Diboron- and Diaza-Doped Anthracenes and Phenanthrenes: Their Electronic Structures for Being Singlet Fission Chromophores

Supporting Information

Ekadashi Pradhan,[†] Seunghoon Lee,[‡] Cheol Ho Choi,[¶] and Tao Zeng[*,†]

†*Department of Chemistry, York University, Toronto, Ontario, M3J1P3, Canada*

‡*Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125, USA*

¶*Department of Chemistry, Kyungpook National University, Daegu 702-701, South Korea*

E-mail: tzeng@yorku.ca

Phone: +1 (416) 7362100 ext. 33673

Section S1. Comparison of excitation energies calculated using cc-pVDZ and cc-pVTZ basis sets.

AB1B8 was chosen as the test system to study the basis set convergence. Using the cc-pVTZ basis set, the vertical $E(S_1)$, adiabatic $E(S_1)$, adiabatic $E(T_1)$, and adiabatic $E(T_2)$ were calculated to be 1.63, 1.39, 0.38, and 1.88 eV, respectively. The counterparts obtained using the cc-pVDZ basis set are 1.63, 1.38, 0.36, and 1.88 eV. The ≤ 0.02 eV discrepancies indicate the appropriateness of using the more economical cc-pVDZ basis set in our calculations.

Section S2. Low-lying electronic states of anthracene and phenanthrene

The calculated vertical and adiabatic $E(S_1)\,s$ of anthracene are 3.42 and 3.11 eV, agree well with the absorption spectrum reported by Steiner and Michl.[1] Our calculated 1.89 eV adiabatic $E(T_1)$ is consistent with the 1.869 eV[2] experimental value. The S_1 state is dominated by HOMO→LUMO excitation, with $r_{HL} = 28.4$, a typical Class I chromophore according to the classification of Smith and Michl.[3] According to Smith and Michl, Class I, II, and III chromophores have their S_1 dominated by HOMO→LUMO excitation, mixture of HOMO−1 →LUMO and HOMO→LUMO+1 excitations, and HOMO⇉LUMO excitation, respectively. The 1.56 a.u. (atomic unit) transition dipole integral between the two orbitals result in a decent oscillator strength $f_{S_1} = 0.090$. HOMO, LUMO, and their localized orbital are shown in Figure S1. The localized orbitals have their largest lobe at the central atoms 9 and 10, respectively. And those lobes remain largely nonbonding after the localized orbitals interact to form HOMO and LUMO, reflecting that the diradical character of anthracene is mostly concentrated at the two positions. This is consistent with the diradical Lewis structure shown in Figure 1 in the main text, which contains two Clar sextets on the two sides. All these results about anthracene are well known.[4–6]

The a and b orbitals are localized on the upper and lower edges of the molecule. Consequently, the HOMO→LUMO excitation involves a CT along the short axis, with a CT energy $2K_{H,L} = 2.28$ eV, compared to $2K_{H-1,L} = 1.66$ eV and $2K_{H,L+1} = 1.58$ eV. The 5.15 eV $\Delta_{H,L}$ is 3 eV smaller than the 8.24 eV $\Delta_{H-1,L}$ and 8.68 eV $\Delta_{H,L+1}$ and cannot be compensated by the differences between the CT energies. Therefore, the HOMO→LUMO configuration dominates the S_1 state, and the two sites model is applicable. For any alternant hydrocarbons (AHs) with antiferromatnetic coupling, The Coulson-Rushbrooke pairing theorem[7,8] determines that the a and b orbitals are mainly localized on the starred set and the unstarred set of C atoms, respectively, only with their orthogonalization tails extended

to the other set. This pairing symmetry leads to a small $K_{a,b} = 0.04$ eV, which is of no significance in determining the $E(S_1) \sim 2E(T_1)$ relation for anthracene (and other AHs too; $K_{a,b} = 0.05$ eV for phenanthrene). With a not large $n_{\mathrm{LUNO}} = 0.14$, anthracene does not satisfy Eq. 1 in the main text ($\Delta_{SF}^{(1)} = -0.66$ eV). Longer polyacenes like tetracene and pentacene have the amplitudes of a and b orbitals further attenuated, and then weaker interactions between them. With smaller $\Delta_{H,L}$s and increased diradical characters, their excitation energies satisfy Eq. 1 in the main text.[9–13] Actually, SF research has been "overwhelmingly limited" to the two longer polyacenes and their derivatives.[14] This fact motivates the thriving studies in proposing other SF chromophores.

Phenanthrene has a very different S_1, which mainly consists of almost equal percentages of HOMO−1 →LUMO and HOMO→LUMO+1 configurations. It is a typical Class II chromophore, with $r_{HL} = 0$. HOMO−1 to LUMO+1 of phenanthrene are shown in Figure S2. Those frontier orbitals show clear characters of the HOMOs and LUMOs of the sextets at the two sides, interacting with the π and π^* orbitals of the top vinyl fragment. These characters are even more obvious in the natural orbitals (Figure S3), which, unlike the state-averaged canonical orbitals, only reflect the ground state electronic structure. The canonical and natural orbitals, as well as the bond lengths clearly point to the 2 terminal sextets + 1 top vinyl Lewis structure for the molecule (Figure 1 in the main text). This lack of diradical Lewis structure is consistent with the 8.11 eV large HOMO-LUMO gap. HOMO and HOMO−1 are close in energy, differing by 1.13 eV only, and so are LUMO and LUMO+1, differing by 1.19 eV. With the not too different orbital energy gaps, the HOMO-1→LUMO and HOMO→LUMO+1 configurations can compete with the HOMO→LUMO configuration to dominate the S_1 state.

The localized orbitals transformed from the HOMO-LUMO; HOMO-LUMO+1; HOMO−1-LUMO pairs are shown in Figure S2(e); (f) and (g); (h) and (i). Since the HOMO-LUMO localized orbitals are symmetry images of each other, only one of them is shown in Figure S2(e). Henceforth, only one of each pair of symmetry-image localized orbitals

is shown. Evidently, the HOMO→LUMO configuration involves CT along the long axis, while the HOMO→LUMO+1 and HOMO−1 →LUMO configurations involve CTs along the short axis. Correspondingly, $2K_{H-1,L} = 1.78$ eV and $2K_{H,L+1} = 1.62$ eV are smaller than $2K_{H,L} = 2.12$ eV. The configuration interaction between HOMO→LUMO+1 and HOMO−1 →LUMO generates their combination with an even lower energy. The similar orbital energy gaps, the lower CT energies, and the configuration interaction, altogether make the HOMO→LUMO+1 and HOMO−1 →LUMO configurations dominate the S_1 state. In the language of Platt's Perimeter Model,[15] it is a ^1L_b state with a destructive interference of the transition dipole moments of the two excitations, which results in $f_{S_1} = 0.0003$. The calculated adiabatic and vertical $E(S_1)$s are 3.81 and 3.98 eV, in qualitative consistence with the 3.64 eV experimental value reported by Hager and Wallace.[16] The T_1 state is dominated by HOMO→LUMO excitation. Despite the competing orbital energy gaps, the large $K_{H,L}$ is a stabilizing factor for the HOMO→LUMO triplet configuration. With $E(T_1) = 2.82$ eV, phenanthrene does not satisfy Eq. 1 in the main text.

We should not solely rely on the small diradical character ($n_{\mathrm{LUNO}} = 0.12$) to explain this failure of satisfying Eq. 1 in the main text, since S_1 involves excitations out of the 2o2e space. However, had the ground state possessed more diradical character, $\Delta_{H,L}$ might be further smaller than $\Delta_{H-1,L}$ and $\Delta_{H,L+1}$, and the two sites model would be more likely applicable. Also, $E(T_1)$ would be further pushed down by a smaller $\Delta_{H,L}$ and/or a larger $K_{H,L}$, so that even if S_1 remains being the ^1L_b state, there is still more likelihood to satisfy Eq. 1 in the main text. Diradical character still matters, even if the two sites model is invalid to determine the $E(S_1) \sim 2E(T_1)$ relation.

Section S3. 2B-doped phenanthrenes

All the studied 2B-doped phenanthrenes have relatively mild diradical characters (Figure 3(a) in the main text). Yet, five of the six (except **PB2B7**) have low enough $E(T_1)$s to satisfy Eq. 1 in the main text. All the calculated results for the excited states of the 2B- and 2N-doped phenanthrenes are summarized in Table S1. According to its HONO, LUNO (Figure S17(a) and (b)), and bond lengths, **PB4B5** shares a similar PQDP resonance structure with **AB4B8**. The diradical characters of the two molecules are comparable ($n_{\mathrm{LUNO}} = 0.27$ for both). The S_1 state of **PB4B5** is dominated by HOMO→LUMO ($r_{HL} = 6.61$). This difference from **AB4B8** arises from the lower CT energy ($2K_{H,L} = 2.72$ vs. 3.52 eV) of **PB4B5** in the excitation (Figure S16(e) for a HOMO-LUMO localized orbital). In both molecules, the CT can be viewed as occuring between the terminal allyl fragments along the long axis. However, the long axis of phenanthrene is shorter than that of anthracene, and then the CT energy of **PB4B5** is lower. The HOMO−1-LUMO localized orbitals of **PB4B5** are shown in Figure S16(f) and (g). They have even better spatial overlap than the **AB4B8** counterparts, leading to the smaller $2K_{H-1,L} = 1.06$ eV. However, the small difference between $2K_{H,L}$ and $2K_{H-1,L}$ of **PB4B5** does not compensate the 2.88 eV difference between $\Delta_{H,L}$ and $\Delta_{H-1,L}$. The HOMO−1 →LUMO configuration is thus of higher energy than HOMO→LUMO. The different IRREPs of the two configurations (B_1 and A_1) dictate that they cannot mix. The S_1 state does not contain the HOMO−1 →LUMO configuration. The two sites model is applicable for **PB4B5**. The HOMO-LUMO transition dipole moment integral is as large as 3.11 a.u. Without suffering substantial destructive interference, this integral gives a decently large $f_{S_1} = 0.054$.

Despite the similar diradical characters, **PB4B5** has a smaller $E(T_1) = 0.34$ eV than **AB4B8**, and it comes along with a lower $E(S_1) = 1.50$ eV. The lower energies of both S_1 and T_1 are induced by a larger $K_{a,b} = 0.16$ eV (vs. $K_{a,b} = 0.06$ eV of **AB4B8**). The better spatial overlap between the HOMO-LUMO localized orbitals enlarges their exchange integral. With the low $E(T_1)$, **PB4B5** is not a good candidate of SF chromophore.

Table S1: Calculated quantities for the 2B- and 2N-doped phenanthrenes discussed in this paper. All energies are given in eV. Excitation energies are relative to $E(S_0)$ of respective molecules.

	$E_v(S_1)^a$	$E(S_1)$	$E(T_1)$	$E(T_2)$	f_{S_1}	$\Delta E_{SF}^{(1)}$	$\Delta E_{SF}^{(2)}$	r_{HL}
P^b	3.98	3.81	2.82	3.60	0.0003	−1.83	−2.03	0
PB4B5	1.78	1.50	0.34	2.09	0.054	0.82	1.41	6.61
PB1B8	1.87	1.59	0.37	2.04	0.067	0.85	1.30	4.33
PB1*a***B8***a*	1.90	1.41	0.62	1.80	0.018	0.17	0.56	11.86
PB3B6	2.51	2.03	0.86	1.80^c	0.009	0.31	0.08	0.48
PB4*a***B5***a*	1.37	1.18	0.50	1.66	0.029	0.18	0.66	14.06
PB2B7	2.37	1.94	1.05	1.73	0.004	−0.16	−0.37	3.8^d
PN4N5	1.96	1.44	0.49	2.13	0.061	0.46	1.15	7.84
PN1N8	1.39	1.04	0.23	1.89	0.044	0.58	1.43	9.32
PN1*a***N8***a*	1.32	0.89	0.46	1.48	0.006	−0.03	0.56	9.00
PN3N6	1.62	0.96	0.16	0.76	0.002	0.64	0.44	0.10
PN4*a***N5***a*	1.53	1.12	0.61	1.85	0.020	−0.10	0.63	14.53
PN2N7	2.38	1.93	1.10	1.99	0.002	−0.27	−0.21	2.97

^{a} The subscript v indicates vertical $E(S_1)$, which was calculated at the S_0 structure and with ZPE-correction. ^{b} The undoped phenanthrene. ^{c} This is the $E(T_2)$ calculated at the T_1 structure. ^{d} This r_{HL} is for the S_1 wave function expressed using the natural orbitals of the state.

The same problem exists for **PB1B8**, whose $E(T_1) = 0.37$ eV. The molecule's HONO, LUNO (Figure S17(e),(f)), and bond lengths indicate an *o*-quinodipropane (OQDP) Lewis structure with two allyl fragments on the side rings (Figure S18(c)). **PB1B8** possesses a similar diradical character ($n_{\text{LUNO}} = 0.27$) as **PB4B5**, a reflection of the connection between *o*- and *p*-arrangement of exocyclic groups. However, the better adjacency of the allyl fragments brought by the *o*-arrangement leads to a larger spatial overlap between the HOMO-LUMO localized orbitals (Figure S19(g)), and consequently a larger $K_{a,b} = 0.24$ eV and a smaller $2K_{H,L} = 2.44$ eV than the **PB4B6** analogues. The opposite changes partially cancel and the two molecules have similar $E(S_1)$ and $E(T_1)$. The S_1 state is dominated by HOMO→LUMO ($r_{HL} = 4.33$) for the same reason as for **PB4B5**, and also has a decently large $f_{S1} = 0.067$.

PB1a**B8**a possesses less diradical character ($n_{\mathrm{LUNO}} = 0.19$), and thus a higher $E(T_1) =$ 0.62 eV. This is beneficial for triplet harvesting and high voltage. The diradical character arises from the long decapentenyl fragment (see Figure S17(i) and (j)). As expected for polyenes, the HOMO-LUMO localized orbitals (Figure S20(e)) have amplitudes on the alternating starred and unstarred C atoms of the decapentenyl and the top vinyl fragments (Figure S18(e)). The good spatial overlap results in a small CT energy ($2K_{H,L} = 1.14$ eV) for the HOMO→LUMO excitation. The 0.86 eV $2K_{H-1,L}$ (see Figure S20(f) and (g) for the localized orbitals) is not much smaller. The S_1 state is thus dominated by HOMO→LUMO with a large $r_{HL} = 11.86$. The relatively small $f_{S_1} = 0.018$ is attributed to the 1.53 a.u. small HOMO-LUMO transition dipole integral. The $K_{H,L}$ is small, yet adequate to raise $E(S_1)$ to be greater than $2E(T_1)$.

The two sites model breaks for **PB3B6**, whose $r_{HL} = 0.48$. The bond lengths of the molecule suggest a Lewis structure with an *o*-quinodimethane (OQDM) moiety + two vinyl fragments at the sides. Another Lewis structure compatible with the bond lengths is an octatrenyl fragment on top + a butadiene fragment at the bottom (see Figure S18(g) for the Lewis structures). The natural orbitals support such a resonance of Lewis structures. The HONO−1 to LUNO+1 are shown in Figure S21(a)-(d). The HONO and LUNO certainly exhibit characters of OQDM. However, the HONO is pseudo-degenerate with the HONO−1 ($n_{\mathrm{HONO-1}} = 1.88$ vs $n_{\mathrm{HONO}} = 1.81$). The $\frac{1}{\sqrt{2}}(\mathrm{HONO} \pm \mathrm{HONO} - 1)$ transformed orbitals are shown in Figure S21(e) and (f), and because of the pseudo-degeneracy, they reflect the ground state wave function to a similar extent as the HONO and HONO−1. These orbitals resemble the HONOs of octatetraene and butadiene, respectively. The similar transformation of LUNO and LUNO+1 also result in orbitals that resemble LUNOs of the two polyenes (Figure S21(g) and (h)). The substantial promotion of 0.32 electron from HONO and HONO−1 to LUNO and LUNO+1 is a reflection of the multiple diradical characters of OQDM and the polyenes. Since octatetraene has a larger diradical character than butadiene,[17] and also the radical centers of the butadiene fragments coincide with those of OQDM,

we only consider the OQDM and octatetraene diradical Lewis structures in the resonance in Figure S18(g). The two structures must have not too different energies, so that the ground state features the multiple diradical characters. For comparison, the $E(T_1)$ s of isolated OQDM and octatetraene molecules are calculated to be 1.18 and 1.67 eV, respectively, at the MRSF-TDDFT/cc-pVDZ level.

An immediate consequence of the multiple diradical characters is a low-lying T_2 state. The HOMO-LUMO and HOMO$-$1-LUMO localized orbitals are shown in Figure S22(i) and (j). They can be viewed as linear combinations of the SOMOs of OQDM and octatraene diradicals (compare the combined orbitals in Figure S23 and Figure S22(i) and (j)). Therefore, the T_1 state with the two parallel spin electrons in HOMO and LUMO can be understood as a bonding linear combination of the OQDM and octatraene diradical valence bond structures. The T_2 state with the unpaired electrons in HOMO$-$1 and LUMO is the corresponding antibonding combination of the diradical structures. $E(T_1) = 0.86$ eV. At the T_1-optimized structure, $E(T_2) = 1.80$ eV, slightly higher than $2E(T_1)$. Our T_2-geometry optimization starting at the T_1 structure failed with a T_2-T_1 crossing, which suggests that T_2 and T_1 are not well separated in the reorganization to the T_2 structure, despite their $\sim$1 eV difference at the T_1 structure. In reality, two **PB3B6** molecules at T_1 state and T_1 structure may interact to form a molecule at T_2 state and another molecule at S_0. Frozen at T_1 structures of the two molecules, the endoergocity for this conversion is 0.26 eV, which is attainable for the transient species. Then the molecules relax at their respective potential energy surfaces. The T_2 relaxation is likely to convert to T_1 through a conical intersection. The SF-generated T_1 pair is then lost. Therefore, although **PB3B6** satisfy Eq. 1 in the main text and has a fairly high $E(T_1)$, it is not a good candidate of SF chromophore.

The HOMO-LUMO and HOMO$-$1-LUMO localized orbitals exhibit different spatial overlaps, smaller for the former pair and larger for the latter, and consequently, $2K_{H,L} =$ 2.74 eV vs. $2K_{H-1,L} = 1.20$ eV. The higher CT energy, and the relatively small difference between $\Delta_{H,L} = 2.95$ eV and $\Delta_{H-1,L} = 4.18$ eV (Figure 2(c) in the main text), leads to the

S_1 dominated by the HOMO-1 $\rightarrow$LUMO excitation, and invalidates the two sites model for **PB3B6**. The HOMO-LUMO and HOMO-1-LUMO transition dipole integrals are 2.94 and 0.62 a.u., respectively. When multiplied by the respective coefficients, they interfere destructively and give the small $f_{S_1} = 0.009$.

The natural orbitals (Figure S24(a)-(d)) and bond lengths point to a Lewis structure with a dodecahexaeneyl fragment for **PB4***a***B5***a* (Figure S18(i)). The diradical character ($n_{\mathrm{LUNO}} = 0.19$) arises from the long polyenyl fragment. The polyenyl character determines that the HOMO-LUMO localized orbitals have amplitudes on alternating starred and unstarred C atoms (Figure S25(e)). The good spatial overlap results in the small $2K_{H,L} = 1.12$ eV. With such a low CT energy (vs. $2K_{H-1,L} = 0.72$ eV), the S_1 is dominated by HOMO$\rightarrow$LUMO, with the largest $r_{HL} = 14.06$ among the 2B-doped phenanthrenes. The 1.40 a.u. HOMO-LUMO transition dipole integral does not suffer destructive interference and leads to the decent $f_{S_1} = 0.029$. This molecule does not possess a large diradical character, nor an exceptionally large $K_{a,b} = 0.20$. It satisfies Eq. 1 in the main text mainly because of the large T_1 reorganization energy: $E(S_1)$ changes from 1.37 to 1.18 eV in S_1 reorganization and $E(T_1)$ changes from 1.18 to 0.50 eV in the T_1 reorganization. The quantity that can explain the different reorganization energies is $2K_{H,L}$, which increases significantly by 0.72 eV along the T_1 reorganization. The bond lengths of the S_1 and T_1 optimized structures are shown in Figure S26. It is clear that the two states' reorganizations occur along the same direction. The enhancement of $2K_{H,L}$ further lowers $E(T_1)$ while diminishing S_1 stabilization along the reorganization. Therefore, many of the bond lengths of the S_1 structure are hence in-between those of the S_0 and T_1 structures. The fact that the vertical $E(S_1)$ and $E(T_1)$ do not satisfy Eq. 1 in the main text but the 0-0 analogues do manifests the importance of optimizing excited states' geometries in proposing SF chromophores. The 0.50 eV $E(T_1)$, however, might be too low for triplet harvesting and a useful voltage.

PB2B7 shares a similarity with **PB3B6**, that it features pseudo-degenerate HONO-1 and HONO with $n_{\mathrm{HONO}-1} = 1.88$ and $n_{\mathrm{HONO}} = 1.82$. The transformation of the two or-

bitals results in those that resemble HONOs of the two hexatrienyl fragments shown in Figure S27(e) and (f). Therefore, in addition to the Lewis structure with a PQDM moiety, we can also view the molecule as consisting of a top and a bottom hexatrienyl fragment. All these Lewis structures participate in the ground state resonance (Figure S18(k)), and there are multiple diradical characters from PQDM and the bottom hexatrienyl fragment. The 1.73 eV low $E(T_2)$ is attributed to the multiple diradical characters. Unlike for **PB3B6**, we could optimize the T_2 structure for this molecule. However, $E(T_2) < 2E(T_1)$. The natural orbitals that accommodate about one electron of the T_1 and T_2 states are shown in Figure S29. They clearly appear as linear combinations of HONOs and LUNOs of the PQDM and hexatrienyl moieties. This corroborates our view of T_1 and T_2 as combinations of the PQDM and hexatrienyl diradical valence bond structures.

Consistent with the multiple diradical characters is the pseudo-degenerate HOMO-1 and HOMO, whose energies are -7.46 and -6.84 eV (Figure 2(c) in the main text). Canonical orbitals with similar energies give natural orbitals with similar occupancies. However, the pseudo-degenerate orbitals makes the r_{HL} ratio less meaningful in characterizing the S_1 character. The S_1 state has $r_{HL} = 0.86$, which is the ratio of the weights of the HOMO$\rightarrow$LUMO and HOMO-1 $\rightarrow$LUMO configurations. The pseudo-degeneracy in energy implies ambiguity of the HOMO-1 and HOMO. They may transform within themselves, and the r_{HL} may correspondingly change. Given this situation, it is less ambiguous to use natural orbitals to describe the S_1 state. The HONO and LUNO of S_1 are shown in Figure S28(h) and (i). Their occupancies are 1.25 and 1.17, respectively. The S_1 state can then be viewed as a one-electron excitation involving the two orbitals. $r_{HL} = 3.80$ when the S_1 is expressed using the natural orbitals. The natural orbitals differ substantially from the T_1 HONO and LUNO in Figure S29(a) and (b). This is especially true when comparing the two HONOs. As already discussed, this is related to the different polarizations of the hole orbitals in S_1 and T_1 through different mixings the pseudo-degenerate HOMO-1 and HOMO, to minimize and maximize $2K_{\text{HONO,LUNO}}$ (0.86 and 4.81 eV), respectively. With the hole polarization, a

small $f_{S_1} = 0.004$ is obtained. This molecule does not satisfy Eq. 1 in the main text either, with $\Delta_{SF}^{(1)} = -0.16$ eV.

Among the 2B-doped phenanthrenes that satisfy Eqs. 1 and 2 in the main text, **PB1aB8a** is the best SF chromophore candidate, as it has the highest 0.62 eV $E\left(T_1\right)$. The disadvantage of its 0.018 low f_{S_1} can be counterpoised by the high irradiance at the $\sim$ 1.90 eV (vertical $E\left(S_1\right)$) region of the solar spectrum.

Section S4. Molecular Orbitals

Summarized in this section are the canonical orbitals and natural orbitals of the molecules that are studied in this work.

Figure S1: (a)-(d) HOMO−1 to LUMO+1 of anthracene, (e)-(f) localized orbitals of HOMO and LUMO.

Figure S2: (a)-(d) HOMO−1 to LUMO+1 of anthracene, (e) a localized orbital of HOMO and LUMO, (f),(g) localized orbitals of HOMO and LUMO+1, (h),(i) localized orbitals of HOMO−1 and LUMO.

Figure S3: (a)-(d) HONO−1, HONO, LUNO, and LUNO+1 of phenanthrene.

Figure S4: (a),(b) HONO and LUNO of **AB1B8**; (c),(d) HONO and LUNO of **AN1N8**; (e),(f) HONO and LUNO of **AB2B7**; (g),(h) HONO and LUNO of **AN2N7**; (i),(j) HONO and LUNO of **AB1***a***B8***a*; (k)-(n) HONO−1 to LUNO+1 of **AN1***a***N8***a*.

Figure S5: (a)-(d) HOMO−1 to LUMO+1 of **AB1B8**, (e) a HOMO-LUMO localized orbital of **AB1B8**, (f) HOMO−1-LUMO localized orbital of **AB1B8**, (g)-(j) HOMO−1 to LUMO+1 of **AN1N8**, (k) a HOMO-LUMO localized orbital of **AN1N8**, (l) a HOMO-LUMO+1 localized orbital of **AN1N8**, (m) correlations between molecular orbitals. In (m), the central straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S6: (a)-(f) HOMO−2 to LUMO+2 of **AB2B7**, (g) a HOMO-LUMO localized orbital of **AB2B7**, (h) a HOMO−1-LUMO localized orbital of **AB2B7**, (i)-(n) HOMO−2 to LUMO+2 of **AN2N7**, (o) a HOMO-LUMO localized orbital of **AN2N7**, (p) a HOMO-LUMO+1 localized orbital of **AN2N7**, (q) correlations between molecular orbitals. In (q), the central straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S7: (a),(b) HONO and LUNO of the S_1 state of **AB1B8**; (c),(d) HONO and LUNO of the T_1 state of **AB1B8**; (e),(f) HONO and LUNO of the S_1 state of **AB2B7**; (g),(h) HONO and LUNO of the T_1 state of **AB2B7**; (i),(j) HONO and LUNO of the S_1 state of **AN1N8**; (k),(l) HONO and LUNO of the T_1 state of **AN1N8** Natural occupancies are given under the orbitals.

Figure S8: (a)-(d) HOMO−1 to LUMO+1 of **AB1***a***B8***a*; (e),(f) HOMO-LUMO localized orbitals of **AB1***a***B8***a*; (g),(h) HOMO−1-LUMO localized orbitals of **AB1***a***B8***a*; (i),(j) SOMOs of the T_1 state of **AB1***a***B8***a*; (k)-(n) HOMO−1 to LUMO+1 of **AN1***a***N8***a*; (o) HOMO-LUMO localized orbital of **AN1***a***N8***a*; (p) HOMO−1-LUMO localized orbital of **AN1***a***N8***a*.

Figure S9: Densities of unpaired electrons of (a) **AB1B8**, (b) **AB2B7**, and (c) **AB1***a***B8***a*. The density is defined as $\frac{1}{2}n_{\mathrm{LUNO}}\,(\mathrm{HONO}^2 + \mathrm{LUNO}^2)$.

Figure S10: (a),(b) HONO and LUNO of **AB4B8**; (c),(d) HONO and LUNO of **AN4N8**.

Figure S11: (a)-(f) HOMO−2 to LUMO+2 of **AB4B8**; (g) a HOMO-LUMO localized orbital of **AB4B8**; (h),(i) HOMO−1-LUMO localized orbitals of **AB4B8**; (j)-(o) HOMO−2 to LUMO+2 of **AN4N8**; (p) a HOMO-LUMO localized orbital of **AN4N8**; (q),(r) HOMO-LUMO+1 localized orbitals of **AN4N8**; (s) correlations between molecular orbitals. In (s), the central straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S12: (a)-(b) HONO−1 to LUNO+1 of **AB4***a***B8***a*; (e)-(h) localized orbitals of the HONO−1-HONO pair and the LUNO-LUNO+1 pair of **AB4***a***B8***a*; (i)-(l) HONO−1 to LUNO+1 of **AN4***a***N8***a*; (m)-(p) localized orbitals of the HONO−1-HONO pair and the LUNO-LUNO+1 pair of **AN4***a***N8***a*.

Figure S13: (a)-(d) HOMO−1 to LUMO+1 of **AB4***a***B8***a*; (e),(f) the HOMO-LUMO localized orbitals of **AB4***a***B8***a*; (g) a HOMO−1-LUMO localized orbitals of **AB4***a***B8***a*; (h)-(k) HOMO−1 to LUMO+1 of **AN4***a***N8***a*; (l),(m) the HOMO-LUMO localized orbitals of **AN4***a***N8***a*; (n) a HOMO-LUMO+1 localized orbitals of **AN4***a***N8***a*; (o) correlations between molecular orbitals. In (o), the central straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S14: (a)-(b) HONO−1 to LUNO+1 of **AB3B7**; (e),(f) localized orbitals of the HONO−1-HONO pair and the LUNO-LUNO+1 pair of **AB3B87**; (g)-(j) HONO−1 to LUNO+1 of **AN3N7**; (k),(l) localized orbitals of the HONO−1-HONO pair and the LUNO-LUNO+1 pair of **AN3N7**.

Figure S15: (a)-(d) HOMO−1 to LUMO+1 of **AB7B7**; (e) a HOMO-LUMO localized orbital of **AB3B7**; (f),(g) the HOMO−1-LUMO localized orbitals of **AB7B7**; (h)-(k) HOMO−1 to LUMO+1 of **AN3N7**; (l) a HOMO-LUMO localized orbital of **AN3N7**; (m),(n) the HOMO-LUMO+1 localized orbitals of **AN3N7**; (o) correlations between molecular orbitals. In (o), the central straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S16: (a)-(d) HOMO−1 to LUMO+1 of **PB4B5**; (e) a HOMO-LUMO localized orbital of **PB4B5**; (f),(g) the HOMO−1-LUMO localized orbitals of **PB4B5**; (h)-(k) HOMO−1 to LUMO+1 of **PN4N5**; (l) a HOMO-LUMO localized orbital of **PN4N5**; (m),(n) the HOMO-LUMO+1 localized orbitals of **PN4N5**; (o) correlations between molecular orbitals. In (o), the central straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S17: (a),(b) HONO and LUNO of **PB4B5**; (c),(d) HONO and LUNO of **PN4N5**; (e),(f) HONO and LUNO of **PB1B8**; (g),(h) HONO and LUNO of **PN1N8**; (i),(j) HONO and LUNO of **PB1***a***B8***a*; (k),(l) HONO and LUNO of **PN1***a***N8***a*.

Figure S18: Dominant Lewis structures of the studied 2B-doped and 2N-doped phenanthrenes. The bond lengths are given in Å. The Lewis structures and bond lengths are given for ground states of the molecules.

Figure S19: (a)-(f) HOMO−2 to LUMO+2 of **PB1B8**; (g) a HOMO-LUMO localized orbital of **PB1B8**; (h) a HOMO−1-LUMO localized orbital of **PB1B8**; (i)-(n) HOMO−2 to LUMO+2 of **PN1N8**; (o) a HOMO-LUMO localized orbital of **PN1N8**; (p) a HOMO-LUMO+1 localized orbital of **PN1N8**; (r) correlations between molecular orbitals. In (r), the central blue straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing, and the central red dashed lines correlate orbitals of the two molecules according to alternant hydrocarbon pairing.

Figure S20: (a)-(e) HOMO−1 to LUMO+1 of **PB1***a***B8***a*; (f) a HOMO-LUMO localized orbital of **PB1***a***B8***a*; (f),(g) the HOMO−1-LUMO localized orbitals of **PB1***a***B8***a*; (h)-(k) HOMO−1 to LUMO+1 of **PN1***a***N8***a*; (l) a HOMO-LUMO localized orbital of **PN1***a***N8***a*; (p) the HOMO-LUMO+1 localized orbitals of **PN1***a***N8***a*; (o) correlations between molecular orbitals. In (o), the central blue straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S21: (a)-(d) HONO−1 to LUNO+1 of **PB3B6**; (e),(f) $\frac{1}{\sqrt{2}}(\mathrm{HONO}-1 \pm \mathrm{HONO})$ of **PB3B6**; (g),(h) $\frac{1}{\sqrt{2}}(\mathrm{LUNO} \pm \mathrm{LUNO}+1)$ of **PB3B6**; (i)-(l) HONO−1 to LUNO+1 of **PN3N6**.

Figure S22: (a)-(d) HOMO−1 to LUMO+1 of **PB3B6**; (e),(f) $\frac{1}{\sqrt{2}}(\mathrm{HOMO}-1-\mathrm{HOMO})$ and $\frac{1}{\sqrt{2}}(\mathrm{HOMO}-1+\mathrm{HOMO})$ of **PB3B6**; (g),(h) $\frac{1}{\sqrt{2}}(\mathrm{LUMO}-\mathrm{LUMO}+1)$ and $\frac{1}{\sqrt{2}}(\mathrm{LUMO}+\mathrm{LUMO}+1)$ of **PB3B6**; (i) a HOMO-LUMO localized orbital of **PB3B6**; (j) a HOMO−1-LUMO localized orbital of **PB3B6**; (k)-(n) HOMO−1 to LUMO+1 of **PN3N6**; (o) a HOMO-LUMO localized orbital of **PN3N6**; (p) a HOMO-LUMO+1 localized orbital of **PN3N6**; (q) correlations between molecular orbitals. In (q), the central blue straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S23: Qualitative sketches of SOMOs of octatetraenyl diradical ((a),(b)) and orthoquinodimethane diradical ((c),(d)), and the linear combinations of the orbitals.

Figure S24: (a)-(d) HONO−1 to LUNO+1 of **PB4***a***B5***a*; (e)-(h) HONO−1 to LUNO+1 of **PN4***a***N5***a*.

Figure S25: (a)-(d) HOMO−1 to LUMO+1 of **PB4***a***B5***a*; (e) a HOMO-LUMO localized orbital of **PB4***a***B5***a*; (f),(g) the HOMO−1-LUMO localized orbitals of **PB4***a***B5***a*; (h)-(k) HOMO−1 to LUMO+1 of **PN4***a***N5***a*; (l) a HOMO-LUMO localized orbital of **PN4***a***N5***a*; (m),(n) the HOMO-LUMO+1 localized orbital of **PN4***a***N5***a*; (o) correlations between molecular orbitals. In (o), the central blue straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S26: Optimized structures of S_0, T_1, and S_1 states of **PB**4a**B**5a.

Figure S27: (a)-(d) HONO−1 to LUNO+1 of **PB2B7**; (e),(f) $\frac{1}{\sqrt{2}}(\mathrm{HONO}-1 \pm \mathrm{HONO})$; (g),(h) $\frac{1}{\sqrt{2}}(\mathrm{LUNO} \pm \mathrm{LUNO}+1)$; (i)-(l) HONO−1 to LUNO+1 of **PN2N7**.

Figure S28: (a)-(d) HOMO−1 to LUMO+1 of **PB2B7**; (e) a HOMO-LUMO localized orbital of **PB2B7**; (f) a HOMO−1-LUMO localized orbital of **PB2B7**; (g)-(j) HONO−1 to LUNO+1 of the S_1 state of **PB2B7**; (k) an S_1 HONO-LUNO localized orbital of **PB2B7**; (l) an S_1 HONO−1-LUMO localized orbital of **PB2B7**; (m)-(p) HOMO−1 to LUMO+1 of **PN2N7**; (q) a HOMO-LUMO localized orbital of **PN2N7**; (r) a HOMO-LUMO+1 localized orbital of **PN2N7**; (s) correlations between the **PB2B7** S_1 natural orbitals and the **PN2N7** canonical orbitals. In (s), the central blue straight lines correlate orbitals of the two molecules according to their C-C bonding/antibonding patterns, and the side brackets correlate orbitals within each molecule according to alternant hydrocarbon pairing.

Figure S29: (a),(b) HONO and LUNO of the T_1 state; (c),(d) HONO and LUNO of the T_2 state of **PB2B7**. The occupancies are given below the orbitals.

Section S5. Coordinates of all studied molecules in this work

All cartesian coordinates in this section are given in Å.

Anthracene S_0:

C	-0.0000000000	-1.3942272189	-0.0000000000
C	0.0000000000	1.3942272189	-0.0000000000
C	-1.2145427813	-0.7170563672	0.0000000000
C	1.2145427813	-0.7170563672	0.0000000000
C	-1.2145427813	0.7170563672	0.0000000000
C	1.2145427813	0.7170563672	0.0000000000
C	-2.4662031295	-1.3996617732	0.0000000000
C	2.4662031295	-1.3996617732	-0.0000000000
C	-2.4662031295	1.3996617732	-0.0000000000
C	2.4662031295	1.3996617732	-0.0000000000
C	-3.6403859821	-0.7098636611	-0.0000000000
C	3.6403859821	-0.7098636611	0.0000000000
C	-3.6403859821	0.7098636611	0.0000000000
C	3.6403859821	0.7098636611	0.0000000000
H	-0.0000000000	-2.4795529326	0.0000000000
H	-0.0000000000	2.4795529326	0.0000000000
H	-2.4645544662	-2.4842873021	0.0000000000
H	2.4645544662	-2.4842873021	-0.0000000000
H	-2.4645544662	2.4842873021	-0.0000000000
H	2.4645544662	2.4842873021	-0.0000000000
H	-4.5844369710	-1.2426442649	0.0000000000
H	4.5844369710	-1.2426442649	0.0000000000

H	-4.5844369710	1.2426442649	0.0000000000
H	4.5844369710	1.2426442649	0.0000000000

Anthracene S_1:

C	-0.0000000000	-1.3824508105	0.0000000000
C	0.0000000000	1.3824508105	0.0000000000
C	-1.2321549447	-0.7203397696	0.0000000000
C	1.2321549447	-0.7203397696	-0.0000000000
C	-1.2321549447	0.7203397696	-0.0000000000
C	1.2321549447	0.7203397696	-0.0000000000
C	-2.4609945730	-1.3926137633	0.0000000000
C	2.4609945730	-1.3926137633	-0.0000000000
C	-2.4609945730	1.3926137633	-0.0000000000
C	2.4609945730	1.3926137633	-0.0000000000
C	-3.6786993893	-0.6899068213	0.0000000000
C	3.6786993893	-0.6899068213	-0.0000000000
C	-3.6786993893	0.6899068213	-0.0000000000
C	3.6786993893	0.6899068213	-0.0000000000
H	-0.0000000000	-2.4683666153	0.0000000000
H	0.0000000000	2.4683666153	0.0000000000
H	-2.4656664813	-2.4769256216	0.0000000000
H	2.4656664813	-2.4769256216	0.0000000000
H	-2.4656664813	2.4769256216	0.0000000000
H	2.4656664813	2.4769256216	0.0000000000
H	-4.6132096374	-1.2380856529	0.0000000000
H	4.6132096374	-1.2380856529	0.0000000000
H	-4.6132096374	1.2380856529	0.0000000000

H	4.6132096374	1.2380856529	0.0000000000

Anthracene T_1:

C	-0.0000000000	-1.4003175110	0.0000000000
C	0.0000000000	1.4003175110	0.0000000000
C	-1.2484916965	-0.7168701682	-0.0000000000
C	1.2484916965	-0.7168701682	0.0000000000
C	-1.2484916965	0.7168701682	0.0000000000
C	1.2484916965	0.7168701682	0.0000000000
C	-2.4642578266	-1.3878363163	0.0000000000
C	2.4642578266	-1.3878363163	-0.0000000000
C	-2.4642578266	1.3878363163	-0.0000000000
C	2.4642578266	1.3878363163	-0.0000000000
C	-3.6846042772	-0.6866269000	-0.0000000000
C	3.6846042772	-0.6866269000	0.0000000000
C	-3.6846042772	0.6866269000	0.0000000000
C	3.6846042772	0.6866269000	0.0000000000
H	-0.0000000000	-2.4845408695	0.0000000000
H	0.0000000000	2.4845408695	0.0000000000
H	-2.4682652884	-2.4724270012	0.0000000000
H	2.4682652884	-2.4724270012	-0.0000000000
H	-2.4682652884	2.4724270012	-0.0000000000
H	2.4682652884	2.4724270012	-0.0000000000
H	-4.6184320043	-1.2364805275	-0.0000000000
H	4.6184320043	-1.2364805275	0.0000000000
H	-4.6184320043	1.2364805275	0.0000000000
H	4.6184320043	1.2364805275	0.0000000000

Anthracene T_2:

C	-0.0000000000	-1.4119258900	-0.0000000000
C	0.0000000000	1.4119258900	-0.0000000000
C	-1.2311155874	-0.7365041388	0.0000000000
C	1.2311155874	-0.7365041388	-0.0000000000
C	-1.2311155874	0.7365041388	-0.0000000000
C	1.2311155874	0.7365041388	-0.0000000000
C	-2.4659554436	-1.4058005389	0.0000000000
C	2.4659554436	-1.4058005389	-0.0000000000
C	-2.4659554436	1.4058005389	-0.0000000000
C	2.4659554436	1.4058005389	-0.0000000000
C	-3.6575883744	-0.7123798340	-0.0000000000
C	3.6575883744	-0.7123798340	0.0000000000
C	-3.6575883744	0.7123798340	0.0000000000
C	3.6575883744	0.7123798340	0.0000000000
H	-0.0000000000	-2.4967571531	0.0000000000
H	0.0000000000	2.4967571531	0.0000000000
H	-2.4692287224	-2.4904347683	0.0000000000
H	2.4692287224	-2.4904347683	0.0000000000
H	-2.4692287224	2.4904347683	0.0000000000
H	2.4692287224	2.4904347683	0.0000000000
H	-4.5990567153	-1.2481366669	0.0000000000
H	4.5990567153	-1.2481366669	0.0000000000
H	-4.5990567153	1.2481366669	0.0000000000
H	4.5990567153	1.2481366669	0.0000000000

AB1B8 S_0:

C	0.0000000000	0.0000000000	-1.3352363831
C	-0.0000000000	0.0000000000	1.4341755851
C	-1.2192361262	0.0000000000	-0.6494072288
C	1.2192361262	-0.0000000000	-0.6494072288
C	-1.2355664305	0.0000000000	0.7786825717
C	1.2355664305	-0.0000000000	0.7786825717
C	-2.4288380718	0.0000000000	-1.3911091128
C	2.4288380718	-0.0000000000	-1.3911091128
B	-2.5749406212	0.0000000000	1.4972544294
B	2.5749406212	0.0000000000	1.4972544294
C	-3.6854389486	0.0000000000	-0.7842762476
C	3.6854389486	-0.0000000000	-0.7842762476
C	-3.8197009164	0.0000000000	0.5911515712
C	3.8197009164	-0.0000000000	0.5911515712
H	0.0000000000	0.0000000000	-2.4215556181
H	-0.0000000000	0.0000000000	2.5202388786
H	-2.3638479778	0.0000000000	-2.4745201058
H	2.3638479778	0.0000000000	-2.4745201058
H	-2.6556834972	0.0000000000	2.6932274272
H	2.6556834972	-0.0000000000	2.6932274272
H	-4.5600381067	0.0000000000	-1.4287095982
H	4.5600381067	-0.0000000000	-1.4287095982
H	-4.8327835153	0.0000000000	0.9865953413
H	4.8327835153	0.0000000000	0.9865953413

AB1B8 S_1:

C	-0.0000000000	0.0000000000	-1.4171857754
C	-0.0000000000	0.0000000000	1.3966747257
C	-1.2270923185	0.0000000000	-0.7327608372
C	1.2270923185	-0.0000000000	-0.7327608372
C	-1.2301833864	0.0000000000	0.7407927257
C	1.2301833864	0.0000000000	0.7407927257
C	-2.4354875298	0.0000000000	-1.3991060711
C	2.4354875298	0.0000000000	-1.3991060711
B	-2.5757980106	0.0000000000	1.5067852245
B	2.5757980106	-0.0000000000	1.5067852245
C	-3.6876093689	0.0000000000	-0.7255340392
C	3.6876093689	-0.0000000000	-0.7255340392
C	-3.8250090175	0.0000000000	0.6425187362
C	3.8250090175	-0.0000000000	0.6425187362
H	-0.0000000000	0.0000000000	-2.5021180758
H	0.0000000000	0.0000000000	2.4820736168
H	-2.4326967901	0.0000000000	-2.4837057052
H	2.4326967901	0.0000000000	-2.4837057052
H	-2.5825330208	0.0000000000	2.7045138608
H	2.5825330208	-0.0000000000	2.7045138608
H	-4.5721931318	0.0000000000	-1.3587626257
H	4.5721931318	-0.0000000000	-1.3587626257
H	-4.8342537871	0.0000000000	1.0432367640
H	4.8342537871	0.0000000000	1.0432367640

AB1B8 T_1:

C	0.0000000000	0.0000000000	-1.3618903642

C	-0.0000000000	0.0000000000	1.4141587657
C	-1.2166556714	0.0000000000	-0.6736955544
C	1.2166556714	-0.0000000000	-0.6736955544
C	-1.2270258044	0.0000000000	0.7497128863
C	1.2270258044	0.0000000000	0.7497128863
C	-2.4563050346	0.0000000000	-1.3851821779
C	2.4563050346	-0.0000000000	-1.3851821779
B	-2.5886549559	0.0000000000	1.4915572076
B	2.5886549559	0.0000000000	1.4915572076
C	-3.7071380052	0.0000000000	-0.7611535735
C	3.7071380052	0.0000000000	-0.7611535735
C	-3.8441199185	0.0000000000	0.6120708167
C	3.8441199185	0.0000000000	0.6120708167
H	0.0000000000	0.0000000000	-2.4476536869
H	-0.0000000000	0.0000000000	2.4995818291
H	-2.4143052508	0.0000000000	-2.4697766040
H	2.4143052508	0.0000000000	-2.4697766040
H	-2.6328093923	0.0000000000	2.6886709479
H	2.6328093923	0.0000000000	2.6886709479
H	-4.5833728144	0.0000000000	-1.4040641200
H	4.5833728144	-0.0000000000	-1.4040641200
H	-4.8519654916	0.0000000000	1.0174621784
H	4.8519654916	0.0000000000	1.0174621784

AB1B8 T_2:

C	0.0000000000	0.0000000000	-1.3775539475
C	0.0000000000	0.0000000000	1.4293662506

C	-1.2160810629	0.0000000000	-0.6960022093
C	1.2160810629	-0.0000000000	-0.6960022093
C	-1.2329412058	0.0000000000	0.7789614684
C	1.2329412058	0.0000000000	0.7789614684
C	-2.4385453934	0.0000000000	-1.4191810384
C	2.4385453934	-0.0000000000	-1.4191810384
B	-2.5638638236	0.0000000000	1.5161762659
B	2.5638638236	0.0000000000	1.5161762659
C	-3.6568597275	0.0000000000	-0.7787929730
C	3.6568597275	0.0000000000	-0.7787929730
C	-3.7900207936	0.0000000000	0.6335651540
C	3.7900207936	-0.0000000000	0.6335651540
H	-0.0000000000	0.0000000000	-2.4625959762
H	0.0000000000	0.0000000000	2.5145161299
H	-2.3961956601	0.0000000000	-2.5021642126
H	2.3961956601	0.0000000000	-2.5021642126
H	-2.6113324555	0.0000000000	2.7135453411
H	2.6113324555	0.0000000000	2.7135453411
H	-4.5504676493	0.0000000000	-1.3980695490
H	4.5504676493	0.0000000000	-1.3980695490
H	-4.8065050928	0.0000000000	1.0177958035
H	4.8065050928	0.0000000000	1.0177958035

AB2B7 S_0:

C	-0.0000000000	0.0000000000	-1.4127540799
C	0.0000000000	0.0000000000	1.3475446114
C	-1.2318449387	0.0000000000	-0.7416540833

C	1.2318449387	-0.0000000000	-0.7416540833
C	-1.2252324647	0.0000000000	0.6835114139
C	1.2252324647	-0.0000000000	0.6835114139
C	-2.4453843917	0.0000000000	-1.4628125139
C	2.4453843917	-0.0000000000	-1.4628125139
C	-2.4635689962	0.0000000000	1.3960076838
C	2.4635689962	0.0000000000	1.3960076838
B	-3.7951857147	0.0000000000	-0.7249966422
B	3.7951857147	-0.0000000000	-0.7249966422
C	-3.6893340456	0.0000000000	0.7860903370
C	3.6893340456	0.0000000000	0.7860903370
H	-0.0000000000	0.0000000000	-2.4987586214
H	0.0000000000	0.0000000000	2.4336490305
H	-2.3581890765	0.0000000000	-2.5473446817
H	2.3581890765	0.0000000000	-2.5473446817
H	-2.3890149909	0.0000000000	2.4818363085
H	2.3890149909	0.0000000000	2.4818363085
H	-4.8325243303	0.0000000000	-1.3233987453
H	4.8325243303	-0.0000000000	-1.3233987453
H	-4.5606015903	0.0000000000	1.4356207315
H	4.5606015903	0.0000000000	1.4356207315

AB2B7 S_1:

C	-0.0026723098	-1.4764492141	0.0000000000
C	0.0316609121	1.3321979741	0.0000000000
C	-1.2692705018	-0.8097948994	0.0000000000
C	1.2442993659	-0.8098491487	0.0000000000

C	-1.2311747951	0.6755810758	0.0000000000
C	1.2283138021	0.6823030877	0.0000000000
C	-2.4528736479	-1.4800203870	0.0000000000
C	2.4335712449	-1.4803531707	0.0000000000
C	-2.4089142914	1.4284442827	0.0000000000
C	2.4588670889	1.4250717400	0.0000000000
B	-3.7655802480	-0.7192660718	0.0000000000
B	3.7629224966	-0.7160731098	0.0000000000
C	-3.6464385197	0.8213438611	0.0000000000
C	3.6733406103	0.8239653959	0.0000000000
H	-0.0015717844	-2.5600881924	0.0000000000
H	0.0275422622	2.4179698986	0.0000000000
H	-2.3986235291	-2.5656660403	0.0000000000
H	2.3830557724	-2.5661406352	0.0000000000
H	-2.3123834016	2.5107936620	0.0000000000
H	2.3614027066	2.5082747723	0.0000000000
H	-4.8356520653	-1.2583996517	0.0000000000
H	4.8170380157	-1.2850321768	0.0000000000
H	-4.5163059025	1.4738200956	0.0000000000
H	4.5522109589	1.4627684918	0.0000000000

AB2B7 T_1:

C	0.0000000000	0.0000000000	-1.4597126155
C	-0.0000000000	0.0000000000	1.3188482543
C	-1.2361033282	0.0000000000	-0.7907229078
C	1.2361033282	0.0000000000	-0.7907229078
C	-1.2216343724	0.0000000000	0.6547760218

C	1.2216343724	0.0000000000	0.6547760218
C	-2.4558805144	0.0000000000	-1.4731528469
C	2.4558805144	-0.0000000000	-1.4731528469
C	-2.4532113412	0.0000000000	1.4111458206
C	2.4532113412	-0.0000000000	1.4111458206
B	-3.7841593495	0.0000000000	-0.7105428446
B	3.7841593495	-0.0000000000	-0.7105428446
C	-3.6730615934	0.0000000000	0.8296600768
C	3.6730615934	-0.0000000000	0.8296600768
H	0.0000000000	0.0000000000	-2.5445142672
H	0.0000000000	0.0000000000	2.4042443627
H	-2.4024500237	0.0000000000	-2.5590834728
H	2.4024500237	-0.0000000000	-2.5590834728
H	-2.3438098500	0.0000000000	2.4932783805
H	2.3438098500	-0.0000000000	2.4932783805
H	-4.8381457301	0.0000000000	-1.2790377068
H	4.8381457301	-0.0000000000	-1.2790377068
H	-4.5420978124	0.0000000000	1.4819468907
H	4.5420978124	-0.0000000000	1.4819468907

AB2B7 T_2:

C	-0.0000000000	0.0000000000	-1.4141162617
C	0.0000000000	0.0000000000	1.3637146680
C	-1.2258693803	0.0000000000	-0.7391842814
C	1.2258693803	-0.0000000000	-0.7391842814
C	-1.2203381313	0.0000000000	0.6959004414
C	1.2203381313	0.0000000000	0.6959004414

C	-2.4800670475	0.0000000000	-1.4625980724
C	2.4800670475	-0.0000000000	-1.4625980724
C	-2.4539162893	0.0000000000	1.3955094342
C	2.4539162893	0.0000000000	1.3955094342
B	-3.8078662268	0.0000000000	-0.7405844897
B	3.8078662268	-0.0000000000	-0.7405844897
C	-3.6989875131	0.0000000000	0.7729795687
C	3.6989875131	-0.0000000000	0.7729795687
H	-0.0000000000	0.0000000000	-2.4985188313
H	0.0000000000	0.0000000000	2.4496440041
H	-2.3840491599	0.0000000000	-2.5457091728
H	2.3840491599	-0.0000000000	-2.5457091728
H	-2.3919453934	0.0000000000	2.4818396096
H	2.3919453934	-0.0000000000	2.4818396096
H	-4.8548494267	0.0000000000	-1.3222709106
H	4.8548494267	-0.0000000000	-1.3222709106
H	-4.5636558156	0.0000000000	1.4314563623
H	4.5636558156	-0.0000000000	1.4314563623

AB1a**B8**a S_0:

C	-0.0491083127	-1.6602356911	0.0000000000
C	0.0585112673	1.3474828426	0.0000000000
B	-1.3312931112	-0.8895722535	0.0000000000
B	1.3079206639	-0.8616153197	0.0000000000
C	-1.2355835089	0.6542271414	0.0000000000
C	1.2485579395	0.7007520266	0.0000000000
C	-2.7458151527	-1.4774648084	0.0000000000

C	2.7060361289	-1.4623724302	0.0000000000
C	-2.3936236591	1.3829404909	0.0000000000
C	2.4899362260	1.4496219981	0.0000000000
C	-3.8445730538	-0.6305031051	0.0000000000
C	3.7791182721	-0.6252727956	0.0000000000
C	-3.6675671943	0.7489867832	0.0000000000
C	3.6811478979	0.8193928793	0.0000000000
H	-0.0343559665	-2.7511158647	0.0000000000
H	0.0337562318	2.4396555228	0.0000000000
H	-2.9357825106	-2.5489912065	0.0000000000
H	2.9018366677	-2.5321864198	0.0000000000
H	-2.3740562163	2.4708528263	0.0000000000
H	2.4507351889	2.5365989778	0.0000000000
H	-4.8590016263	-1.0178710019	0.0000000000
H	4.7881033873	-1.0344716769	0.0000000000
H	-4.5481814291	1.3843380296	0.0000000000
H	4.6017842600	1.3922197445	0.0000000000

AB1a**B8**a S_1:

C	0.0000000000	0.0000000000	-1.6518035307
C	-0.0000000000	0.0000000000	1.3159247889
B	-1.3270579638	0.0000000000	-0.8769225627
B	1.3270579638	0.0000000000	-0.8769225627
C	-1.2458938835	0.0000000000	0.6500552149
C	1.2458938835	-0.0000000000	0.6500552149
C	-2.7067231255	0.0000000000	-1.4628862587
C	2.7067231255	0.0000000000	-1.4628862587

C	-2.4243959913	0.0000000000	1.4020119954
C	2.4243959913	-0.0000000000	1.4020119954
C	-3.8114873863	0.0000000000	-0.6000363246
C	3.8114873863	-0.0000000000	-0.6000363246
C	-3.6797596360	0.0000000000	0.7858674658
C	3.6797596360	0.0000000000	0.7858674658
H	-0.0000000000	0.0000000000	-2.7441970011
H	0.0000000000	0.0000000000	2.4098313123
H	-2.9161487182	0.0000000000	-2.5304696072
H	2.9161487182	0.0000000000	-2.5304696072
H	-2.3801864444	0.0000000000	2.4899145371
H	2.3801864444	-0.0000000000	2.4899145371
H	-4.8199636933	0.0000000000	-1.0072003276
H	4.8199636933	-0.0000000000	-1.0072003276
H	-4.5714535583	0.0000000000	1.4024883617
H	4.5714535583	0.0000000000	1.4024883617

AB1a**B8**a T_1:

C	-0.0000000000	0.0000000000	-1.6719945727
C	0.0000000000	0.0000000000	1.3367107341
B	-1.3170429452	0.0000000000	-0.8905839316
B	1.3170429452	-0.0000000000	-0.8905839316
C	-1.2334316822	0.0000000000	0.6736873514
C	1.2334316822	-0.0000000000	0.6736873514
C	-2.7387028841	0.0000000000	-1.4759565525
C	2.7387028841	0.0000000000	-1.4759565525
C	-2.4367965726	0.0000000000	1.4230642661

C	2.4367965726	0.0000000000	1.4230642661
C	-3.8029266017	0.0000000000	-0.6315410396
C	3.8029266017	-0.0000000000	-0.6315410396
C	-3.6534854314	0.0000000000	0.7998375791
C	3.6534854314	0.0000000000	0.7998375791
H	-0.0000000000	0.0000000000	-2.7625767696
H	-0.0000000000	0.0000000000	2.4289181979
H	-2.9382540213	0.0000000000	-2.5452133138
H	2.9382540213	0.0000000000	-2.5452133138
H	-2.3976104178	0.0000000000	2.5096803150
H	2.3976104178	0.0000000000	2.5096803150
H	-4.8209236488	0.0000000000	-1.0140174488
H	4.8209236488	0.0000000000	-1.0140174488
H	-4.5554741689	0.0000000000	1.4032142587
H	4.5554741689	0.0000000000	1.4032142587

AB1a**B8**a T_2:

C	-0.0006566835	-1.6924739388	0.0000000000
C	-0.0104883948	1.3084749151	0.0000000000
B	-1.3408597339	-0.8916670138	0.0000000000
B	1.3306582112	-0.8949177261	0.0000000000
C	-1.2444007623	0.6639606795	0.0000000000
C	1.2307665165	0.6301824744	0.0000000000
C	-2.7632390480	-1.4694306383	0.0000000000
C	2.7574049948	-1.4523536599	0.0000000000
C	-2.4446526318	1.4197569240	0.0000000000
C	2.4280629830	1.3841746101	0.0000000000

C	-3.8248059903	-0.6160221619	0.0000000000
C	3.8627315369	-0.5804415931	0.0000000000
C	-3.6731064444	0.8095277040	0.0000000000
C	3.7060719439	0.7971392488	0.0000000000
H	-0.0086155220	-2.7835980437	0.0000000000
H	0.0025913421	2.4011512292	0.0000000000
H	-2.9725946271	-2.5370213379	0.0000000000
H	2.9787075279	-2.5176642819	0.0000000000
H	-2.3957645380	2.5066690537	0.0000000000
H	2.3706793345	2.4714486728	0.0000000000
H	-4.8431547219	-0.9982873696	0.0000000000
H	4.8720675841	-0.9827389127	0.0000000000
H	-4.5693816536	1.4205602776	0.0000000000
H	4.5789147751	1.4390538886	0.0000000000

AB4B8 S_0:

C	-0.0080758166	-1.3928763308	-0.0000000000
C	0.0080758166	1.3928763308	0.0000000000
C	-1.2165294694	0.7721868985	-0.0000000000
C	1.2165294694	-0.7721868985	0.0000000000
C	-1.2384907033	-0.6707131715	-0.0000000000
C	1.2384907033	0.6707131715	0.0000000000
B	-2.5447174237	1.5466856313	-0.0000000000
B	2.5447174237	-1.5466856313	0.0000000000
C	-2.4471201547	-1.3399139094	0.0000000000
C	2.4471201547	1.3399139094	-0.0000000000
C	-3.8184237511	0.6904747389	-0.0000000000

C	3.8184237511	-0.6904747389	0.0000000000
C	-3.7068521445	-0.6687237282	0.0000000000
C	3.7068521445	0.6687237282	-0.0000000000
H	-0.0498180509	-2.4784106482	-0.0000000000
H	0.0498180509	2.4784106482	0.0000000000
H	-2.5579373657	2.7455485190	-0.0000000000
H	2.5579373657	-2.7455485190	0.0000000000
H	-2.4413851801	-2.4252189878	0.0000000000
H	2.4413851801	2.4252189878	-0.0000000000
H	-4.8199523972	1.1119396769	-0.0000000000
H	4.8199523972	-1.1119396769	0.0000000000
H	-4.5940994727	-1.2971742732	-0.0000000000
H	4.5940994727	1.2971742732	0.0000000000

AB4B8 S_1:

C	-0.0314348419	-1.4040014411	0.0000000000
C	0.0314348419	1.4040014411	-0.0000000000
C	-1.2095059704	0.7725726220	0.0000000000
C	1.2095059704	-0.7725726220	-0.0000000000
C	-1.2360891783	-0.7003390381	0.0000000000
C	1.2360891783	0.7003390381	-0.0000000000
B	-2.5349532126	1.5502644998	0.0000000000
B	2.5349532126	-1.5502644998	0.0000000000
C	-2.4787526877	-1.3804798316	0.0000000000
C	2.4787526877	1.3804798316	0.0000000000
C	-3.7775875096	0.7033644535	-0.0000000000
C	3.7775875096	-0.7033644535	0.0000000000

C	-3.6851058549	-0.7046834402	0.0000000000
C	3.6851058549	0.7046834402	0.0000000000
H	-0.0567931174	-2.4889243501	-0.0000000000
H	0.0567931174	2.4889243501	0.0000000000
H	-2.5410160294	2.7488144363	0.0000000000
H	2.5410160294	-2.7488144363	0.0000000000
H	-2.4685245266	-2.4643997385	0.0000000000
H	2.4685245266	2.4643997385	0.0000000000
H	-4.7814896739	1.1193384943	-0.0000000000
H	4.7814896739	-1.1193384943	0.0000000000
H	-4.5939788688	-1.3009189696	0.0000000000
H	4.5939788688	1.3009189696	-0.0000000000

AB4B8 T_1:

C	-0.0379056589	-1.3854931723	-0.0000000000
C	0.0379056589	1.3854931723	0.0000000000
C	-1.2046697606	0.7573762649	-0.0000000000
C	1.2046697606	-0.7573762649	0.0000000000
C	-1.2351863973	-0.6614390956	-0.0000000000
C	1.2351863973	0.6614390956	0.0000000000
B	-2.5449790275	1.5323026206	0.0000000000
B	2.5449790275	-1.5323026206	-0.0000000000
C	-2.5005567917	-1.3491783976	-0.0000000000
C	2.5005567917	1.3491783976	0.0000000000
C	-3.8205648104	0.6846114897	-0.0000000000
C	3.8205648104	-0.6846114897	0.0000000000
C	-3.7271028074	-0.7005319217	-0.0000000000

C	3.7271028074	0.7005319217	0.0000000000
H	-0.0757391298	-2.4707114299	0.0000000000
H	0.0757391298	2.4707114299	-0.0000000000
H	-2.5646979824	2.7305183740	0.0000000000
H	2.5646979824	-2.7305183740	-0.0000000000
H	-2.4777783141	-2.4342496761	0.0000000000
H	2.4777783141	2.4342496761	-0.0000000000
H	-4.8166422683	1.1187728482	-0.0000000000
H	4.8166422683	-1.1187728482	0.0000000000
H	-4.6230696625	-1.3150380876	-0.0000000000
H	4.6230696625	1.3150380876	0.0000000000

AB4B8 T_2:

C	-0.0237677898	-1.4059351999	0.0000000000
C	0.0237677898	1.4059351999	-0.0000000000
C	-1.2109435226	0.7788165931	0.0000000000
C	1.2109435226	-0.7788165931	-0.0000000000
C	-1.2341466101	-0.6997187781	-0.0000000000
C	1.2341466101	0.6997187781	0.0000000000
B	-2.5337867795	1.5563197532	0.0000000000
B	2.5337867795	-1.5563197532	-0.0000000000
C	-2.4690981134	-1.3782708091	0.0000000000
C	2.4690981134	1.3782708091	0.0000000000
C	-3.7768557159	0.7085913002	0.0000000000
C	3.7768557159	-0.7085913002	-0.0000000000
C	-3.6757025894	-0.7025572662	0.0000000000
C	3.6757025894	0.7025572662	-0.0000000000

H	-0.0532993534	-2.4907617388	0.0000000000
H	0.0532993534	2.4907617388	0.0000000000
H	-2.5389874390	2.7549403465	-0.0000000000
H	2.5389874390	-2.7549403465	0.0000000000
H	-2.4606402631	-2.4621694444	0.0000000000
H	2.4606402631	2.4621694444	-0.0000000000
H	-4.7830638432	1.1183780722	0.0000000000
H	4.7830638432	-1.1183780722	-0.0000000000
H	-4.5834531326	-1.3008957943	-0.0000000000
H	4.5834531326	1.3008957943	0.0000000000

AB4*a***B8***a* S_0:

C	-0.1348628117	-1.5008929108	0.0000000000
C	0.1348628117	1.5008929108	0.0000000000
B	-1.2562437321	0.7666405169	0.0000000000
B	1.2562437321	-0.7666405169	0.0000000000
C	-1.2962717293	-0.8010799948	0.0000000000
C	1.2962717293	0.8010799948	0.0000000000
C	-2.6086104684	1.4709145360	0.0000000000
C	2.6086104684	-1.4709145360	0.0000000000
C	-2.5923788786	-1.4585740348	0.0000000000
C	2.5923788786	1.4585740348	0.0000000000
C	-3.7326683891	0.7110062729	0.0000000000
C	3.7326683891	-0.7110062729	0.0000000000
C	-3.7316136183	-0.7426355444	0.0000000000
C	3.7316136183	0.7426355444	0.0000000000
H	-0.1824339940	-2.5927543211	0.0000000000

H	0.1824339940	2.5927543211	0.0000000000
H	-2.7276683862	2.5517542006	0.0000000000
H	2.7276683862	-2.5517542006	0.0000000000
H	-2.6301282531	-2.5452045472	0.0000000000
H	2.6301282531	2.5452045472	0.0000000000
H	-4.7124353298	1.1853170251	0.0000000000
H	4.7124353298	-1.1853170251	0.0000000000
H	-4.6916320665	-1.2472488044	0.0000000000
H	4.6916320665	1.2472488044	0.0000000000

AB4a**B8**a S_1:

C	-0.0809853010	-1.4948816644	0.0000000000
C	0.0809853010	1.4948816644	0.0000000000
B	-1.2633858620	0.7881816377	0.0000000000
B	1.2633858620	-0.7881816377	0.0000000000
C	-1.2837022175	-0.7601606074	0.0000000000
C	1.2837022175	0.7601606074	0.0000000000
C	-2.6157842671	1.4806409629	0.0000000000
C	2.6157842671	-1.4806409629	0.0000000000
C	-2.5260560554	-1.4082388505	0.0000000000
C	2.5260560554	1.4082388505	0.0000000000
C	-3.7694903447	0.7102065224	0.0000000000
C	3.7694903447	-0.7102065224	0.0000000000
C	-3.7251285699	-0.6935322900	0.0000000000
C	3.7251285699	0.6935322900	0.0000000000
H	-0.1592428148	-2.5849426653	0.0000000000
H	0.1592428148	2.5849426653	0.0000000000

H	-2.7385217035	2.5617350727	0.0000000000
H	2.7385217035	-2.5617350727	0.0000000000
H	-2.5722684034	-2.4956862547	0.0000000000
H	2.5722684034	2.4956862547	0.0000000000
H	-4.7495672430	1.1802077106	0.0000000000
H	4.7495672430	-1.1802077106	0.0000000000
H	-4.6606264270	-1.2430171018	0.0000000000
H	4.6606264270	1.2430171018	0.0000000000

AB4a**B8**a T_1:

C	-0.0803427262	-1.4999522257	0.0000000000
C	0.0803427262	1.4999522257	0.0000000000
B	-1.2623617659	0.7896926767	0.0000000000
B	1.2623617659	-0.7896926767	0.0000000000
C	-1.2816717240	-0.7697306477	0.0000000000
C	1.2816717240	0.7697306477	0.0000000000
C	-2.6305862043	1.4866997899	0.0000000000
C	2.6305862043	-1.4866997899	0.0000000000
C	-2.5341069668	-1.4176517305	0.0000000000
C	2.5341069668	1.4176517305	0.0000000000
C	-3.7649458260	0.7251933020	0.0000000000
C	3.7649458260	-0.7251933020	0.0000000000
C	-3.7121437126	-0.6992641229	0.0000000000
C	3.7121437126	0.6992641229	0.0000000000
H	-0.1558174378	-2.5895297046	0.0000000000
H	0.1558174378	2.5895297046	0.0000000000
H	-2.7471625254	2.5684622556	0.0000000000

H	2.7471625254	-2.5684622556	0.0000000000
H	-2.5830251490	-2.5041778910	0.0000000000
H	2.5830251490	2.5041778910	0.0000000000
H	-4.7504221570	1.1835133197	0.0000000000
H	4.7504221570	-1.1835133197	0.0000000000
H	-4.6524894444	-1.2419668750	0.0000000000
H	4.6524894444	1.2419668750	0.0000000000

AB4a**B8**a T_2:

C	-0.1090297297	-1.5018843736	0.0000000000
C	0.1090297297	1.5018843736	0.0000000000
B	-1.2596478936	0.7791775641	0.0000000000
B	1.2596478936	-0.7791775641	0.0000000000
C	-1.2863469679	-0.7695672734	0.0000000000
C	1.2863469679	0.7695672734	0.0000000000
C	-2.6345231521	1.4689094856	0.0000000000
C	2.6345231521	-1.4689094856	0.0000000000
C	-2.5524781334	-1.4108610171	0.0000000000
C	2.5524781334	1.4108610171	0.0000000000
C	-3.7895861713	0.7047179852	0.0000000000
C	3.7895861713	-0.7047179852	0.0000000000
C	-3.7519924547	-0.6998967697	0.0000000000
C	3.7519924547	0.6998967697	0.0000000000
H	-0.1828706143	-2.5919958382	0.0000000000
H	0.1828706143	2.5919958382	0.0000000000
H	-2.7567571724	2.5503130455	0.0000000000
H	2.7567571724	-2.5503130455	0.0000000000

H	-2.5982301223	-2.4983170270	0.0000000000
H	2.5982301223	2.4983170270	0.0000000000
H	-4.7658044735	1.1823391735	0.0000000000
H	4.7658044735	-1.1823391735	0.0000000000
H	-4.6868820108	-1.2495562514	0.0000000000
H	4.6868820108	1.2495562514	0.0000000000

AB3B7 S_0:

C	-0.0649253771	-1.3898004176	0.0000000000
C	0.0649253771	1.3898004176	0.0000000000
C	-1.2206867134	0.7383346850	0.0000000000
C	1.2206867134	-0.7383346850	0.0000000000
C	-1.2455093891	-0.7148199699	0.0000000000
C	1.2455093891	0.7148199699	0.0000000000
C	-2.3862484119	1.4510786574	0.0000000000
C	2.3862484119	-1.4510786574	0.0000000000
C	-2.5080815522	-1.4298883762	-0.0000000000
C	2.5080815522	1.4298883762	0.0000000000
B	-3.7509151257	0.7276761708	0.0000000000
B	3.7509151257	-0.7276761708	-0.0000000000
C	-3.7050808299	-0.8057848777	0.0000000000
C	3.7050808299	0.8057848777	0.0000000000
H	-0.0695310557	-2.4753883300	0.0000000000
H	0.0695310557	2.4753883300	-0.0000000000
H	-2.3021996639	2.5355229710	0.0000000000
H	2.3021996639	-2.5355229710	0.0000000000
H	-2.4336005935	-2.5154124673	0.0000000000

H	2.4336005935	2.5154124673	0.0000000000
H	-4.7786180770	1.3434052701	0.0000000000
H	4.7786180770	-1.3434052701	0.0000000000
H	-4.5990506411	-1.4230677067	0.0000000000
H	4.5990506411	1.4230677067	0.0000000000

AB3B7 S_1:

C	-0.0067470362	-1.3920937427	0.0000000000
C	0.0067470362	1.3920937427	0.0000000000
C	-1.2320475347	0.7666975034	-0.0000000000
C	1.2320475347	-0.7666975034	0.0000000000
C	-1.2287539762	-0.6956428264	0.0000000000
C	1.2287539762	0.6956428264	-0.0000000000
C	-2.4447355996	1.4883575504	-0.0000000000
C	2.4447355996	-1.4883575504	0.0000000000
C	-2.4426005440	-1.4047580925	0.0000000000
C	2.4426005440	1.4047580925	-0.0000000000
B	-3.7650745911	0.7765487667	-0.0000000000
B	3.7650745911	-0.7765487667	0.0000000000
C	-3.6674394219	-0.7644806910	-0.0000000000
C	3.6674394219	0.7644806910	0.0000000000
H	-0.0386699798	-2.4769371540	0.0000000000
H	0.0386699798	2.4769371540	-0.0000000000
H	-2.3484729077	2.5711747637	0.0000000000
H	2.3484729077	-2.5711747637	-0.0000000000
H	-2.3841397438	-2.4901928936	0.0000000000
H	2.3841397438	2.4901928936	0.0000000000

H	-4.8227320763	1.3386283127	-0.0000000000
H	4.8227320763	-1.3386283127	0.0000000000
H	-4.5468319103	-1.4045300140	-0.0000000000
H	4.5468319103	1.4045300140	0.0000000000

AB3B7 T_1:

C	-0.0369355165	-1.3827650546	0.0000000000
C	0.0369355165	1.3827650546	0.0000000000
C	-1.2040363902	0.7339240757	0.0000000000
C	1.2040363902	-0.7339240757	-0.0000000000
C	-1.2417505028	-0.6873376457	-0.0000000000
C	1.2417505028	0.6873376457	0.0000000000
C	-2.4346422672	1.4644652513	-0.0000000000
C	2.4346422672	-1.4644652513	0.0000000000
C	-2.5080439454	-1.4024656811	-0.0000000000
C	2.5080439454	1.4024656811	0.0000000000
B	-3.7894215724	0.7397780358	0.0000000000
B	3.7894215724	-0.7397780358	-0.0000000000
C	-3.7137982537	-0.7933714716	0.0000000000
C	3.7137982537	0.7933714716	-0.0000000000
H	-0.0540705761	-2.4678816085	0.0000000000
H	0.0540705761	2.4678816085	-0.0000000000
H	-2.3451100790	2.5481237086	-0.0000000000
H	2.3451100790	-2.5481237086	0.0000000000
H	-2.4299873434	-2.4878316822	-0.0000000000
H	2.4299873434	2.4878316822	0.0000000000
H	-4.8194755954	1.3497946855	0.0000000000

H	4.8194755954	-1.3497946855	-0.0000000000
H	-4.5964044611	-1.4268662200	0.0000000000
H	4.5964044611	1.4268662200	-0.0000000000

AB3B7 T_2:

C	1.395744	0.023966	0.000000
C	-1.395744	-0.023966	0.000000
C	-0.738281	-1.254445	0.000000
C	0.738281	1.254445	0.000000
C	0.733014	-1.215568	0.000000
C	-0.733014	1.215568	0.000000
C	-1.422674	-2.473153	0.000000
C	1.422674	2.473153	0.000000
C	1.477112	-2.412560	0.000000
C	-1.477112	2.412560	0.000000
B	-0.672643	-3.777233	0.000000
B	0.672643	3.777233	0.000000
C	0.870445	-3.645037	0.000000
C	-0.870445	3.645037	0.000000
H	2.481135	0.021318	0.000000
H	-2.481135	-0.021318	0.000000
H	-2.508095	-2.410262	0.000000
H	2.508095	2.410262	0.000000
H	2.560668	-2.324314	0.000000
H	-2.560668	2.324314	0.000000
H	-1.206774	-4.849070	0.000000
H	1.206774	4.849070	0.000000

H	1.527573	-4.512056	0.000000
H	-1.527573	4.512056	0.000000

AN1N8 S_0:

C	-0.0000000000	0.0000000000	-1.4343052759
C	-0.0000000000	0.0000000000	1.3569914135
C	-1.2316522545	0.0000000000	-0.7696827233
C	1.2316522545	-0.0000000000	-0.7696827233
C	-1.2087562442	0.0000000000	0.6640370127
C	1.2087562442	-0.0000000000	0.6640370127
C	-2.4963131231	0.0000000000	-1.3959047122
C	2.4963131231	-0.0000000000	-1.3959047122
N	-2.3883526220	0.0000000000	1.3279725201
N	2.3883526220	0.0000000000	1.3279725201
C	-3.6742813401	0.0000000000	-0.6425563496
C	3.6742813401	-0.0000000000	-0.6425563496
C	-3.6272979310	0.0000000000	0.7189017175
C	3.6272979310	-0.0000000000	0.7189017175
H	-0.0000000000	0.0000000000	-2.5183771824
H	0.0000000000	0.0000000000	2.4428622186
H	-2.5450112549	0.0000000000	-2.4776878885
H	2.5450112549	0.0000000000	-2.4776878885
H	-2.3523713775	0.0000000000	2.3306558709
H	2.3523713775	0.0000000000	2.3306558709
H	-4.6388765996	0.0000000000	-1.1350937210
H	4.6388765996	-0.0000000000	-1.1350937210
H	-4.4848545280	0.0000000000	1.3734729654

H	4.4848545280	-0.0000000000	1.3734729654

AN1N8 S_1:

C	-0.0000000000	0.0000000000	-1.4337943279
C	-0.0000000000	0.0000000000	1.3944123400
C	-1.2249922954	0.0000000000	-0.7695516597
C	1.2249922954	-0.0000000000	-0.7695516597
C	-1.2024642374	0.0000000000	0.7014131925
C	1.2024642374	0.0000000000	0.7014131925
C	-2.4867111978	0.0000000000	-1.4005236009
C	2.4867111978	0.0000000000	-1.4005236009
N	-2.4080416315	0.0000000000	1.3382404180
N	2.4080416315	0.0000000000	1.3382404180
C	-3.6672944872	0.0000000000	-0.6771342163
C	3.6672944872	-0.0000000000	-0.6771342163
C	-3.6115137575	0.0000000000	0.7180722034
C	3.6115137575	0.0000000000	0.7180722034
H	0.0000000000	0.0000000000	-2.5196132676
H	-0.0000000000	0.0000000000	2.4816876071
H	-2.5203510829	0.0000000000	-2.4849596391
H	2.5203510829	0.0000000000	-2.4849596391
H	-2.3968908283	0.0000000000	2.3423341517
H	2.3968908283	0.0000000000	2.3423341517
H	-4.6297178427	0.0000000000	-1.1695880808
H	4.6297178427	0.0000000000	-1.1695880808
H	-4.4811660297	0.0000000000	1.3580513343
H	4.4811660297	0.0000000000	1.3580513343

AN1N8 T_1:

C	0.0000000000	0.0000000000	-1.4015348711
C	-0.0000000000	0.0000000000	1.3671265398
C	-1.2284626004	0.0000000000	-0.7349956178
C	1.2284626004	-0.0000000000	-0.7349956178
C	-1.2062275554	0.0000000000	0.6783963757
C	1.2062275554	0.0000000000	0.6783963757
C	-2.4893832289	0.0000000000	-1.4146575395
C	2.4893832289	0.0000000000	-1.4146575395
N	-2.4190465609	0.0000000000	1.3584783822
N	2.4190465609	0.0000000000	1.3584783822
C	-3.6690634823	0.0000000000	-0.6656506168
C	3.6690634823	0.0000000000	-0.6656506168
C	-3.6296408828	0.0000000000	0.6995861198
C	3.6296408828	0.0000000000	0.6995861198
H	0.0000000000	0.0000000000	-2.4863113198
H	0.0000000000	0.0000000000	2.4534997592
H	-2.5123184401	0.0000000000	-2.4960981854
H	2.5123184401	0.0000000000	-2.4960981854
H	-2.4055821786	0.0000000000	2.3591051615
H	2.4055821786	0.0000000000	2.3591051615
H	-4.6346677340	0.0000000000	-1.1562001701
H	4.6346677340	0.0000000000	-1.1562001701
H	-4.5118834486	0.0000000000	1.3233463153
H	4.5118834486	0.0000000000	1.3233463153

AN1N8 T_2:

C	-0.0000000000	0.0000000000	-1.4380064053
C	-0.0000000000	0.0000000000	1.3928047335
C	-1.2245314001	0.0000000000	-0.7745769025
C	1.2245314001	-0.0000000000	-0.7745769025
C	-1.2015745010	0.0000000000	0.6995055713
C	1.2015745010	0.0000000000	0.6995055713
C	-2.4886716880	0.0000000000	-1.3993062379
C	2.4886716880	0.0000000000	-1.3993062379
N	-2.4023149866	0.0000000000	1.3353334306
N	2.4023149866	0.0000000000	1.3353334306
C	-3.6669714422	0.0000000000	-0.6777973180
C	3.6669714422	-0.0000000000	-0.6777973180
C	-3.6077473103	0.0000000000	0.7237111900
C	3.6077473103	0.0000000000	0.7237111900
H	0.0000000000	0.0000000000	-2.5238810503
H	-0.0000000000	0.0000000000	2.4801088959
H	-2.5243470709	0.0000000000	-2.4839736589
H	2.5243470709	0.0000000000	-2.4839736589
H	-2.3873606625	0.0000000000	2.3399441867
H	2.3873606625	0.0000000000	2.3399441867
H	-4.6299291178	0.0000000000	-1.1687485387
H	4.6299291178	-0.0000000000	-1.1687485387
H	-4.4738123237	0.0000000000	1.3680954691
H	4.4738123237	0.0000000000	1.3680954691

AN2N7 S_0:

C	-0.0000000000	0.0000000000	-1.4305656488
C	0.0000000000	0.0000000000	1.3612677045
C	-1.2287761888	0.0000000000	-0.7511118339
C	1.2287761888	-0.0000000000	-0.7511118339
C	-1.2218631297	0.0000000000	0.6893124397
C	1.2218631297	-0.0000000000	0.6893124397
C	-2.4751973085	0.0000000000	-1.3833939775
C	2.4751973085	0.0000000000	-1.3833939775
C	-2.4658918993	0.0000000000	1.3743846494
C	2.4658918993	0.0000000000	1.3743846494
N	-3.6403934595	0.0000000000	-0.6514656039
N	3.6403934595	0.0000000000	-0.6514656039
C	-3.6469505703	0.0000000000	0.6845336276
C	3.6469505703	0.0000000000	0.6845336276
H	-0.0000000000	0.0000000000	-2.5151350251
H	0.0000000000	0.0000000000	2.4464348495
H	-2.5889641688	0.0000000000	-2.4567941269
H	2.5889641688	0.0000000000	-2.4567941269
H	-2.4834957743	0.0000000000	2.4565475344
H	2.4834957743	0.0000000000	2.4565475344
H	-4.5127418320	0.0000000000	-1.1445546445
H	4.5127418320	-0.0000000000	-1.1445546445
H	-4.6142494984	0.0000000000	1.1692412745
H	4.6142494984	-0.0000000000	1.1692412745

AN2N7 S_1:

C	0.0000000000	0.0000000000	-1.4348457037

C	-0.0000000000	0.0000000000	1.4215330771
C	-1.2335493702	0.0000000000	-0.7383491476
C	1.2335493702	-0.0000000000	-0.7383491476
C	-1.2200004127	0.0000000000	0.7545056211
C	1.2200004127	-0.0000000000	0.7545056211
C	-2.4337236810	0.0000000000	-1.3739413091
C	2.4337236810	0.0000000000	-1.3739413091
C	-2.4854516791	0.0000000000	1.3851151130
C	2.4854516791	-0.0000000000	1.3851151130
N	-3.6142203828	0.0000000000	-0.7013772486
N	3.6142203828	-0.0000000000	-0.7013772486
C	-3.6490594871	0.0000000000	0.6769825369
C	3.6490594871	-0.0000000000	0.6769825369
H	0.0000000000	0.0000000000	-2.5202762674
H	-0.0000000000	0.0000000000	2.5078064213
H	-2.5064767352	0.0000000000	-2.4550901222
H	2.5064767352	-0.0000000000	-2.4550901222
H	-2.5395037678	0.0000000000	2.4679577981
H	2.5395037678	-0.0000000000	2.4679577981
H	-4.4712432071	0.0000000000	-1.2170232125
H	4.4712432071	0.0000000000	-1.2170232125
H	-4.6287285823	0.0000000000	1.1318114862
H	4.6287285823	-0.0000000000	1.1318114862

AN2N7 T_1:

C	-0.0000000000	0.0000000000	-1.4130850221
C	-0.0000000000	0.0000000000	1.3919203291

C	-1.2269223289	0.0000000000	-0.7253825123
C	1.2269223289	-0.0000000000	-0.7253825123
C	-1.2167891103	0.0000000000	0.7240401341
C	1.2167891103	-0.0000000000	0.7240401341
C	-2.4434071006	0.0000000000	-1.3905969521
C	2.4434071006	-0.0000000000	-1.3905969521
C	-2.4967806502	0.0000000000	1.3856801481
C	2.4967806502	-0.0000000000	1.3856801481
N	-3.6299067933	0.0000000000	-0.6940693850
N	3.6299067933	0.0000000000	-0.6940693850
C	-3.6450630054	0.0000000000	0.6864045427
C	3.6450630054	0.0000000000	0.6864045427
H	-0.0000000000	0.0000000000	-2.4982536384
H	-0.0000000000	0.0000000000	2.4784441261
H	-2.5163885160	0.0000000000	-2.4688819696
H	2.5163885160	0.0000000000	-2.4688819696
H	-2.5389939167	0.0000000000	2.4681455127
H	2.5389939167	0.0000000000	2.4681455127
H	-4.4943529159	0.0000000000	-1.1964325274
H	4.4943529159	0.0000000000	-1.1964325274
H	-4.6225741389	0.0000000000	1.1492803904
H	4.6225741389	-0.0000000000	1.1492803904

AN2N7 T_2:

C	-0.0130000137	-1.4058797477	0.0000000000
C	-0.0099927530	1.3793756700	0.0000000000
C	-1.2245547784	-0.7340821564	0.0000000000

C	1.2162652052	-0.7241406449	0.0000000000
C	-1.2151935614	0.6991659579	0.0000000000
C	1.2308721729	0.7112698688	0.0000000000
C	-2.5039316823	-1.4079928506	0.0000000000
C	2.4752175776	-1.3977886994	0.0000000000
C	-2.4711541836	1.3951142235	0.0000000000
C	2.4579553159	1.3955946400	0.0000000000
N	-3.6458569748	-0.6592509916	0.0000000000
N	3.6082166994	-0.6884584456	0.0000000000
C	-3.6421364506	0.6905440341	0.0000000000
C	3.6642662910	0.6654602956	0.0000000000
H	-0.0090523921	-2.4924613409	0.0000000000
H	-0.0174501141	2.4641672255	0.0000000000
H	-2.6149039549	-2.4805512835	0.0000000000
H	2.5696972733	-2.4739268269	0.0000000000
H	-2.4924681470	2.4759822913	0.0000000000
H	2.4851961028	2.4761001623	0.0000000000
H	-4.5281425916	-1.1344695472	0.0000000000
H	4.4762410261	-1.1932460266	0.0000000000
H	-4.6137442502	1.1666039522	0.0000000000
H	4.6478211641	1.1082727990	0.0000000000

AN1a**N8**a S_0:

C	-0.8316503222	-1.2426659761	0.0000000000
C	-0.4622555987	1.4091503104	0.0000000000
N	-0.2487130841	-0.6274889151	-1.1820132701
N	-0.2487130841	-0.6274889151	1.1820132701

C	-0.2390485372	0.7404614976	-1.2153490783
C	-0.2390485372	0.7404614976	1.2153490783
C	0.0737154158	-1.3477102771	-2.2640415056
C	0.0737154158	-1.3477102771	2.2640415056
C	0.0328887304	1.3656594725	-2.4464386583
C	0.0328887304	1.3656594725	2.4464386583
C	0.3259773306	-0.7688986357	-3.4867215105
C	0.3259773306	-0.7688986357	3.4867215105
C	0.2900195664	0.6228279232	-3.5742028122
C	0.2900195664	0.6228279232	3.5742028122
H	-0.5363261072	-2.2930028468	0.0000000000
H	-0.4777850469	2.4896581371	0.0000000000
H	0.0689126861	-2.4202650250	-2.1225336479
H	0.0689126861	-2.4202650250	2.1225336479
H	0.0299206516	2.4476055244	-2.4766751044
H	0.0299206516	2.4476055244	2.4766751044
H	0.5433464250	-1.3942663170	-4.3414169763
H	0.5433464250	-1.3942663170	4.3414169763
H	0.4769893530	1.1182052184	-4.5198626375
H	0.4769893530	1.1182052184	4.5198626375

AN1a**N8**a S_1:

C	-0.0000000000	0.0000000000	-1.3248003430
C	0.0000000000	0.0000000000	1.4146962102
N	-1.1952864230	0.0000000000	-0.6664658839
N	1.1952864230	0.0000000000	-0.6664658839
C	-1.2253668067	0.0000000000	0.7517888020

C	1.2253668067	0.0000000000	0.7517888020
C	-2.3805356247	0.0000000000	-1.3701808121
C	2.3805356247	-0.0000000000	-1.3701808121
C	-2.4866028958	0.0000000000	1.3742490023
C	2.4866028958	0.0000000000	1.3742490023
C	-3.5857549592	0.0000000000	-0.7544223368
C	3.5857549592	-0.0000000000	-0.7544223368
C	-3.6570272844	0.0000000000	0.6678851240
C	3.6570272844	0.0000000000	0.6678851240
H	-0.0000000000	0.0000000000	-2.4006503869
H	-0.0000000000	0.0000000000	2.4960326451
H	-2.2738255593	0.0000000000	-2.4466230983
H	2.2738255593	-0.0000000000	-2.4466230983
H	-2.4922235833	0.0000000000	2.4581443026
H	2.4922235833	0.0000000000	2.4581443026
H	-4.4802768871	0.0000000000	-1.3629840433
H	4.4802768871	-0.0000000000	-1.3629840433
H	-4.6131934316	0.0000000000	1.1736701592
H	4.6131934316	0.0000000000	1.1736701592

AN1a**N8**a T_1:

C	-0.0000000000	0.0000000000	-1.3025593071
C	0.0000000000	0.0000000000	1.4247458110
N	-1.1903397196	0.0000000000	-0.6552109168
N	1.1903397196	-0.0000000000	-0.6552109168
C	-1.2269179651	0.0000000000	0.7616726518
C	1.2269179651	0.0000000000	0.7616726518

C	-2.3775790985	0.0000000000	-1.3751329049
C	2.3775790985	0.0000000000	-1.3751329049
C	-2.4875294032	0.0000000000	1.3731431742
C	2.4875294032	0.0000000000	1.3731431742
C	-3.5808881315	0.0000000000	-0.7614270740
C	3.5808881315	0.0000000000	-0.7614270740
C	-3.6592147645	0.0000000000	0.6581447941
C	3.6592147645	-0.0000000000	0.6581447941
H	-0.0000000000	0.0000000000	-2.3792252877
H	0.0000000000	0.0000000000	2.5057041728
H	-2.2605619334	0.0000000000	-2.4500109271
H	2.2605619334	-0.0000000000	-2.4500109271
H	-2.4999300395	0.0000000000	2.4567918870
H	2.4999300395	0.0000000000	2.4567918870
H	-4.4737574133	0.0000000000	-1.3731716844
H	4.4737574133	0.0000000000	-1.3731716844
H	-4.6179383302	0.0000000000	1.1585685842
H	4.6179383302	-0.0000000000	1.1585685842

AN1a**N8**a T_2:

C	0.0000755867	-1.3735178647	-0.0619789562
C	0.0001292716	1.4189144302	-0.0218680796
N	-1.1902382759	-0.6321611714	-0.0320875721
N	1.1904260367	-0.6323795066	-0.0299646697
C	-1.2175929525	0.7431638932	-0.0206992155
C	1.2176765023	0.7432137230	-0.0192333898
C	-2.3572383951	-1.3811553180	-0.0112951137

C	2.3576703207	-1.3809626418	-0.0064241475
C	-2.4720381819	1.3816571531	-0.0059148841
C	2.4720373972	1.3816923254	-0.0034171427
C	-3.5786529525	-0.7596659320	0.0178938772
C	3.5786295562	-0.7594420269	0.0243294423
C	-3.6453263494	0.6357726356	0.0204723418
C	3.6453555758	0.6362808090	0.0255012224
H	-0.0006559872	-2.2529973633	0.5924208628
H	0.0000001359	2.4985715716	-0.0078711240
H	-2.2184441695	-2.4499517135	-0.0562915319
H	2.2190050706	-2.4498640533	-0.0498015646
H	-2.4873645128	2.4626038670	-0.0187579250
H	2.4874082351	2.4626381040	-0.0175140459
H	-4.4758195328	-1.3646705006	0.0311482156
H	4.4757820393	-1.3644218257	0.0398004401
H	-4.6065019143	1.1343188337	0.0388994565
H	4.6064354953	1.1349245717	0.0446465038

AN4N8 S_0:

C	0.0353646210	-1.3994695006	-0.0000000000
C	-0.0353646210	1.3994695006	0.0000000000
C	-1.2116214489	0.6970288522	0.0000000000
C	1.2116214489	-0.6970288522	-0.0000000000
C	-1.2302727910	-0.7471704452	0.0000000000
C	1.2302727910	0.7471704452	-0.0000000000
N	-2.4317414651	1.3304499611	0.0000000000
N	2.4317414651	-1.3304499611	-0.0000000000

C	-2.4454670842	-1.3999095858	0.0000000000
C	2.4454670842	1.3999095858	-0.0000000000
C	-3.6396159371	0.6747842531	-0.0000000000
C	3.6396159371	-0.6747842531	0.0000000000
C	-3.6698555618	-0.6733988407	0.0000000000
C	3.6698555618	0.6733988407	0.0000000000
H	0.0555518685	-2.4844472784	0.0000000000
H	-0.0555518685	2.4844472784	-0.0000000000
H	-2.4298737712	2.3329764733	0.0000000000
H	2.4298737712	-2.3329764733	-0.0000000000
H	-2.4651506504	-2.4833038230	0.0000000000
H	2.4651506504	2.4833038230	-0.0000000000
H	-4.5188998834	1.3033821156	0.0000000000
H	4.5188998834	-1.3033821156	-0.0000000000
H	-4.6205776823	-1.1896606948	0.0000000000
H	4.6205776823	1.1896606948	-0.0000000000

AN4N8 S_1:

C	0.0200579611	-1.4146097411	-0.0000000000
C	-0.0200579611	1.4146097411	0.0000000000
C	-1.2121155721	0.7054650922	-0.0000000000
C	1.2121155721	-0.7054650922	0.0000000000
C	-1.2123363931	-0.7660249220	0.0000000000
C	1.2123363931	0.7660249220	-0.0000000000
N	-2.4321040479	1.3267697106	0.0000000000
N	2.4321040479	-1.3267697106	-0.0000000000
C	-2.4648310298	-1.4144741912	0.0000000000

C	2.4648310298	1.4144741912	-0.0000000000
C	-3.6179416341	0.6950658959	0.0000000000
C	3.6179416341	-0.6950658959	-0.0000000000
C	-3.6541657469	-0.7032791674	0.0000000000
C	3.6541657469	0.7032791674	-0.0000000000
H	0.0391145846	-2.5011218045	0.0000000000
H	-0.0391145846	2.5011218045	-0.0000000000
H	-2.4309472259	2.3314019859	-0.0000000000
H	2.4309472259	-2.3314019859	0.0000000000
H	-2.4874051271	-2.4991735353	0.0000000000
H	2.4874051271	2.4991735353	0.0000000000
H	-4.4990156423	1.3195922205	0.0000000000
H	4.4990156423	-1.3195922205	-0.0000000000
H	-4.6103638171	-1.2078236893	0.0000000000
H	4.6103638171	1.2078236893	0.0000000000

AN4N8 T_1:

C	0.0183068292	-1.3832130853	-0.0000000000
C	-0.0183068292	1.3832130853	0.0000000000
C	-1.2136594660	0.6793447249	0.0000000000
C	1.2136594660	-0.6793447249	0.0000000000
C	-1.2180214218	-0.7317894522	0.0000000000
C	1.2180214218	0.7317894522	0.0000000000
N	-2.4322755094	1.3461122484	0.0000000000
N	2.4322755094	-1.3461122484	0.0000000000
C	-2.4789329091	-1.4279227289	0.0000000000
C	2.4789329091	1.4279227289	0.0000000000

C	-3.6359891683	0.6797479044	0.0000000000
C	3.6359891683	-0.6797479044	0.0000000000
C	-3.6576493090	-0.6924628872	0.0000000000
C	3.6576493090	0.6924628872	0.0000000000
H	0.0360763099	-2.4687472939	0.0000000000
H	-0.0360763099	2.4687472939	0.0000000000
H	-2.4243307955	2.3471695213	0.0000000000
H	2.4243307955	-2.3471695213	0.0000000000
H	-2.4920436607	-2.5095886485	0.0000000000
H	2.4920436607	2.5095886485	0.0000000000
H	-4.5249444029	1.2930714037	0.0000000000
H	4.5249444029	-1.2930714037	0.0000000000
H	-4.6188027190	-1.1922875468	0.0000000000
H	4.6188027190	1.1922875468	0.0000000000

AN4N8 T_2:

C	0.0246399381	-1.4149400869	0.0000000000
C	-0.0246399381	1.4149400869	-0.0000000000
C	-1.2099238184	0.7106456327	0.0000000000
C	1.2099238184	-0.7106456327	-0.0000000000
C	-1.2143351959	-0.7635923110	-0.0000000000
C	1.2143351959	0.7635923110	0.0000000000
N	-2.4286948651	1.3291159732	-0.0000000000
N	2.4286948651	-1.3291159732	0.0000000000
C	-2.4625020441	-1.4092706723	-0.0000000000
C	2.4625020441	1.4092706723	0.0000000000
C	-3.6186291326	0.6964814305	0.0000000000

C	3.6186291326	-0.6964814305	-0.0000000000
C	-3.6534576333	-0.7068862995	0.0000000000
C	3.6534576333	0.7068862995	-0.0000000000
H	0.0426839225	-2.5014946932	-0.0000000000
H	-0.0426839225	2.5014946932	0.0000000000
H	-2.4279632200	2.3337711641	-0.0000000000
H	2.4279632200	-2.3337711641	0.0000000000
H	-2.4818932226	-2.4945266966	0.0000000000
H	2.4818932226	2.4945266966	0.0000000000
H	-4.4984011420	1.3223811390	0.0000000000
H	4.4984011420	-1.3223811390	0.0000000000
H	-4.6078298945	-1.2142807467	-0.0000000000
H	4.6078298945	1.2142807467	0.0000000000

AN4*a***N8***a* S_0:

C	0.0013612989	-1.3646176325	0.0000000000
C	-0.0013612989	1.3646176325	0.0000000000
N	-1.2473497585	0.6736684891	0.0000000000
N	1.2473497585	-0.6736684891	0.0000000000
C	-1.1849763001	-0.7265232898	0.0000000000
C	1.1849763001	0.7265232898	0.0000000000
C	-2.4196795492	1.3398713456	0.0000000000
C	2.4196795492	-1.3398713456	0.0000000000
C	-2.4629303223	-1.4040913485	0.0000000000
C	2.4629303223	1.4040913485	0.0000000000
C	-3.6250302844	0.7155723875	0.0000000000
C	3.6250302844	-0.7155723875	0.0000000000

C	-3.6211893180	-0.7130410982	0.0000000000
C	3.6211893180	0.7130410982	0.0000000000
H	0.0592592592	-2.4412129419	0.0000000000
H	-0.0592592592	2.4412129419	0.0000000000
H	-2.3274580727	2.4189543172	0.0000000000
H	2.3274580727	-2.4189543172	0.0000000000
H	-2.4533203782	-2.4867583432	0.0000000000
H	2.4533203782	2.4867583432	0.0000000000
H	-4.5398579326	1.2887137036	0.0000000000
H	4.5398579326	-1.2887137036	0.0000000000
H	-4.5631254892	-1.2505953323	0.0000000000
H	4.5631254892	1.2505953323	0.0000000000

AN4*a***N8***a* S_1:

C	0.0282848538	-1.3561815297	0.0000000000
C	-0.0282848538	1.3561815297	0.0000000000
N	-1.2137720244	0.6933507059	0.0000000000
N	1.2137720244	-0.6933507059	0.0000000000
C	-1.2132338685	-0.7170295923	0.0000000000
C	1.2132338685	0.7170295923	0.0000000000
C	-2.4215137252	1.3607216036	0.0000000000
C	2.4215137252	-1.3607216036	0.0000000000
C	-2.4363939033	-1.3854447664	0.0000000000
C	2.4363939033	1.3854447664	0.0000000000
C	-3.6122218007	0.6994660109	0.0000000000
C	3.6122218007	-0.6994660109	0.0000000000
C	-3.6435641154	-0.7094178726	0.0000000000

C	3.6435641154	0.7094178726	0.0000000000
H	0.0787709652	-2.4339993759	0.0000000000
H	-0.0787709652	2.4339993759	0.0000000000
H	-2.3456048798	2.4388528556	0.0000000000
H	2.3456048798	-2.4388528556	0.0000000000
H	-2.4074220033	-2.4686140256	0.0000000000
H	2.4074220033	2.4686140256	0.0000000000
H	-4.5243641164	1.2822910722	0.0000000000
H	4.5243641164	-1.2822910722	0.0000000000
H	-4.5819503924	-1.2466569194	0.0000000000
H	4.5819503924	1.2466569194	0.0000000000

AN4*a***N8***a* T_1:

C	0.0252897350	-1.3585272309	0.0000000000
C	-0.0252897350	1.3585272309	0.0000000000
N	-1.2136162167	0.6914720152	0.0000000000
N	1.2136162167	-0.6914720152	0.0000000000
C	-1.2078105428	-0.7193529621	0.0000000000
C	1.2078105428	0.7193529621	0.0000000000
C	-2.4246916268	1.3632302398	0.0000000000
C	2.4246916268	-1.3632302398	0.0000000000
C	-2.4400903588	-1.3879423772	0.0000000000
C	2.4400903588	1.3879423772	0.0000000000
C	-3.6073924673	0.7033918239	0.0000000000
C	3.6073924673	-0.7033918239	0.0000000000
C	-3.6384514433	-0.7142935529	0.0000000000
C	3.6384514433	0.7142935529	0.0000000000

H	0.0772603826	-2.4363295655	0.0000000000
H	-0.0772603826	2.4363295655	0.0000000000
H	-2.3463348721	2.4412200825	0.0000000000
H	2.3463348721	-2.4412200825	0.0000000000
H	-2.4120044508	-2.4713432099	0.0000000000
H	2.4120044508	2.4713432099	0.0000000000
H	-4.5215438467	1.2832640218	0.0000000000
H	4.5215438467	-1.2832640218	0.0000000000
H	-4.5785790531	-1.2484231917	0.0000000000
H	4.5785790531	1.2484231917	0.0000000000

AN4a**N8**a T_2:

C	0.0199762623	-1.3475856388	0.0000000000
C	-0.0199762623	1.3475856388	0.0000000000
N	-1.2235381579	0.6629162999	0.0000000000
N	1.2235381579	-0.6629162999	0.0000000000
C	-1.2042494133	-0.7160700784	0.0000000000
C	1.2042494133	0.7160700784	0.0000000000
C	-2.4134779198	1.3669778729	0.0000000000
C	2.4134779198	-1.3669778729	0.0000000000
C	-2.4434587234	-1.4107160498	0.0000000000
C	2.4434587234	1.4107160498	0.0000000000
C	-3.6212210454	0.6927048327	0.0000000000
C	3.6212210454	-0.6927048327	0.0000000000
C	-3.6389204113	-0.6965627707	0.0000000000
C	3.6389204113	0.6965627707	0.0000000000
H	0.0842622583	-2.4233278172	0.0000000000

H	-0.0842622583	2.4233278172	0.0000000000
H	-2.3161095181	2.4409330190	0.0000000000
H	2.3161095181	-2.4409330190	0.0000000000
H	-2.4227486440	-2.4911281723	0.0000000000
H	2.4227486440	2.4911281723	0.0000000000
H	-4.5384675019	1.2665315907	0.0000000000
H	4.5384675019	-1.2665315907	0.0000000000
H	-4.5835624378	-1.2266046758	0.0000000000
H	4.5835624378	1.2266046758	0.0000000000

AN3N7 S_0:

C	-0.0205900127	-1.4067527266	0.0000000000
C	0.0205900127	1.4067527266	-0.0000000000
C	-1.2420323792	0.7158586882	0.0000000000
C	1.2420323792	-0.7158586882	-0.0000000000
C	-1.2072582161	-0.7410818794	-0.0000000000
C	1.2072582161	0.7410818794	0.0000000000
C	-2.4387862047	1.3587181222	-0.0000000000
C	2.4387862047	-1.3587181222	0.0000000000
C	-2.4963083195	-1.4020988645	-0.0000000000
C	2.4963083195	1.4020988645	0.0000000000
N	-3.6358104502	0.6659612775	0.0000000000
N	3.6358104502	-0.6659612775	-0.0000000000
C	-3.6422817175	-0.6940036759	0.0000000000
C	3.6422817175	0.6940036759	-0.0000000000
H	-0.0172955253	-2.4922263729	0.0000000000
H	0.0172955253	2.4922263729	-0.0000000000

H	-2.5180566292	2.4372120268	0.0000000000
H	2.5180566292	-2.4372120268	-0.0000000000
H	-2.5421666814	-2.4837609057	0.0000000000
H	2.5421666814	2.4837609057	-0.0000000000
H	-4.4990605104	1.1700196723	0.0000000000
H	4.4990605104	-1.1700196723	-0.0000000000
H	-4.6169365164	-1.1657890040	-0.0000000000
H	4.6169365164	1.1657890040	0.0000000000

AN3N7 S_1:

C	0.0077041309	-1.4145742988	0.0000000000
C	-0.0077041309	1.4145742988	0.0000000000
C	-1.2125271098	0.7184053707	0.0000000000
C	1.2125271098	-0.7184053707	0.0000000000
C	-1.2298163803	-0.7578320717	0.0000000000
C	1.2298163803	0.7578320717	0.0000000000
C	-2.4512902027	1.3606964150	0.0000000000
C	2.4512902027	-1.3606964150	0.0000000000
C	-2.4731705909	-1.4020217898	0.0000000000
C	2.4731705909	1.4020217898	0.0000000000
N	-3.6035307897	0.6760645854	0.0000000000
N	3.6035307897	-0.6760645854	0.0000000000
C	-3.6576678033	-0.7026780013	0.0000000000
C	3.6576678033	0.7026780013	0.0000000000
H	0.0264468232	-2.5005294232	0.0000000000
H	-0.0264468232	2.5005294232	0.0000000000
H	-2.5336340850	2.4401103566	0.0000000000

H	2.5336340850	-2.4401103566	0.0000000000
H	-2.5108922680	-2.4853482484	0.0000000000
H	2.5108922680	2.4853482484	0.0000000000
H	-4.4634440022	1.1910428236	0.0000000000
H	4.4634440022	-1.1910428236	0.0000000000
H	-4.6392848792	-1.1491874450	0.0000000000
H	4.6392848792	1.1491874450	0.0000000000

AN3N7 T_1:

C	-0.0029380998	-1.3864339853	-0.0000000000
C	0.0029380998	1.3864339853	0.0000000000
C	-1.2252422036	0.7160463348	-0.0000000000
C	1.2252422036	-0.7160463348	0.0000000000
C	-1.2148463629	-0.7021346034	-0.0000000000
C	1.2148463629	0.7021346034	0.0000000000
C	-2.4737955321	1.4070123346	-0.0000000000
C	2.4737955321	-1.4070123346	0.0000000000
C	-2.4928264915	-1.3931632063	0.0000000000
C	2.4928264915	1.3931632063	-0.0000000000
N	-3.6458369460	0.6708333206	-0.0000000000
N	3.6458369460	-0.6708333206	0.0000000000
C	-3.6424037805	-0.6925363539	0.0000000000
C	3.6424037805	0.6925363539	-0.0000000000
H	-0.0135865709	-2.4719859629	0.0000000000
H	0.0135865709	2.4719859629	-0.0000000000
H	-2.5634115766	2.4811504768	0.0000000000
H	2.5634115766	-2.4811504768	-0.0000000000

H	-2.5229374719	-2.4747309911	0.0000000000
H	2.5229374719	2.4747309911	0.0000000000
H	-4.5222377408	1.1536870597	-0.0000000000
H	4.5222377408	-1.1536870597	0.0000000000
H	-4.6159153286	-1.1664134683	0.0000000000
H	4.6159153286	1.1664134683	0.0000000000

AN3N7 T_2:

C	-0.007244	-1.388071	-0.000003
C	-0.005284	1.389390	0.000000
C	-1.228171	0.718808	-0.000002
C	1.215454	-0.717652	-0.000005
C	-1.219321	-0.702079	-0.000007
C	1.206860	0.703560	-0.000008
C	-2.478402	1.410279	0.000006
C	2.465919	-1.408744	0.000003
C	-2.498672	-1.391083	-0.000004
C	2.485981	1.392296	-0.000007
N	-3.653488	0.672513	0.000007
N	3.640584	-0.671347	0.000006
C	-3.643360	-0.693335	0.000001
C	3.630979	0.694543	0.000000
H	-0.017670	-2.473923	-0.000000
H	0.004220	2.475249	-0.000002
H	-2.565999	2.484890	0.000007
H	2.553096	-2.483422	0.000010
H	-2.527682	-2.473056	-0.000015

H	2.514717	2.474277	-0.000014
H	-4.529940	1.154275	0.000012
H	4.516876	-1.153462	0.000012
H	-4.615269	-1.170729	-0.000001
H	4.602808	1.172001	0.000002

Phenanthrene S_0:

C	-0.7273345321	0.0000000000	-0.0490848705
C	0.7273345321	-0.0000000000	-0.0490848705
C	-1.4154161891	0.0000000000	1.1877051185
C	1.4154161891	0.0000000000	1.1877051185
C	-0.6755523926	0.0000000000	2.4103761730
C	0.6755523926	0.0000000000	2.4103761730
C	-1.4911709322	0.0000000000	-1.2300213065
C	1.4911709322	-0.0000000000	-1.2300213065
C	-2.8243161123	0.0000000000	1.2004409209
C	2.8243161123	0.0000000000	1.2004409209
C	-2.8660202007	0.0000000000	-1.1950053717
C	2.8660202007	-0.0000000000	-1.1950053717
C	-3.5424714366	0.0000000000	0.0322457990
C	3.5424714366	-0.0000000000	0.0322457990
H	-1.2254520685	0.0000000000	3.3450921737
H	1.2254520685	0.0000000000	3.3450921737
H	-0.9976753944	0.0000000000	-2.1925660572
H	0.9976753944	0.0000000000	-2.1925660572
H	-3.3348920007	0.0000000000	2.1574553318
H	3.3348920007	0.0000000000	2.1574553318

H	-3.4271289112	0.0000000000	-2.1223256322
H	3.4271289112	0.0000000000	-2.1223256322
H	-4.6261324714	0.0000000000	0.0556877209
H	4.6261324714	0.0000000000	0.0556877209

Phenanthrene S_1:

C	-0.7084788500	0.0000000000	-0.0630329708
C	0.7084788500	0.0000000000	-0.0630329708
C	-1.4289519717	0.0000000000	1.2171755843
C	1.4289519717	0.0000000000	1.2171755843
C	-0.6959777345	0.0000000000	2.3971122009
C	0.6959777345	-0.0000000000	2.3971122009
C	-1.4922812757	0.0000000000	-1.2390462581
C	1.4922812757	-0.0000000000	-1.2390462581
C	-2.8401680978	0.0000000000	1.2158642856
C	2.8401680978	-0.0000000000	1.2158642856
C	-2.8833164464	0.0000000000	-1.1934323891
C	2.8833164464	0.0000000000	-1.1934323891
C	-3.5649913310	0.0000000000	0.0293755787
C	3.5649913310	0.0000000000	0.0293755787
H	-1.2273421431	0.0000000000	3.3427384467
H	1.2273421431	-0.0000000000	3.3427384467
H	-1.0097696432	0.0000000000	-2.2066409996
H	1.0097696432	-0.0000000000	-2.2066409996
H	-3.3558183562	0.0000000000	2.1697236016
H	3.3558183562	-0.0000000000	2.1697236016
H	-3.4428522611	0.0000000000	-2.1214631202

H	3.4428522611	0.0000000000	-2.1214631202
H	-4.6476621920	0.0000000000	0.0516260395
H	4.6476621920	0.0000000000	0.0516260395

Phenanthrene T_1:

C	-0.7435988046	0.0000000000	-0.0557850558
C	0.7435988046	0.0000000000	-0.0557850558
C	-1.4396886497	0.0000000000	1.2119483012
C	1.4396886497	-0.0000000000	1.2119483012
C	-0.7323955490	0.0000000000	2.3906047981
C	0.7323955490	-0.0000000000	2.3906047981
C	-1.4891758505	0.0000000000	-1.2079401770
C	1.4891758505	-0.0000000000	-1.2079401770
C	-2.8699180328	0.0000000000	1.2012850553
C	2.8699180328	0.0000000000	1.2012850553
C	-2.8995707877	0.0000000000	-1.1915935785
C	2.8995707877	-0.0000000000	-1.1915935785
C	-3.5779120441	0.0000000000	0.0213090236
C	3.5779120441	-0.0000000000	0.0213090236
H	-1.2590292703	0.0000000000	3.3369085576
H	1.2590292703	0.0000000000	3.3369085576
H	-0.9972135442	0.0000000000	-2.1720717571
H	0.9972135442	0.0000000000	-2.1720717571
H	-3.3885341712	0.0000000000	2.1533835154
H	3.3885341712	0.0000000000	2.1533835154
H	-3.4440652261	0.0000000000	-2.1276412379
H	3.4440652261	-0.0000000000	-2.1276412379

H	-4.6618765280	0.0000000000	0.0395925550
H	4.6618765280	-0.0000000000	0.0395925550

Phenanthrene T_2:

C	-0.7032909952	0.0000000000	-0.0633946820
C	0.7032909952	0.0000000000	-0.0633946820
C	-1.4236691664	0.0000000000	1.2130715673
C	1.4236691664	0.0000000000	1.2130715673
C	-0.6951801490	0.0000000000	2.3841914335
C	0.6951801490	-0.0000000000	2.3841914335
C	-1.4939441058	0.0000000000	-1.2417100542
C	1.4939441058	-0.0000000000	-1.2417100542
C	-2.8428945262	0.0000000000	1.2189700287
C	2.8428945262	-0.0000000000	1.2189700287
C	-2.8903896969	0.0000000000	-1.1825058294
C	2.8903896969	0.0000000000	-1.1825058294
C	-3.5731096679	0.0000000000	0.0321491601
C	3.5731096679	0.0000000000	0.0321491601
H	-1.2242041172	0.0000000000	3.3317670634
H	1.2242041172	-0.0000000000	3.3317670634
H	-1.0182248254	0.0000000000	-2.2121334293
H	1.0182248254	0.0000000000	-2.2121334293
H	-3.3517357482	0.0000000000	2.1764147742
H	3.3517357482	-0.0000000000	2.1764147742
H	-3.4507683002	0.0000000000	-2.1108313977
H	3.4507683002	-0.0000000000	-2.1108313977
H	-4.6553359961	0.0000000000	0.0540113658

H	4.6553359961	0.0000000000	0.0540113658

PB4B5 S_0:

C	-0.6953449781	0.0000000000	-0.0529961395
C	0.6953449781	0.0000000000	-0.0529961395
C	-1.4062516085	0.0000000000	1.2084150742
C	1.4062516085	0.0000000000	1.2084150742
C	-0.6734001473	0.0000000000	2.4420846088
C	0.6734001473	-0.0000000000	2.4420846088
B	-1.5626243911	0.0000000000	-1.3686037697
B	1.5626243911	-0.0000000000	-1.3686037697
C	-2.7847897953	0.0000000000	1.2268933781
C	2.7847897953	0.0000000000	1.2268933781
C	-3.0854555592	0.0000000000	-1.1994222329
C	3.0854555592	0.0000000000	-1.1994222329
C	-3.6063065013	0.0000000000	0.0534275884
C	3.6063065013	0.0000000000	0.0534275884
H	-1.2281205335	0.0000000000	3.3742990923
H	1.2281205335	0.0000000000	3.3742990923
H	-1.0651696951	0.0000000000	-2.4485109507
H	1.0651696951	0.0000000000	-2.4485109507
H	-3.2825527993	0.0000000000	2.1916484484
H	3.2825527993	-0.0000000000	2.1916484484
H	-3.7714076636	0.0000000000	-2.0413619420
H	3.7714076636	0.0000000000	-2.0413619420
H	-4.6819442860	0.0000000000	0.2141268441
H	4.6819442860	0.0000000000	0.2141268441

PB4B5 S_1:

C	-0.7231191779	-0.1199115172	0.0000000000
C	0.7015307783	-0.1030286790	0.0000000000
C	-1.4222309105	1.1786823940	0.0000000000
C	1.3906447986	1.1364821403	0.0000000000
C	-0.6936763210	2.3843651879	0.0000000000
C	0.6727416108	2.3700391229	0.0000000000
B	-1.5740593745	-1.3790225032	0.0000000000
B	1.5811042282	-1.3707670138	0.0000000000
C	-2.8389166307	1.2677636706	0.0000000000
C	2.7860361573	1.2179103110	0.0000000000
C	-3.0589511739	-1.1651662845	0.0000000000
C	3.1288403926	-1.1552609288	0.0000000000
C	-3.6153930617	0.1358587075	0.0000000000
C	3.6553095312	0.1019444375	0.0000000000
H	-1.2307031757	3.3259450768	0.0000000000
H	1.2274142989	3.3030549784	0.0000000000
H	-1.1048389119	-2.4785533127	0.0000000000
H	1.1460527861	-2.4766177908	0.0000000000
H	-3.2940260189	2.2507183068	0.0000000000
H	3.2301599026	2.2097226247	0.0000000000
H	-3.7718955625	-1.9861812233	0.0000000000
H	3.8216652719	-1.9933175344	0.0000000000
H	-4.6960943216	0.2610870090	0.0000000000
H	4.7251085044	0.2842531503	0.0000000000

PB4B5 T_1:

C	-0.7093410051	0.0000000000	-0.0768492887
C	0.7093410051	0.0000000000	-0.0768492887
C	-1.3994390072	0.0000000000	1.1670172301
C	1.3994390072	-0.0000000000	1.1670172301
C	-0.6869882074	0.0000000000	2.3774937335
C	0.6869882074	-0.0000000000	2.3774937335
B	-1.5824598219	0.0000000000	-1.3591029159
B	1.5824598219	0.0000000000	-1.3591029159
C	-2.8325666054	0.0000000000	1.2268174256
C	2.8325666054	-0.0000000000	1.2268174256
C	-3.1067224047	0.0000000000	-1.1653996542
C	3.1067224047	-0.0000000000	-1.1653996542
C	-3.6510842573	0.0000000000	0.1059685973
C	3.6510842573	-0.0000000000	0.1059685973
H	-1.2302186222	0.0000000000	3.3166519652
H	1.2302186222	0.0000000000	3.3166519652
H	-1.1173287957	0.0000000000	-2.4562994196
H	1.1173287957	-0.0000000000	-2.4562994196
H	-3.2876806091	0.0000000000	2.2122935417
H	3.2876806091	-0.0000000000	2.2122935417
H	-3.7955508202	0.0000000000	-2.0062794924
H	3.7955508202	0.0000000000	-2.0062794924
H	-4.7267850614	0.0000000000	0.2576882773
H	4.7267850614	0.0000000000	0.2576882773

PB4B5 T_2:

C	-0.7076866417	0.0000000000	-0.0888340046
C	0.7076866417	0.0000000000	-0.0888340046
C	-1.4130932571	0.0000000000	1.1723585136
C	1.4130932571	0.0000000000	1.1723585136
C	-0.6685328163	0.0000000000	2.4203233162
C	0.6685328163	0.0000000000	2.4203233162
B	-1.5660087662	0.0000000000	-1.3804535787
B	1.5660087662	-0.0000000000	-1.3804535787
C	-2.8196155089	0.0000000000	1.2359691140
C	2.8196155089	-0.0000000000	1.2359691140
C	-3.0716693658	0.0000000000	-1.1896534210
C	3.0716693658	0.0000000000	-1.1896534210
C	-3.6201936261	0.0000000000	0.1074402081
C	3.6201936261	0.0000000000	0.1074402081
H	-1.2250178637	0.0000000000	3.3511571472
H	1.2250178637	0.0000000000	3.3511571472
H	-1.0891537184	0.0000000000	-2.4709318519
H	1.0891537184	0.0000000000	-2.4709318519
H	-3.2850213433	0.0000000000	2.2155688544
H	3.2850213433	-0.0000000000	2.2155688544
H	-3.7718602166	0.0000000000	-2.0202653385
H	3.7718602166	0.0000000000	-2.0202653385
H	-4.6980263162	0.0000000000	0.2473210411
H	4.6980263162	0.0000000000	0.2473210411

PB1B8 S_0:

C	-0.7305065360	0.0000000000	-0.0291619777

C	0.7305065360	-0.0000000000	-0.0291619777
C	-1.4330990323	0.0000000000	1.2347935012
C	1.4330990323	0.0000000000	1.2347935012
C	-0.7113807077	0.0000000000	2.3980665774
C	0.7113807077	0.0000000000	2.3980665774
C	-1.4929913661	0.0000000000	-1.1770317524
C	1.4929913661	-0.0000000000	-1.1770317524
B	-2.9892127156	0.0000000000	1.2752988194
B	2.9892127156	-0.0000000000	1.2752988194
C	-2.9270640393	0.0000000000	-1.1926622637
C	2.9270640393	-0.0000000000	-1.1926622637
C	-3.6992383552	0.0000000000	-0.0728477852
C	3.6992383552	-0.0000000000	-0.0728477852
H	-1.2379094253	0.0000000000	3.3467654370
H	1.2379094253	0.0000000000	3.3467654370
H	-1.0045407920	0.0000000000	-2.1435024898
H	1.0045407920	-0.0000000000	-2.1435024898
H	-3.5521717676	0.0000000000	2.3332958580
H	3.5521717676	0.0000000000	2.3332958580
H	-3.3870013336	0.0000000000	-2.1784944807
H	3.3870013336	-0.0000000000	-2.1784944807
H	-4.7781224062	0.0000000000	-0.1945194441
H	4.7781224062	-0.0000000000	-0.1945194441

PB1B8 S_1:

C	-0.7222730940	0.0359324402	0.0000000000
C	0.7312082555	0.0124723291	0.0000000000

C	-1.4393439525	1.2742787222	0.0000000000
C	1.4510104579	1.2641023019	0.0000000000
C	-0.6999748297	2.4617006732	0.0000000000
C	0.6890050927	2.4465505194	0.0000000000
C	-1.4377456966	-1.1569005189	0.0000000000
C	1.4546868159	-1.2083265182	0.0000000000
B	-2.9612476902	1.2679231700	0.0000000000
B	2.9629628114	1.2824747518	0.0000000000
C	-2.8597241735	-1.2439462498	0.0000000000
C	2.8414458362	-1.2337339763	0.0000000000
C	-3.6400905548	-0.1281314946	0.0000000000
C	3.6296865467	-0.0781616774	0.0000000000
H	-1.2276731882	3.4088445791	0.0000000000
H	1.2273699093	3.3888606343	0.0000000000
H	-0.9036497955	-2.0959547895	0.0000000000
H	0.9367555335	-2.1546887493	0.0000000000
H	-3.5951666658	2.2832803702	0.0000000000
H	3.5733805379	2.3161513183	0.0000000000
H	-3.2921816869	-2.2399657770	0.0000000000
H	3.3162284286	-2.2121128608	0.0000000000
H	-4.7182878417	-0.2660031660	0.0000000000
H	4.7066640137	-0.2246463922	0.0000000000

PB1B8 T_1:

C	-0.7149362559	0.0000000000	0.0371398274
C	0.7149362559	0.0000000000	0.0371398274
C	-1.4208599561	0.0000000000	1.2660649527

C	1.4208599561	-0.0000000000	1.2660649527
C	-0.6909103748	0.0000000000	2.4618667872
C	0.6909103748	-0.0000000000	2.4618667872
C	-1.4705555311	0.0000000000	-1.1840099775
C	1.4705555311	0.0000000000	-1.1840099775
B	-2.9619318337	0.0000000000	1.2650346742
B	2.9619318337	0.0000000000	1.2650346742
C	-2.8627231916	0.0000000000	-1.2435028577
C	2.8627231916	0.0000000000	-1.2435028577
C	-3.6458389577	0.0000000000	-0.1055802121
C	3.6458389577	0.0000000000	-0.1055802121
H	-1.2327476402	0.0000000000	3.4015860623
H	1.2327476402	0.0000000000	3.4015860623
H	-0.9425623641	0.0000000000	-2.1271774315
H	0.9425623641	-0.0000000000	-2.1271774315
H	-3.5754803057	0.0000000000	2.2944191221
H	3.5754803057	-0.0000000000	2.2944191221
H	-3.3169741276	0.0000000000	-2.2304604955
H	3.3169741276	0.0000000000	-2.2304604955
H	-4.7246067274	0.0000000000	-0.2353804517
H	4.7246067274	0.0000000000	-0.2353804517

PB1B8 T_2:

C	-0.7331812248	-0.0147798555	0.0000000000
C	0.7321959532	-0.0395786028	0.0000000000
C	-1.4092951856	1.2157615221	0.0000000000
C	1.4633817830	1.2415015601	0.0000000000

C	-0.6560604699	2.4465353487	0.0000000000
C	0.7003747183	2.4488555685	0.0000000000
C	-1.4999152801	-1.1893619303	0.0000000000
C	1.4631638970	-1.2143500987	0.0000000000
B	-2.9746887615	1.2516193436	0.0000000000
B	2.9899407564	1.2912078789	0.0000000000
C	-2.9194623125	-1.2218538721	0.0000000000
C	2.8606241003	-1.2091787900	0.0000000000
C	-3.6836533866	-0.0913208820	0.0000000000
C	3.6585942270	-0.0376838842	0.0000000000
H	-1.2093198005	3.3787048747	0.0000000000
H	1.2469257449	3.3850137548	0.0000000000
H	-0.9941625835	-2.1457546687	0.0000000000
H	0.9647235213	-2.1725681566	0.0000000000
H	-3.5378043447	2.3088223357	0.0000000000
H	3.5585599303	2.3474015257	0.0000000000
H	-3.3789620858	-2.2068504446	0.0000000000
H	3.3501692082	-2.1807263212	0.0000000000
H	-4.7638557869	-0.2015958369	0.0000000000
H	4.7339540921	-0.1898202698	0.0000000000

PB1a**B8**a S_0:

C	-0.6919764147	0.0000000000	-0.0915934393
C	0.6919764147	-0.0000000000	-0.0915934393
B	-1.4641644039	0.0000000000	1.2876638956
B	1.4641644039	0.0000000000	1.2876638956
C	-0.6713615849	0.0000000000	2.6361416362

C	0.6713615849	0.0000000000	2.6361416362
C	-1.4880503653	0.0000000000	-1.3019402329
C	1.4880503653	0.0000000000	-1.3019402329
C	-2.9962490222	0.0000000000	1.2083127957
C	2.9962490222	0.0000000000	1.2083127957
C	-2.8348068487	0.0000000000	-1.2538933810
C	2.8348068487	-0.0000000000	-1.2538933810
C	-3.5856404824	0.0000000000	-0.0063401882
C	3.5856404824	-0.0000000000	-0.0063401882
H	-1.2102501645	0.0000000000	3.5848485217
H	1.2102501645	0.0000000000	3.5848485217
H	-1.0075652875	0.0000000000	-2.2731576142
H	1.0075652875	0.0000000000	-2.2731576142
H	-3.6350235166	0.0000000000	2.0882264421
H	3.6350235166	0.0000000000	2.0882264421
H	-3.4014086831	0.0000000000	-2.1790972027
H	3.4014086831	-0.0000000000	-2.1790972027
H	-4.6697587483	0.0000000000	-0.0991712337
H	4.6697587483	-0.0000000000	-0.0991712337

PB1*a***B8***a* S_1:

C	-0.6957724188	-0.0864697175	0.0000000000
C	0.7363136268	-0.0616952414	0.0000000000
B	-1.4867055846	1.2959593621	0.0000000000
B	1.4718680319	1.2705951634	0.0000000000
C	-0.7161934925	2.5863613955	0.0000000000
C	0.6718402765	2.5788877807	0.0000000000

C	-1.4791202790	-1.2666867715	0.0000000000
C	1.4929490161	-1.2404485176	0.0000000000
C	-3.0321511653	1.2106540648	0.0000000000
C	2.9756158896	1.2004960652	0.0000000000
C	-2.8474200440	-1.2084754396	0.0000000000
C	2.9024047234	-1.2417091560	0.0000000000
C	-3.6309168527	-0.0048493647	0.0000000000
C	3.6157896341	-0.0586871933	0.0000000000
H	-1.2319138437	3.5473237533	0.0000000000
H	1.1861946620	3.5423591415	0.0000000000
H	-1.0194908062	-2.2484718911	0.0000000000
H	1.0079500156	-2.2129169799	0.0000000000
H	-3.6628375195	2.0968427504	0.0000000000
H	3.6227635136	2.0753349124	0.0000000000
H	-3.3913801324	-2.1494302729	0.0000000000
H	3.4272415354	-2.1895643305	0.0000000000
H	-4.7110566706	-0.1176266947	0.0000000000
H	4.7015683242	-0.1177826187	0.0000000000

PB1a**B8**a T_1:

C	-0.7315231544	0.0000000000	-0.1011338585
C	0.7315231544	0.0000000000	-0.1011338585
B	-1.4836058892	0.0000000000	1.2631674932
B	1.4836058892	-0.0000000000	1.2631674932
C	-0.6804934555	0.0000000000	2.5806223496
C	0.6804934555	-0.0000000000	2.5806223496
C	-1.4948109304	0.0000000000	-1.2553601386

C	1.4948109304	0.0000000000	-1.2553601386
C	-3.0231160357	0.0000000000	1.2019327143
C	3.0231160357	0.0000000000	1.2019327143
C	-2.8952902396	0.0000000000	-1.2138986504
C	2.8952902396	0.0000000000	-1.2138986504
C	-3.6457254760	0.0000000000	-0.0150589149
C	3.6457254760	-0.0000000000	-0.0150589149
H	-1.2015304643	0.0000000000	3.5399500607
H	1.2015304643	0.0000000000	3.5399500607
H	-1.0341335447	0.0000000000	-2.2384215145
H	1.0341335447	0.0000000000	-2.2384215145
H	-3.6463305930	0.0000000000	2.0937782310
H	3.6463305930	-0.0000000000	2.0937782310
H	-3.4339870393	0.0000000000	-2.1563604935
H	3.4339870393	0.0000000000	-2.1563604935
H	-4.7289376419	0.0000000000	-0.0992172784
H	4.7289376419	-0.0000000000	-0.0992172784

PB1a**B8**a T_2:

C	-0.7092649389	0.0000000000	-0.0577856736
C	0.7092649389	-0.0000000000	-0.0577856736
B	-1.4630273631	0.0000000000	1.2941585447
B	1.4630273631	0.0000000000	1.2941585447
C	-0.6730571967	0.0000000000	2.6362093402
C	0.6730571967	-0.0000000000	2.6362093402
C	-1.4834667501	0.0000000000	-1.2503488264
C	1.4834667501	0.0000000000	-1.2503488264

C	-2.9916670624	0.0000000000	1.1878031205
C	2.9916670624	-0.0000000000	1.1878031205
C	-2.8823820469	0.0000000000	-1.2477251888
C	2.8823820469	-0.0000000000	-1.2477251888
C	-3.6158106505	0.0000000000	-0.0612432782
C	3.6158106505	0.0000000000	-0.0612432782
H	-1.2052102375	0.0000000000	3.5895639807
H	1.2052102375	0.0000000000	3.5895639807
H	-0.9996151043	0.0000000000	-2.2219159182
H	0.9996151043	-0.0000000000	-2.2219159182
H	-3.6418751210	0.0000000000	2.0603385196
H	3.6418751210	0.0000000000	2.0603385196
H	-3.4066081102	0.0000000000	-2.1964718020
H	3.4066081102	-0.0000000000	-2.1964718020
H	-4.7002597838	0.0000000000	-0.1325828191
H	4.7002597838	0.0000000000	-0.1325828191

PB3B6 S_0:

C	-0.7484396169	0.0000000000	-0.1413970541
C	0.7484396169	0.0000000000	-0.1413970541
C	-1.4385687170	0.0000000000	1.1494385141
C	1.4385687170	0.0000000000	1.1494385141
C	-0.7061066925	0.0000000000	2.3087499177
C	0.7061066925	-0.0000000000	2.3087499177
C	-1.4930772057	0.0000000000	-1.2714841471
C	1.4930772057	0.0000000000	-1.2714841471
C	-2.8816115155	0.0000000000	1.2451175583

C	2.8816115155	0.0000000000	1.2451175583
B	-3.0334257593	0.0000000000	-1.2290269366
B	3.0334257593	-0.0000000000	-1.2290269366
C	-3.6865597025	0.0000000000	0.1629292059
C	3.6865597025	-0.0000000000	0.1629292059
H	-1.2265825719	0.0000000000	3.2603183696
H	1.2265825719	0.0000000000	3.2603183696
H	-0.9747025930	0.0000000000	-2.2242486936
H	0.9747025930	-0.0000000000	-2.2242486936
H	-3.2838383959	0.0000000000	2.2557448274
H	3.2838383959	-0.0000000000	2.2557448274
H	-3.6794441253	0.0000000000	-2.2385207231
H	3.6794441253	-0.0000000000	-2.2385207231
H	-4.7610485208	0.0000000000	0.3223791614
H	4.7610485208	0.0000000000	0.3223791614

PB3B6 T_1:

C	-0.7312884612	0.0000000000	-0.0882261825
C	0.7312884612	-0.0000000000	-0.0882261825
C	-1.4227122572	0.0000000000	1.1438442852
C	1.4227122572	-0.0000000000	1.1438442852
C	-0.6803373828	0.0000000000	2.3559016147
C	0.6803373828	-0.0000000000	2.3559016147
C	-1.4897957029	0.0000000000	-1.2698930293
C	1.4897957029	-0.0000000000	-1.2698930293
C	-2.8691716784	0.0000000000	1.2224968230
C	2.8691716784	-0.0000000000	1.2224968230

B	-3.0316861137	0.0000000000	-1.2511006235
B	3.0316861137	0.0000000000	-1.2511006235
C	-3.6771113975	0.0000000000	0.1402462615
C	3.6771113975	-0.0000000000	0.1402462615
H	-1.2219195839	0.0000000000	3.2953358592
H	1.2219195839	-0.0000000000	3.2953358592
H	-0.9549283469	0.0000000000	-2.2122599705
H	0.9549283469	-0.0000000000	-2.2122599705
H	-3.2802898902	0.0000000000	2.2297625142
H	3.2802898902	0.0000000000	2.2297625142
H	-3.6585690652	0.0000000000	-2.2714227199
H	3.6585690652	0.0000000000	-2.2714227199
H	-4.7506244092	0.0000000000	0.3053151678
H	4.7506244092	0.0000000000	0.3053151678

PB4a**B5**a S_0:

B	-0.8625314801	-0.0021835769	-0.2566492191
B	0.8625314801	0.0021835769	-0.2566492191
C	-1.5215027508	-0.0020839444	1.1684493467
C	1.5215027508	0.0020839444	1.1684493467
C	-0.7277189275	-0.0012623966	2.2772662380
C	0.7277189275	0.0012623966	2.2772662380
C	-1.8607516975	-0.0074466651	-1.4131717302
C	1.8607516975	0.0074466651	-1.4131717302
C	-2.9615672656	-0.0046488580	1.3020295316
C	2.9615672656	0.0046488580	1.3020295316
C	-3.1903644103	-0.0106857541	-1.1381369119

C	3.1903644103	0.0106857541	-1.1381369119
C	-3.7434806758	-0.0085602188	0.2052376344
C	3.7434806758	0.0085602188	0.2052376344
H	-1.1919312697	-0.0025853919	3.2633771731
H	1.1919312697	0.0025853919	3.2633771731
H	-1.5675159378	-0.0089252216	-2.4602245465
H	1.5675159378	0.0089252216	-2.4602245465
H	-3.4095884267	-0.0034980949	2.2929928428
H	3.4095884267	0.0034980949	2.2929928428
H	-3.9172132552	-0.0150950547	-1.9488320130
H	3.9172132552	0.0150950547	-1.9488320130
H	-4.8231800353	-0.0101798626	0.3076616540
H	4.8231800353	0.0101798626	0.3076616540

PB4*a***B5***a* S_1:

B	-0.8293901445	-0.2588944895	0.0000000000
B	0.8151901556	-0.2583688095	0.0000000000
C	-1.4718415390	1.1266712390	0.0000000000
C	1.4882454365	1.1986479021	0.0000000000
C	-0.6799069323	2.3185186944	0.0000000000
C	0.7091284505	2.3585452769	0.0000000000
C	-1.8325364130	-1.3976121217	0.0000000000
C	1.8470049917	-1.4254273285	0.0000000000
C	-2.8505942934	1.2687969888	0.0000000000
C	2.9063082395	1.3044656083	0.0000000000
C	-3.2256150461	-1.1345662065	0.0000000000
C	3.1748527472	-1.1666029978	0.0000000000

C	-3.7243819582	0.1466106646	0.0000000000
C	3.6838033231	0.1848483963	0.0000000000
H	-1.1992169831	3.2774853963	0.0000000000
H	1.1943821952	3.3312625462	0.0000000000
H	-1.5483753595	-2.4484029671	0.0000000000
H	1.5364233375	-2.4678566317	0.0000000000
H	-3.3032972878	2.2605458956	0.0000000000
H	3.3816289902	2.2820791447	0.0000000000
H	-3.9348932081	-1.9588368975	0.0000000000
H	3.9136748529	-1.9637749846	0.0000000000
H	-4.7950123606	0.3142743258	0.0000000000
H	4.7633915756	0.3075915854	0.0000000000

PB4a**B5**a T_1:

B	-0.8428976461	0.0000000000	-0.2521448935
B	0.8428976461	-0.0000000000	-0.2521448935
C	-1.4976848720	0.0000000000	1.1699259488
C	1.4976848720	-0.0000000000	1.1699259488
C	-0.6831046357	0.0000000000	2.3524987109
C	0.6831046357	-0.0000000000	2.3524987109
C	-1.8514984890	0.0000000000	-1.4214019200
C	1.8514984890	-0.0000000000	-1.4214019200
C	-2.8852244778	0.0000000000	1.2918380601
C	2.8852244778	-0.0000000000	1.2918380601
C	-3.1911613071	0.0000000000	-1.1648074606
C	3.1911613071	0.0000000000	-1.1648074606
C	-3.6978851051	0.0000000000	0.1665156310

C	3.6978851051	-0.0000000000	0.1665156310
H	-1.1874096529	0.0000000000	3.3172192570
H	1.1874096529	-0.0000000000	3.3172192570
H	-1.5423388147	0.0000000000	-2.4645781941
H	1.5423388147	0.0000000000	-2.4645781941
H	-3.3557032710	0.0000000000	2.2728137627
H	3.3557032710	0.0000000000	2.2728137627
H	-3.9206712298	0.0000000000	-1.9707957168
H	3.9206712298	0.0000000000	-1.9707957168
H	-4.7748750138	0.0000000000	0.3029168146
H	4.7748750138	-0.0000000000	0.3029168146

PB4a**B5**a T_2:

B	-0.8521569929	0.0000000000	-0.2592230568
B	0.8521569929	0.0000000000	-0.2592230568
C	-1.4929793835	0.0000000000	1.1485284131
C	1.4929793835	0.0000000000	1.1485284131
C	-0.6991633186	0.0000000000	2.3118088162
C	0.6991633186	0.0000000000	2.3118088162
C	-1.8818826353	0.0000000000	-1.4027288608
C	1.8818826353	-0.0000000000	-1.4027288608
C	-2.8994529618	0.0000000000	1.2803230784
C	2.8994529618	0.0000000000	1.2803230784
C	-3.2483350844	0.0000000000	-1.1337836328
C	3.2483350844	0.0000000000	-1.1337836328
C	-3.7492353006	0.0000000000	0.1725816952
C	3.7492353006	0.0000000000	0.1725816952

H	-1.1924815270	0.0000000000	3.2826987717
H	1.1924815270	-0.0000000000	3.2826987717
H	-1.5988014821	0.0000000000	-2.4536408056
H	1.5988014821	-0.0000000000	-2.4536408056
H	-3.3485432651	0.0000000000	2.2722804652
H	3.3485432651	-0.0000000000	2.2722804652
H	-3.9672313123	0.0000000000	-1.9494374622
H	3.9672313123	-0.0000000000	-1.9494374622
H	-4.8217824967	0.0000000000	0.3305925781
H	4.8217824967	0.0000000000	0.3305925781

PB2B7 S_0:

C	-0.6932568155	0.0000000000	-0.0157877004
C	0.6932568155	0.0000000000	-0.0157877004
C	-1.4220067597	0.0000000000	1.2523340244
C	1.4220067597	0.0000000000	1.2523340244
C	-0.6687988465	0.0000000000	2.4870599003
C	0.6687988465	0.0000000000	2.4870599003
C	-1.4593305146	0.0000000000	-1.2639928458
C	1.4593305146	-0.0000000000	-1.2639928458
C	-2.7859256989	0.0000000000	1.2791526390
C	2.7859256989	-0.0000000000	1.2791526390
C	-2.8042116569	0.0000000000	-1.3181373585
C	2.8042116569	0.0000000000	-1.3181373585
B	-3.6180507782	0.0000000000	-0.0133722643
B	3.6180507782	0.0000000000	-0.0133722643
H	-1.2297129963	0.0000000000	3.4145983157

H	1.2297129963	0.0000000000	3.4145983157
H	-0.8986890668	0.0000000000	-2.1876377239
H	0.8986890668	0.0000000000	-2.1876377239
H	-3.2494652571	0.0000000000	2.2628046002
H	3.2494652571	0.0000000000	2.2628046002
H	-3.2636227432	0.0000000000	-2.3025426278
H	3.2636227432	0.0000000000	-2.3025426278
H	-4.8152770496	0.0000000000	0.0055210415
H	4.8152770496	-0.0000000000	0.0055210415

PB2B7 S_1:

C	-0.713029	0.000000	-0.043957
C	0.713029	0.000000	-0.043957
C	-1.439651	0.000000	1.216701
C	1.439651	0.000000	1.216701
C	-0.689915	0.000000	2.412761
C	0.689915	0.000000	2.412761
C	-1.472349	0.000000	-1.238961
C	1.472349	0.000000	-1.238961
C	-2.832810	0.000000	1.273409
C	2.832810	0.000000	1.273409
C	-2.852822	0.000000	-1.263443
C	2.852822	0.000000	-1.263443
B	-3.674946	0.000000	0.018399
B	3.674946	0.000000	0.018399
H	-1.226721	0.000000	3.354791
H	1.226721	0.000000	3.354791

H	-0.939615	0.000000	-2.180997
H	0.939615	0.000000	-2.180997
H	-3.259307	0.000000	2.274557
H	3.259307	0.000000	2.274557
H	-3.307415	0.000000	-2.251602
H	3.307415	0.000000	-2.251602
H	-4.872219	0.000000	0.028350
H	4.872219	0.000000	0.028350

PB2B7 T_1:

C	-0.7066589228	0.0000000000	-0.0103488513
C	0.7066589228	0.0000000000	-0.0103488513
C	-1.4076031754	0.0000000000	1.2347738397
C	1.4076031754	0.0000000000	1.2347738397
C	-0.6904521765	0.0000000000	2.4384910414
C	0.6904521765	-0.0000000000	2.4384910414
C	-1.4840137543	0.0000000000	-1.2354637129
C	1.4840137543	-0.0000000000	-1.2354637129
C	-2.8337160589	0.0000000000	1.2711482165
C	2.8337160589	0.0000000000	1.2711482165
C	-2.8405851098	0.0000000000	-1.2913440927
C	2.8405851098	0.0000000000	-1.2913440927
B	-3.6685501159	0.0000000000	-0.0129859562
B	3.6685501159	0.0000000000	-0.0129859562
H	-1.2364298650	0.0000000000	3.3749878342
H	1.2364298650	-0.0000000000	3.3749878342
H	-0.9302880150	0.0000000000	-2.1657489138

H	0.9302880150	0.0000000000	-2.1657489138
H	-3.2747952327	0.0000000000	2.2651355209
H	3.2747952327	0.0000000000	2.2651355209
H	-3.2870912343	0.0000000000	-2.2820303000
H	3.2870912343	0.0000000000	-2.2820303000
H	-4.8654250802	0.0000000000	0.0133853740
H	4.8654250802	-0.0000000000	0.0133853740

PB2B7 T_2:

C	-0.7493775908	0.0000000000	-0.0352886571
C	0.7493775908	0.0000000000	-0.0352886571
C	-1.4606901439	0.0000000000	1.2276808708
C	1.4606901439	-0.0000000000	1.2276808708
C	-0.6689824815	0.0000000000	2.4471667849
C	0.6689824815	0.0000000000	2.4471667849
C	-1.4557099603	0.0000000000	-1.2489425665
C	1.4557099603	0.0000000000	-1.2489425665
C	-2.8251649353	0.0000000000	1.2766048823
C	2.8251649353	-0.0000000000	1.2766048823
C	-2.8331209809	0.0000000000	-1.2913226783
C	2.8331209809	0.0000000000	-1.2913226783
B	-3.6631362289	0.0000000000	0.0179170883
B	3.6631362289	0.0000000000	0.0179170883
H	-1.2143402738	0.0000000000	3.3843719359
H	1.2143402738	-0.0000000000	3.3843719359
H	-0.9059616958	0.0000000000	-2.1786397677
H	0.9059616958	-0.0000000000	-2.1786397677

H	-3.2684339336	0.0000000000	2.2694965044
H	3.2684339336	-0.0000000000	2.2694965044
H	-3.2883122044	0.0000000000	-2.2787056325
H	3.2883122044	0.0000000000	-2.2787056325
H	-4.8599976664	0.0000000000	0.0096612354
H	4.8599976664	0.0000000000	0.0096612354

PN4N5 S_0:

C	-0.6806526152	-0.0105915790	0.0106443286
C	0.6806526152	0.0105915790	0.0106443286
C	-1.4327942517	0.0232269090	1.2305634951
C	1.4327942517	-0.0232269090	1.2305634951
C	-0.6753713969	0.0163712002	2.4503678301
C	0.6753713969	-0.0163712002	2.4503678301
N	-1.3804478624	-0.0306831516	-1.2166430044
N	1.3804478624	0.0306831516	-1.2166430044
C	-2.8045306518	0.0579094894	1.1882302327
C	2.8045306518	-0.0579094894	1.1882302327
C	-2.7646977170	-0.0533949688	-1.2155511679
C	2.7646977170	0.0533949688	-1.2155511679
C	-3.4785482501	0.0297988925	-0.0785822053
C	3.4785482501	-0.0297988925	-0.0785822053
H	-1.2218378793	0.0323447898	3.3870431611
H	1.2218378793	-0.0323447898	3.3870431611
H	-0.9340620766	-0.5733276252	-1.9415654328
H	0.9340620766	0.5733276252	-1.9415654328
H	-3.3745625203	0.0873465387	2.1084875848

H	3.3745625203	-0.0873465387	2.1084875848
H	-3.2259615583	-0.1120395592	-2.1935991297
H	3.2259615583	0.1120395592	-2.1935991297
H	-4.5588096531	0.0671105905	-0.1293956924
H	4.5588096531	-0.0671105905	-0.1293956924

PN4N5 S_1:

C	-0.6983064970	0.0034312250	0.0401343383
C	0.7091363991	0.0876966857	0.0227361670
C	-1.4489933515	0.0491869205	1.2743784423
C	1.4282614855	-0.0079805490	1.2359865021
C	-0.7110518765	0.0494997057	2.4556877472
C	0.6665852593	-0.0102100041	2.4539444100
N	-1.3717295022	-0.1449277070	-1.1123768211
N	1.3620348213	0.2041851630	-1.1991176250
C	-2.8653801675	0.0954647575	1.1481886537
C	2.8278429191	-0.0832467782	1.1597824939
C	-2.7064308516	-0.1716697737	-1.2297146646
C	2.7649070970	0.0752363407	-1.2561447218
C	-3.4886347416	0.0010853809	-0.0643888457
C	3.4575019720	-0.0805446715	-0.1027019223
H	-1.2430925846	0.0956400452	3.4006548690
H	1.2114756082	-0.0140377290	3.3894473930
H	-0.8106108078	-0.2982232432	-1.9365774555
H	0.9836547670	0.9059882182	-1.8181097262
H	-3.4608157654	0.2024087555	2.0491066436
H	3.4117527649	-0.1756041730	2.0653146025

H	-3.1080236180	-0.3479014585	-2.2154580541
H	3.2004918059	0.0813737759	-2.2443454367
H	-4.5658648041	0.0320715019	-0.1518872818
H	4.5327374382	-0.2087928887	-0.1645401079

PN4N5 T_1:

C	-0.6975638733	-0.0159483444	0.0258657832
C	0.6975638733	0.0159483444	0.0258657832
C	-1.4210456815	0.0292036104	1.2401948649
C	1.4210456815	-0.0292036104	1.2401948649
C	-0.6907957462	0.0261039753	2.4343637395
C	0.6907957462	-0.0261039753	2.4343637395
N	-1.3848938294	-0.0645263233	-1.1802487138
N	1.3848938294	0.0645263233	-1.1802487138
C	-2.8523234387	0.0673006771	1.1752000577
C	2.8523234387	-0.0673006771	1.1752000577
C	-2.7684533790	-0.0725968604	-1.2226213458
C	2.7684533790	0.0725968604	-1.2226213458
C	-3.4876297719	0.0237169658	-0.0610376814
C	3.4876297719	-0.0237169658	-0.0610376814
H	-1.2321528020	0.0504910299	3.3732289097
H	1.2321528020	-0.0504910299	3.3732289097
H	-0.9068481800	-0.5001449328	-1.9497583310
H	0.9068481800	0.5001449328	-1.9497583310
H	-3.4226681434	0.1198863794	2.0930876591
H	3.4226681434	-0.1198863794	2.0930876591
H	-3.2135847881	-0.1394229327	-2.2044837897

H	3.2135847881	0.1394229327	-2.2044837897
H	-4.5688090733	0.0540857962	-0.1237911527
H	4.5688090733	-0.0540857962	-0.1237911527

PN4N5 T_2:

C	-0.6897511895	0.0224747349	-0.0067696899
C	0.7110248352	0.0399626873	0.0010103837
C	-1.4374709606	0.0470992088	1.2393088519
C	1.4156800840	-0.0173762389	1.2003374478
C	-0.6805692616	-0.0054299055	2.4639573307
C	0.6625655314	-0.0574276933	2.4519946786
N	-1.4037332685	-0.0746622853	-1.1647303628
N	1.3954497906	0.0744956598	-1.2204540378
C	-2.8212048838	0.0869647070	1.1649659927
C	2.8402168392	-0.0363859953	1.1735336781
C	-2.7425977163	-0.0609143242	-1.2345913362
C	2.7869042667	0.0741127914	-1.2237915425
C	-3.5031169516	0.0719329477	-0.0482861547
C	3.5002697636	-0.0028154168	-0.0427539338
H	-1.2260524542	-0.0154214372	3.4017478929
H	1.2225651768	-0.1147070879	3.3781691103
H	-0.8893990608	-0.2705962785	-2.0061911596
H	0.9744979194	0.6756302254	-1.9173729693
H	-3.3873136510	0.1213033263	2.0910712298
H	3.3910159330	-0.0757167505	2.1047991506
H	-3.1743780380	-0.1768181412	-2.2176338464
H	3.2529025451	0.1306437214	-2.1972887999

H	-4.5806446313	0.1089589511	-0.1003951132
H	4.5820907224	-0.0240081468	-0.0906365011

PN1N8 S_0:

C	-0.7331600441	0.0000000000	-0.0733476877
C	0.7331600441	-0.0000000000	-0.0733476877
C	-1.4038092979	0.0000000000	1.2135265295
C	1.4038092979	-0.0000000000	1.2135265295
C	-0.7162433942	0.0000000000	2.3808662524
C	0.7162433942	0.0000000000	2.3808662524
C	-1.4911116221	0.0000000000	-1.2180153627
C	1.4911116221	-0.0000000000	-1.2180153627
N	-2.8063034993	0.0000000000	1.1798579693
N	2.8063034993	0.0000000000	1.1798579693
C	-2.9226694582	0.0000000000	-1.1730744131
C	2.9226694582	0.0000000000	-1.1730744131
C	-3.5321578653	0.0000000000	0.0277730110
C	3.5321578653	0.0000000000	0.0277730110
H	-1.2475378463	0.0000000000	3.3261813597
H	1.2475378463	0.0000000000	3.3261813597
H	-1.0118451549	0.0000000000	-2.1874694337
H	1.0118451549	0.0000000000	-2.1874694337
H	-3.2875544594	0.0000000000	2.0579177176
H	3.2875544594	0.0000000000	2.0579177176
H	-3.5074461906	0.0000000000	-2.0819953813
H	3.5074461906	-0.0000000000	-2.0819953813
H	-4.6080780109	0.0000000000	0.1477794401

H	4.6080780109	0.0000000000	0.1477794401

PN1N8 S_1:

C	-0.7218542436	-0.1084903627	0.0000000000
C	0.7107022981	-0.0736426589	0.0000000000
C	-1.3930974283	1.1688172946	0.0000000000
C	1.3998088170	1.1890930667	0.0000000000
C	-0.6807604868	2.3715384644	0.0000000000
C	0.7138595600	2.4048923378	0.0000000000
C	-1.5068787547	-1.2540050745	0.0000000000
C	1.5158461259	-1.2399246496	0.0000000000
N	-2.7473695018	1.1788819297	0.0000000000
N	2.7444577628	1.1777719074	0.0000000000
C	-2.9268351446	-1.1633772130	0.0000000000
C	2.8958298017	-1.1774357254	0.0000000000
C	-3.5441512114	0.0351959612	0.0000000000
C	3.5193549160	0.0647672344	0.0000000000
H	-1.2375539341	3.3030769334	0.0000000000
H	1.2513018004	3.3450512290	0.0000000000
H	-1.0500897344	-2.2330132155	0.0000000000
H	1.0389541760	-2.2106984943	0.0000000000
H	-3.1999346119	2.0736838868	0.0000000000
H	3.2025341258	2.0727849993	0.0000000000
H	-3.5257581197	-2.0657355077	0.0000000000
H	3.4988993043	-2.0750897826	0.0000000000
H	-4.6108859740	0.1967598354	0.0000000000
H	4.5873992172	0.2190975141	0.0000000000

PN1N8 T_1:

C	-0.7095414011	0.0000000000	-0.0557937266
C	0.7095414011	0.0000000000	-0.0557937266
C	-1.3903033650	0.0000000000	1.1871618127
C	1.3903033650	0.0000000000	1.1871618127
C	-0.6937353004	0.0000000000	2.3905613439
C	0.6937353004	0.0000000000	2.3905613439
C	-1.4964391452	0.0000000000	-1.2513791740
C	1.4964391452	0.0000000000	-1.2513791740
N	-2.7693931147	0.0000000000	1.1885544221
N	2.7693931147	0.0000000000	1.1885544221
C	-2.8894792693	0.0000000000	-1.1717338461
C	2.8894792693	0.0000000000	-1.1717338461
C	-3.5241652364	0.0000000000	0.0372932690
C	3.5241652364	0.0000000000	0.0372932690
H	-1.2380299116	0.0000000000	3.3286121038
H	1.2380299116	0.0000000000	3.3286121038
H	-1.0183352005	0.0000000000	-2.2184225275
H	1.0183352005	0.0000000000	-2.2184225275
H	-3.2343193327	0.0000000000	2.0757875907
H	3.2343193327	0.0000000000	2.0757875907
H	-3.4880849562	0.0000000000	-2.0743746640
H	3.4880849562	0.0000000000	-2.0743746640
H	-4.5965627410	0.0000000000	0.1637333958
H	4.5965627410	0.0000000000	0.1637333958

PN1N8 T_2:

C	-0.7375271464	-0.0804488460	0.0078857171
C	0.7173084818	-0.0940029128	-0.0024335585
C	-1.3822253502	1.1480951410	0.0291663313
C	1.4075495596	1.1931585358	0.0109650194
C	-0.6651805418	2.3956414981	0.0266483865
C	0.6933824300	2.4163051411	0.0217623032
C	-1.5030886449	-1.2680512509	-0.0019879813
C	1.5028635169	-1.2315550501	-0.0188925948
N	-2.7883133861	1.1914206974	0.0176894370
N	2.7610910027	1.1732672565	0.0087857456
C	-2.9167386216	-1.1718045151	0.0402744682
C	2.8960181141	-1.1946198969	-0.0202046938
C	-3.5257557471	0.0371230072	0.0746986562
C	3.5231654470	0.0814536459	-0.0044303295
H	-1.2252274661	3.3242591417	0.0224374943
H	1.2340736313	3.3575081360	0.0216501266
H	-1.0318866219	-2.2385469085	-0.0233216671
H	1.0209571456	-2.2019424258	-0.0288574977
H	-3.2281977061	2.0524981601	0.2828280971
H	3.2243651713	2.0668388273	0.0184592612
H	-3.5274151755	-2.0660149282	0.0486297445
H	3.4921800727	-2.0935745558	-0.0299899992
H	-4.5999647185	0.1575996766	0.1233123602
H	4.5919720528	0.2347291466	-0.0020637673

PN1a**N8**a S_0:

C	-0.6811478498	0.0000000000	-0.0674676112
C	0.6811478498	-0.0000000000	-0.0674676112
N	-1.4108190653	0.0000000000	1.1649475655
N	1.4108190653	-0.0000000000	1.1649475655
C	-0.6626648400	0.0000000000	2.3491841134
C	0.6626648400	-0.0000000000	2.3491841134
C	-1.5111800734	0.0000000000	-1.2542924948
C	1.5111800734	0.0000000000	-1.2542924948
C	-2.7740474657	0.0000000000	1.1985375333
C	2.7740474657	0.0000000000	1.1985375333
C	-2.8528237584	0.0000000000	-1.1891315585
C	2.8528237584	-0.0000000000	-1.1891315585
C	-3.5330661845	0.0000000000	0.0900354660
C	3.5330661845	-0.0000000000	0.0900354660
H	-1.2246956268	0.0000000000	3.2718036293
H	1.2246956268	0.0000000000	3.2718036293
H	-1.0216861671	0.0000000000	-2.2177408529
H	1.0216861671	-0.0000000000	-2.2177408529
H	-3.2006222405	0.0000000000	2.1944934356
H	3.2006222405	-0.0000000000	2.1944934356
H	-3.4346496407	0.0000000000	-2.1033784878
H	3.4346496407	0.0000000000	-2.1033784878
H	-4.6105534376	0.0000000000	0.1630092625
H	4.6105534376	0.0000000000	0.1630092625

PN1*a***N8***a* S_1:

C	-0.720674	0.003008	-0.053666

C	0.689859	-0.003152	-0.048649
N	-1.425010	0.004582	1.174263
N	1.385219	-0.004898	1.184269
C	-0.707961	0.002448	2.335156
C	0.660039	-0.001866	2.340198
C	-1.508099	0.007546	-1.228083
C	1.485733	-0.007486	-1.217420
C	-2.794798	0.008715	1.186881
C	2.754960	-0.009474	1.206734
C	-2.879855	0.012079	-1.200530
C	2.857188	-0.012028	-1.179979
C	-3.538380	0.012294	0.044746
C	3.506800	-0.012727	0.070015
H	-1.273057	0.005408	3.253848
H	1.218522	-0.003166	3.262842
H	-1.000036	0.007957	-2.180727
H	0.984747	-0.007445	-2.173805
H	-3.235628	0.009129	2.174370
H	3.188509	-0.010506	2.197450
H	-3.444681	0.015866	-2.123617
H	3.428754	-0.015485	-2.098912
H	-4.617451	0.015808	0.120872
H	4.585298	-0.016607	0.153745

PN1a**N8**a T_1:

C	-0.7263773892	-0.0268555869	-0.0747129828
C	0.7263773892	0.0268555869	-0.0747129828

N	-1.3966390659	0.0512364653	1.1649516317
N	1.3966390659	-0.0512364653	1.1649516317
C	-0.6710170423	0.0323500759	2.3352946405
C	0.6710170423	-0.0323500759	2.3352946405
C	-1.4973491155	-0.1347005860	-1.2137997379
C	1.4973491155	0.1347005860	-1.2137997379
C	-2.7827500684	0.1041544253	1.1947951364
C	2.7827500684	-0.1041544253	1.1947951364
C	-2.8890073528	-0.1127162323	-1.1901654546
C	2.8890073528	0.1127162323	-1.1901654546
C	-3.5228716465	0.0274909461	0.0650964359
C	3.5228716465	-0.0274909461	0.0650964359
H	-1.2361988539	0.0585031584	3.2541868115
H	1.2361988539	-0.0585031584	3.2541868115
H	-0.9896545024	-0.2392655347	-2.1628013064
H	0.9896545024	0.2392655347	-2.1628013064
H	-3.2133370750	0.2050620117	2.1810138292
H	3.2133370750	-0.2050620117	2.1810138292
H	-3.4609172682	-0.2001026385	-2.1026615626
H	3.4609172682	0.2001026385	-2.1026615626
H	-4.6015996296	0.0727273906	0.1486654491
H	4.6015996296	-0.0727273906	0.1486654491

PN1a**N8**a T_2:

C	-0.7100770361	-0.0504994403	0.0000000000
C	0.7097617195	-0.0624909818	0.0000000000
N	-1.3862113803	1.1323142419	0.0000000000

N	1.3928148359	1.1684975592	0.0000000000
C	-0.6585399321	2.3448380131	0.0000000000
C	0.6678365153	2.3319692416	0.0000000000
C	-1.4860285328	-1.2529098636	0.0000000000
C	1.4702753282	-1.2284720721	0.0000000000
C	-2.7492235482	1.2219490459	0.0000000000
C	2.7895330850	1.2131601633	0.0000000000
C	-2.8769566144	-1.1654692577	0.0000000000
C	2.8726584649	-1.1855580319	0.0000000000
C	-3.5251778126	0.0550518310	0.0000000000
C	3.5151374010	0.0595217238	0.0000000000
H	-1.2397016411	3.2514881781	0.0000000000
H	1.2350801714	3.2519087846	0.0000000000
H	-0.9934345181	-2.2088662707	0.0000000000
H	0.9628352658	-2.1792894312	0.0000000000
H	-3.1531030503	2.2212517464	0.0000000000
H	3.2192837982	2.2034641575	0.0000000000
H	-3.4597056485	-2.0801028971	0.0000000000
H	3.4457896645	-2.1024973151	0.0000000000
H	-4.6032806080	0.1310815056	0.0000000000
H	4.5959018729	0.1296593993	0.0000000000

PN3N6 S_0:

C	-0.7386026059	-0.0460882789	-0.0614067781
C	0.7386026059	0.0460882789	-0.0614067781
C	-1.4286732928	0.1189664119	1.2310839710
C	1.4286732928	-0.1189664119	1.2310839710

C	-0.7080445367	0.0891615297	2.3912722860
C	0.7080445367	-0.0891615297	2.3912722860
C	-1.4624610835	-0.3038691638	-1.1614131714
C	1.4624610835	0.3038691638	-1.1614131714
C	-2.8645875710	0.2267570470	1.1510270265
C	2.8645875710	-0.2267570470	1.1510270265
N	-2.8383650042	-0.2454061000	-1.1741636664
N	2.8383650042	0.2454061000	-1.1741636664
C	-3.5210104560	0.0340362833	-0.0055885809
C	3.5210104560	-0.0340362833	-0.0055885809
H	-1.2287946173	0.1717013943	3.3393193003
H	1.2287946173	-0.1717013943	3.3393193003
H	-1.0033451406	-0.5397380162	-2.1140226742
H	1.0033451406	0.5397380162	-2.1140226742
H	-3.4321039252	0.4489969135	2.0469853218
H	3.4321039252	-0.4489969135	2.0469853218
H	-3.3347854106	-0.6300288168	-1.9529954896
H	3.3347854106	0.6300288168	-1.9529954896
H	-4.5980641782	0.0957518361	-0.0900975451
H	4.5980641782	-0.0957518361	-0.0900975451

PN3N6 S_1:

C	-0.7190809510	0.0000000000	-0.0556209020
C	0.7190809510	-0.0000000000	-0.0556209020
C	-1.4414516873	0.0000000000	1.2194692539
C	1.4414516873	-0.0000000000	1.2194692539
C	-0.6877883592	0.0000000000	2.4111866639

C	0.6877883592	-0.0000000000	2.4111866639
C	-1.4916552499	0.0000000000	-1.2042069947
C	1.4916552499	-0.0000000000	-1.2042069947
C	-2.8366944614	0.0000000000	1.1965672066
C	2.8366944614	0.0000000000	1.1965672066
N	-2.8380509560	0.0000000000	-1.1600664367
N	2.8380509560	-0.0000000000	-1.1600664367
C	-3.5456313320	0.0000000000	0.0062919194
C	3.5456313320	-0.0000000000	0.0062919194
H	-1.2225231530	0.0000000000	3.3552473773
H	1.2225231530	0.0000000000	3.3552473773
H	-1.0707065424	0.0000000000	-2.1997374473
H	1.0707065424	0.0000000000	-2.1997374473
H	-3.3843041868	0.0000000000	2.1311472109
H	3.3843041868	0.0000000000	2.1311472109
H	-3.3389823208	0.0000000000	-2.0283687059
H	3.3389823208	0.0000000000	-2.0283687059
H	-4.6213265645	0.0000000000	-0.0719091460
H	4.6213265645	0.0000000000	-0.0719091460

PN3N6 T_1:

C	-0.7147092381	0.0023281822	-0.0269713191
C	0.7147092381	-0.0023281822	-0.0269713191
C	-1.4007309182	-0.0093232265	1.2101324197
C	1.4007309182	0.0093232265	1.2101324197
C	-0.6897137753	-0.0078843165	2.4174961403
C	0.6897137753	0.0078843165	2.4174961403

C	-1.4602382608	0.0158198028	-1.2285033492
C	1.4602382608	-0.0158198028	-1.2285033492
C	-2.8472370200	-0.0172643772	1.1885312252
C	2.8472370200	0.0172643772	1.1885312252
N	-2.8463018627	0.0193526110	-1.1671953405
N	2.8463018627	-0.0193526110	-1.1671953405
C	-3.5116497306	-0.0048864478	0.0146228732
C	3.5116497306	0.0048864478	0.0146228732
H	-1.2394603268	-0.0140214203	3.3520168358
H	1.2394603268	0.0140214203	3.3520168358
H	-1.0319213075	0.1105734321	-2.2107859457
H	1.0319213075	-0.1105734321	-2.2107859457
H	-3.3997186486	-0.0321365605	2.1186337124
H	3.3997186486	0.0321365605	2.1186337124
H	-3.3682181377	0.0205185266	-2.0208805926
H	3.3682181377	-0.0205185266	-2.0208805926
H	-4.5926508697	-0.0117991930	-0.0474797895
H	4.5926508697	0.0117991930	-0.0474797895

PN3N6 T_2:

C	-0.713492	0.006044	-0.060613
C	0.713492	-0.006044	-0.060613
C	-1.440790	0.011196	1.218492
C	1.440790	-0.011196	1.218492
C	-0.686688	0.005286	2.410287
C	0.686688	-0.005286	2.410287
C	-1.492581	0.013815	-1.208767

C	1.492581	-0.013815	-1.208767
C	-2.837343	0.022202	1.195827
C	2.837343	-0.022202	1.195827
N	-2.843000	0.024568	-1.162075
N	2.843000	-0.024568	-1.162075
C	-3.544739	0.028288	0.013828
C	3.544739	-0.028288	0.013828
H	-1.222220	0.009505	3.354228
H	1.222220	-0.009505	3.354228
H	-1.074614	0.012123	-2.205932
H	1.074614	-0.012123	-2.205932
H	-3.386040	0.026400	2.130242
H	3.386040	-0.026400	2.130242
H	-3.349441	0.028891	-2.026304
H	3.349441	-0.028891	-2.026304
H	-4.621354	0.039180	-0.058914
H	4.621354	-0.039180	-0.058914

PN4a**N5**a S_0:

N	-0.6876037024	0.0916464343	0.0446594089
N	0.6876037024	-0.0916464343	0.0446594089
C	-1.3784839190	-0.2649975367	1.2279537642
C	1.3784839190	0.2649975367	1.2279537642
C	-0.6904900789	-0.2159297124	2.3902732296
C	0.6904900789	0.2159297124	2.3902732296
C	-1.3113845399	0.6910868055	-1.0092811957
C	1.3113845399	-0.6910868055	-1.0092811957

C	-2.7875337050	-0.5193956783	1.0113231658
C	2.7875337050	0.5193956783	1.0113231658
C	-2.6543998087	0.6458509585	-1.1177399955
C	2.6543998087	-0.6458509585	-1.1177399955
C	-3.3946635068	-0.0668721649	-0.1020867101
C	3.3946635068	0.0668721649	-0.1020867101
H	-1.1833695135	-0.4895996338	3.3137795718
H	1.1833695135	0.4895996338	3.3137795718
H	-0.6580585284	1.1400940417	-1.7475991740
H	0.6580585284	-1.1400940417	-1.7475991740
H	-3.3425349764	-1.0289494852	1.7902385852
H	3.3425349764	1.0289494852	1.7902385852
H	-3.1493157152	1.1069937058	-1.9601025674
H	3.1493157152	-1.1069937058	-1.9601025674
H	-4.4577959696	-0.2288237182	-0.2409522524
H	4.4577959696	0.2288237182	-0.2409522524

PN4a**N5**a S_1:

N	-0.671945	0.069364	-0.169134
N	0.679475	0.070720	0.176655
C	-1.405176	1.247857	0.087352
C	1.413757	1.245623	-0.093362
C	-0.677329	2.453533	0.082922
C	0.687264	2.452225	-0.099166
C	-1.323287	-1.121332	-0.403153
C	1.330158	-1.118036	0.423119
C	-2.786815	1.121952	0.228896

C	2.794866	1.116998	-0.236684
C	-2.671352	-1.219119	-0.277809
C	2.677920	-1.218373	0.296111
C	-3.437848	-0.084985	0.084474
C	3.444668	-0.089307	-0.080704
H	-1.228893	3.378232	0.190958
H	1.239274	3.375546	-0.216019
H	-0.704683	-1.940825	-0.735529
H	0.711483	-1.933118	0.766047
H	-3.344508	2.027528	0.438523
H	3.352487	2.020038	-0.456999
H	-3.142039	-2.168794	-0.498771
H	3.148590	-2.165755	0.526732
H	-4.508890	-0.157814	0.215258
H	4.515274	-0.165481	-0.213157

PN4a**N5**a T_1:

N	-0.6760231105	-0.1600187514	0.0693677260
N	0.6760231105	0.1600187514	0.0693677260
C	-1.4083682865	0.1221762663	1.2392737087
C	1.4083682865	-0.1221762663	1.2392737087
C	-0.6741104295	0.1087475626	2.4518134823
C	0.6741104295	-0.1087475626	2.4518134823
C	-1.3241541307	-0.4412908495	-1.1160051677
C	1.3241541307	0.4412908495	-1.1160051677
C	-2.7802606368	0.2696131224	1.1139952750
C	2.7802606368	-0.2696131224	1.1139952750

C	-2.6720512243	-0.3161640394	-1.2128004255
C	2.6720512243	0.3161640394	-1.2128004255
C	-3.4352197512	0.0922793932	-0.0941796588
C	3.4352197512	-0.0922793932	-0.0941796588
H	-1.2240619593	0.2281312363	3.3763514884
H	1.2240619593	-0.2281312363	3.3763514884
H	-0.7022236706	-0.8020201163	-1.9216582072
H	0.7022236706	0.8020201163	-1.9216582072
H	-3.3364485692	0.4958530730	2.0165969622
H	3.3364485692	-0.4958530730	2.0165969622
H	-3.1470573415	-0.5688005541	-2.1525323589
H	3.1470573415	0.5688005541	-2.1525323589
H	-4.5063309832	0.2194145647	-0.1702228041
H	4.5063309832	-0.2194145647	-0.1702228041

PN4a**N5**a T_2:

N	-0.6892646075	0.0397271593	0.0215009302
N	0.7041060193	0.0495289698	0.0603075021
C	-1.3991266736	1.2331544383	0.2251718736
C	1.3788151713	1.1934719650	-0.2191635440
C	-0.6875584378	2.4312160332	0.0714417165
C	0.6491334013	2.4002676369	-0.2594710764
C	-1.3213432142	-1.0758145637	-0.5376663966
C	1.3014278988	-1.1180802870	0.4632268611
C	-2.7750490128	1.0947530943	0.4160174098
C	2.7987957430	1.1107580382	-0.2959449937
C	-2.6674753252	-1.1779003858	-0.3940249534

C	2.7065164385	-1.2044759873	0.4028164244
C	-3.4066543569	-0.1203023525	0.1865770067
C	3.4293752512	-0.1003724415	0.0073838606
H	-1.2223213398	3.3663951939	0.1732327098
H	1.1996255764	3.3094223028	-0.4582616279
H	-0.6964880120	-1.7786699177	-1.0647817747
H	0.6446149719	-1.8888273062	0.8255047721
H	-3.3444938032	1.9864452101	0.6484206317
H	3.3543774974	2.0117039093	-0.5083277965
H	-3.1704086086	-2.0486583856	-0.7957309899
H	3.1881134874	-2.1288376920	0.6896226307
H	-4.4762956285	-0.2146479827	0.3196342652
H	4.5115831045	-0.1583691090	-0.0347942996

PN2N7 S_0:

C	-0.6817905068	-0.0029837603	-0.0578450553
C	0.6817905068	0.0029837603	-0.0578450553
C	-1.4291709977	-0.0101885583	1.1973103067
C	1.4291709977	0.0101885583	1.1973103067
C	-0.6720862715	-0.0066752531	2.4280028190
C	0.6720862715	0.0066752531	2.4280028190
C	-1.5147424341	-0.0097572077	-1.2570196456
C	1.5147424341	0.0097572077	-1.2570196456
C	-2.7821614063	-0.0138432739	1.2006222225
C	2.7821614063	0.0138432739	1.2006222225
C	-2.8529501643	-0.0103066029	-1.1794611989
C	2.8529501643	0.0103066029	-1.1794611989

N	-3.5140557987	0.0265682740	0.0273526231
N	3.5140557987	-0.0265682740	0.0273526231
H	-1.2170648081	-0.0115722926	3.3666219533
H	1.2170648081	0.0115722926	3.3666219533
H	-1.0629135107	-0.0097171349	-2.2389508353
H	1.0629135107	0.0097171349	-2.2389508353
H	-3.3559112472	-0.0215134949	2.1179472954
H	3.3559112472	0.0215134949	2.1179472954
H	-3.4833528898	-0.0185285575	-2.0596233651
H	3.4833528898	0.0185285575	-2.0596233651
H	-4.4958853256	-0.1613255464	0.0550428794
H	4.4958853256	0.1613255464	0.0550428794

PN2N7 S_1:

C	-0.7213619658	0.0000000000	-0.0961582150
C	0.7213619658	-0.0000000000	-0.0961582150
C	-1.4189888351	0.0000000000	1.1975888068
C	1.4189888351	0.0000000000	1.1975888068
C	-0.6851875017	0.0000000000	2.4142515181
C	0.6851875017	0.0000000000	2.4142515181
C	-1.5165819382	0.0000000000	-1.2387085548
C	1.5165819382	-0.0000000000	-1.2387085548
C	-2.7890677096	0.0000000000	1.1846831747
C	2.7890677096	0.0000000000	1.1846831747
C	-2.9001843501	0.0000000000	-1.1908051282
C	2.9001843501	0.0000000000	-1.1908051282
N	-3.4984084583	0.0000000000	0.0455096230

N	3.4984084583	-0.0000000000	0.0455096230
H	-1.2331789091	0.0000000000	3.3501111372
H	1.2331789091	-0.0000000000	3.3501111372
H	-1.0592341793	0.0000000000	-2.2201552584
H	1.0592341793	-0.0000000000	-2.2201552584
H	-3.3634711327	0.0000000000	2.1028382326
H	3.3634711327	-0.0000000000	2.1028382326
H	-3.5479047456	0.0000000000	-2.0522554690
H	3.5479047456	0.0000000000	-2.0522554690
H	-4.4993456755	0.0000000000	0.1031001331
H	4.4993456755	-0.0000000000	0.1031001331

PN2N7 T_1:

C	-0.7008804017	0.0000000000	-0.0190513337
C	0.7008804017	-0.0000000000	-0.0190513337
C	-1.4181348558	0.0000000000	1.2310729451
C	1.4181348558	0.0000000000	1.2310729451
C	-0.6986653191	0.0000000000	2.4246334797
C	0.6986653191	-0.0000000000	2.4246334797
C	-1.4855281406	0.0000000000	-1.2268950440
C	1.4855281406	0.0000000000	-1.2268950440
C	-2.8343760240	0.0000000000	1.1968825611
C	2.8343760240	0.0000000000	1.1968825611
C	-2.8413690953	0.0000000000	-1.1838754494
C	2.8413690953	0.0000000000	-1.1838754494
N	-3.4989782123	0.0000000000	-0.0038706560
N	3.4989782123	0.0000000000	-0.0038706560

H	-1.2367209910	0.0000000000	3.3661081906
H	1.2367209910	0.0000000000	3.3661081906
H	-1.0116354110	0.0000000000	-2.1966447401
H	1.0116354110	0.0000000000	-2.1966447401
H	-3.4407476094	0.0000000000	2.0891498097
H	3.4407476094	0.0000000000	2.0891498097
H	-3.4546312204	0.0000000000	-2.0752070763
H	3.4546312204	0.0000000000	-2.0752070763
H	-4.5005387148	0.0000000000	-0.0023026867
H	4.5005387148	0.0000000000	-0.0023026867

PN2N7 T_2:

C	0.715245	0.390647	-0.000000
C	-0.715757	0.394229	-0.000000
C	1.415025	-0.893965	-0.000000
C	-1.416819	-0.894425	0.000000
C	0.691158	-2.097722	0.000000
C	-0.692932	-2.097203	0.000000
C	1.507325	1.552808	0.000000
C	-1.504603	1.552029	-0.000000
C	2.802683	-0.872603	-0.000000
C	-2.802222	-0.870292	0.000000
C	2.878734	1.504850	0.000000
C	-2.880582	1.506690	-0.000000
N	3.498624	0.286554	0.000000
N	-3.496378	0.284378	0.000000
H	1.235844	-3.035324	0.000000

H	-1.237769	-3.034961	0.000000
H	1.045620	2.530969	0.000000
H	-1.042282	2.530030	-0.000000
H	3.390044	-1.781328	-0.000000
H	-3.389562	-1.779514	0.000000
H	3.516444	2.375957	0.000000
H	-3.520288	2.375742	-0.000000
H	4.499870	0.248242	-0.000000
H	-4.497829	0.243851	0.000000

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