0.878178000
7	1.042956000	-1.695608000	-2.052707000
5	0.150673000	2.991034000	0.309619000
7	-1.231849000	3.413156000	0.535351000
5	-2.166721000	2.726994000	-0.302856000
7	-1.722247000	2.345063000	-1.658903000
5	-1.323295000	-0.241480000	-2.796175000
5	-0.296489000	-2.248567000	-1.903473000
7	-1.509900000	-1.626689000	-2.310260000
7	-2.492462000	0.468047000	-3.226756000
5	-2.711465000	1.667332000	-2.417169000
7	6.948808000	1.428244000	-0.016421000
6	5.637205000	1.203671000	0.152508000

6	5.195420000	-0.146465000	0.097986000
6	6.199637000	-1.099536000	-0.017285000
7	7.504027000	-0.895358000	-0.152659000
6	7.785728000	0.403604000	-0.165582000
7	5.562680000	-2.322771000	0.044561000
6	4.242880000	-2.099479000	0.175719000
7	3.972699000	-0.812036000	0.206746000
7	4.835105000	2.247940000	0.371713000
1	8.829957000	0.665986000	-0.298791000
1	3.499076000	-2.875605000	0.246826000
1	5.277385000	3.150224000	0.453088000
1	3.871676000	2.096861000	0.670575000
1	6.019320000	-3.221885000	-0.006360000

B24N24 - G1 M06-2X/6-311+G** gas-phase

5	2.386941000	-0.556710000	-0.065813000
7	1.818775000	-1.949261000	-0.578869000
7	-0.603294000	-2.412776000	-1.222924000
5	0.738524000	-1.878913000	-1.527060000
7	1.639895000	0.647296000	-0.645667000
5	0.717367000	1.435975000	0.171438000
5	1.149327000	0.421996000	-1.978979000
7	0.891571000	-0.899273000	-2.590320000
7	-4.466302000	2.166922000	-0.878377000
5	-4.753146000	0.770587000	-1.134520000
5	-3.090298000	2.547421000	-1.119621000
7	-2.221984000	1.749942000	-2.000622000
5	-2.659292000	0.386790000	-2.380129000
7	-4.008012000	-0.084947000	-2.023693000
7	-2.500021000	3.407590000	-0.107717000
5	-4.066857000	-1.465380000	-1.595251000
7	-3.039621000	-2.479424000	-1.814485000
5	-1.737832000	-1.926123000	-2.038726000
7	-1.656494000	-0.632451000	-2.750319000
5	-0.757754000	1.895178000	-1.815224000
5	-1.138920000	3.057427000	0.278223000
7	-0.201662000	2.365980000	-0.532264000
7	0.131254000	1.203464000	-2.692739000
5	-0.323469000	-0.165499000	-2.922467000
5	1.352195000	-2.003182000	0.785046000
7	2.030492000	-0.869696000	1.386494000
7	0.502045000	1.152110000	1.602583000
5	1.046568000	-0.121403000	2.112452000
7	0.110923000	-2.612814000	1.217477000
5	-0.928904000	-2.704274000	0.191143000
5	-0.326726000	-2.053187000	2.471815000
7	0.271501000	-0.864936000	3.102798000

7	-5.291217000	0.371155000	0.184230000
5	-4.601495000	1.608110000	0.484998000
5	-4.614500000	-0.821296000	0.652001000
7	-3.620219000	-0.758437000	1.735147000
5	-3.084093000	0.566058000	2.125469000
7	-3.660322000	1.798056000	1.559817000
7	-4.588751000	-1.925595000	-0.292206000
5	-2.687951000	2.818149000	1.234126000
7	-1.311511000	2.884772000	1.719682000
5	-0.797227000	1.616923000	2.144441000
7	-1.751635000	0.666739000	2.752180000
5	-2.645336000	-1.875243000	1.827792000
5	-3.313263000	-2.624603000	-0.383566000
7	-2.336521000	-2.703385000	0.642822000
7	-1.713655000	-1.892992000	2.912484000
5	-1.151275000	-0.561354000	3.144224000
6	5.037248000	2.986831000	0.018918000
7	4.028597000	2.065637000	-0.162829000
1	3.052776000	2.225755000	-0.371105000
6	4.613662000	0.841156000	-0.143730000
6	5.959457000	1.085932000	0.054198000
7	6.203484000	2.432012000	0.154576000
6	6.887288000	-0.011175000	0.079318000
8	8.076868000	-0.044985000	0.227746000
7	6.177739000	-1.239043000	-0.144428000
1	6.785296000	-2.048107000	-0.184196000
6	4.845134000	-1.427063000	-0.306249000
7	3.993799000	-0.388800000	-0.297723000
7	4.407259000	-2.671091000	-0.483751000
1	4.832585000	4.045900000	0.041481000
1	5.041890000	-3.449430000	-0.435968000
1	3.400062000	-2.792853000	-0.655452000

B24N24 - C1 M06-2X/6-311+G** gas-phase

5	2.663009000	0.318396000	0.109290000
7	2.276231000	0.522814000	1.619463000
7	-0.053405000	0.124817000	2.589816000
5	1.272196000	-0.363684000	2.126793000
7	1.896874000	-0.787812000	-0.590943000
5	0.895983000	-0.492454000	-1.590156000
5	1.550499000	-1.869450000	0.289581000
7	1.408650000	-1.762798000	1.761121000
7	-4.262973000	-1.887396000	-1.197012000
5	-4.425414000	-1.445479000	0.172671000
5	-2.901789000	-2.245388000	-1.549816000
7	-1.917727000	-2.608512000	-0.521926000
5	-2.223199000	-2.292197000	0.891994000

7	-3.559464000	-1.791852000	1.269782000
7	-2.454893000	-1.759979000	-2.845091000
5	-3.543266000	-0.752353000	2.275473000
7	-2.432953000	-0.428220000	3.164703000
5	-1.158195000	-0.853542000	2.657193000
7	-1.128536000	-2.096362000	1.857415000
5	-0.478214000	-2.478411000	-0.884434000
5	-1.097917000	-1.219201000	-2.858913000
7	-0.058350000	-1.571755000	-1.967639000
7	0.514593000	-2.893983000	0.050263000
5	0.178490000	-2.433151000	1.395570000
5	1.729178000	1.727269000	1.087167000
7	2.265750000	1.741253000	-0.279848000
7	0.580387000	0.905637000	-1.996619000
5	1.169519000	1.974177000	-1.175822000
7	0.501000000	2.373380000	1.523465000
5	-0.453457000	1.489644000	2.198572000
5	-0.066549000	3.184293000	0.478986000
7	0.390820000	3.186847000	-0.923260000
7	-5.027110000	-0.111972000	-0.055502000
5	-4.450789000	-0.427815000	-1.346295000
5	-4.296306000	0.889434000	0.695710000
7	-3.389990000	1.834892000	0.025275000
5	-2.980533000	1.550608000	-1.370612000
7	-3.606568000	0.446741000	-2.119543000
7	-4.124355000	0.597143000	2.108426000
5	-2.689685000	-0.306122000	-2.949733000
7	-1.363108000	0.124080000	-3.380198000
5	-0.782891000	1.117424000	-2.523716000
7	-1.708505000	2.085828000	-1.890424000
5	-2.341704000	2.476593000	0.861396000
5	-2.794785000	0.886808000	2.635700000
7	-1.890582000	1.849883000	2.119190000
7	-1.490834000	3.460411000	0.266421000
5	-1.048920000	3.035902000	-1.063177000
6	6.402440000	1.108102000	-0.583489000
6	5.027869000	1.151459000	-0.455651000
7	4.268859000	0.123104000	-0.084590000
6	4.840498000	-1.100166000	0.212413000
8	4.257515000	-2.089640000	0.557177000
7	6.249659000	-1.137166000	0.077485000
1	6.644200000	-2.042675000	0.303418000
6	7.030604000	-0.101820000	-0.294997000
7	8.357070000	-0.292048000	-0.368997000
1	6.967784000	1.974748000	-0.887826000
1	4.465624000	2.058908000	-0.652594000
1	8.787473000	-1.174317000	-0.146019000
1	8.956253000	0.469666000	-0.639819000

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5	2.283971000	-1.196158000	-0.270619000
7	1.508437000	-2.481940000	-0.609600000
7	-0.992102000	-2.618536000	-1.056547000
5	0.396147000	-2.332645000	-1.487579000
7	1.754082000	0.096337000	-0.914065000
5	1.015840000	1.081391000	-0.118773000
5	1.119872000	-0.160213000	-2.187161000
7	0.609455000	-1.465479000	-2.643331000
7	-4.061578000	2.543038000	-0.892703000
5	-4.578890000	1.193786000	-0.998697000
5	-2.666345000	2.676242000	-1.256855000
7	-2.002472000	1.682745000	-2.114243000
5	-2.671689000	0.378094000	-2.333088000
7	-4.046295000	0.160730000	-1.849852000
7	-1.873835000	3.511642000	-0.368201000
5	-4.282970000	-1.153249000	-1.291258000
7	-3.446821000	-2.333110000	-1.481233000
5	-2.093283000	-2.019511000	-1.835571000
7	-1.869548000	-0.813462000	-2.665961000
5	-0.522326000	1.606185000	-2.038961000
5	-0.557485000	2.979218000	-0.040580000
7	0.196679000	2.084974000	-0.842023000
7	0.179818000	0.714965000	-2.903625000
5	-0.497609000	-0.581103000	-2.965773000
5	1.163954000	-2.382211000	0.773247000
7	2.050874000	-1.303958000	1.228210000
7	0.872329000	0.950307000	1.344636000
5	1.247134000	-0.355663000	1.932824000
7	-0.125790000	-2.733297000	1.343838000
5	-1.242858000	-2.738650000	0.395859000
5	-0.372806000	-2.006099000	2.560560000
7	0.447697000	-0.876802000	3.038631000
7	-5.067973000	0.995727000	0.383611000
5	-4.174209000	2.125584000	0.522588000
5	-4.548672000	-0.248821000	0.915779000
7	-3.475437000	-0.258008000	1.922426000
5	-2.712391000	0.989522000	2.151145000
7	-3.133872000	2.249513000	1.512573000
7	-4.768458000	-1.415447000	0.079393000
5	-2.044715000	3.069467000	1.031359000
7	-0.639851000	2.954953000	1.419381000
5	-0.296309000	1.657497000	1.923062000
7	-1.334465000	0.925813000	2.675936000
5	-2.679526000	-1.507657000	2.053298000
5	-3.626454000	-2.316866000	-0.028662000

7	-2.597005000	-2.467923000	0.935253000
7	-1.680168000	-1.585215000	3.072928000
5	-0.902597000	-0.348304000	3.140086000
6	7.906189000	2.227608000	0.388778000
6	6.775374000	1.288867000	0.113388000
6	5.492771000	1.662052000	-0.017053000
7	4.475211000	0.753690000	-0.264004000
1	3.517540000	1.041286000	-0.466721000
6	4.706774000	-0.561958000	-0.388671000
8	3.809945000	-1.410386000	-0.627446000
7	5.985986000	-0.967771000	-0.263087000
1	6.157859000	-1.965487000	-0.335058000
6	7.103564000	-0.135666000	-0.018098000
8	8.202962000	-0.614309000	0.070086000
1	8.406019000	1.952741000	1.319590000
1	8.651990000	2.162840000	-0.405755000
1	7.551206000	3.254998000	0.463853000
1	5.170885000	2.692183000	0.063370000

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7	4.065014000	-0.533855000	-2.050256000
5	4.906425000	-0.241129000	-0.925506000
5	2.929096000	-1.402487000	-1.655808000
5	2.928978000	0.416993000	-2.129527000
7	5.073237000	1.085997000	-0.282834000
7	2.947815000	-2.332673000	-0.553101000
7	1.813276000	-0.539127000	-2.070405000
7	2.947862000	1.766758000	-1.620765000
5	3.906384000	1.890125000	-0.492241000
5	4.906384000	0.241105000	0.925468000
5	3.906367000	-1.890143000	0.492218000
5	2.011994000	-1.920483000	0.500208000
5	0.757808000	-0.280641000	-1.077351000
5	2.011992000	1.920479000	-0.500304000
7	2.947828000	2.332559000	0.553067000
7	4.064929000	0.533825000	2.050199000
7	2.947843000	-1.766693000	1.620695000
7	0.811520000	-1.145626000	0.298754000
7	0.811427000	1.145916000	-0.298353000
5	2.929055000	1.402518000	1.655851000
5	2.928914000	-0.416997000	2.129573000
5	0.757574000	0.280706000	1.077739000
7	1.813204000	0.539202000	2.070575000
7	5.073220000	-1.086017000	0.282811000
7	-1.813261000	-2.070617000	0.539167000
5	-0.757823000	-1.077517000	0.280632000
5	-2.929075000	-1.655846000	1.402500000

5	-2.928969000	-2.129594000	-0.416980000
7	-0.811304000	-0.298700000	-1.145939000
7	-2.947848000	-0.553063000	2.332621000
7	-4.064996000	-2.050208000	0.533859000
7	-2.947848000	-1.620754000	-1.766693000
5	-2.011956000	-0.500293000	-1.920494000
5	-0.757687000	1.077498000	-0.280681000
5	-2.012095000	0.500311000	1.920532000
5	-3.906385000	0.492254000	1.890055000
5	-4.906409000	-0.925468000	0.241089000
5	-3.906343000	-0.492247000	-1.890110000
7	-2.947790000	0.553053000	-2.332621000
7	-1.813224000	2.070480000	-0.539230000
7	-2.947859000	1.620794000	1.766720000
7	-5.073210000	0.282855000	1.085939000
7	-5.073216000	-0.282815000	-1.086027000
5	-2.929051000	1.655819000	-1.402539000
5	-2.928910000	2.129565000	0.416938000
5	-4.906397000	0.925512000	-0.241177000
7	-4.064954000	2.050244000	-0.533881000
7	-0.811573000	0.298439000	1.145638000