Supporting information

The enhancement of nonlinear optical properties of azulene-based nanographene by N atoms: a finishing touch

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[#]Y. Q. Zhang and C. C. Yang contributed equally to this work.

Supporting Information list:

Figure S1 The structure of B, N doped nanographenes. H or P in square brackets indicates that the carbon atom at

the end of a heptagon (H) or pentagon (P) in azulene of A1A2A3 is replaced by B and N atoms.

Figure S2 The proposed Kekulé structures of all investigated molecules according to bond distance and spin distribution.

Figure S3 Evolution of the static first hyperpolarizability ($<\beta_0>$) and the static second hyperpolarizability ($<\gamma_0>$) with

the numbers of excited states in A1[H_N]A3[P_N] and A1[H_N]A2[$H_N P_N$]A3[P_N], respectively.

Figure S4a The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3,

A2[$H_B P_B$], A2[$H_B P_N$] and A2[$H_N P_N$] predicted with B3LYP/6-31G (d, p).

Figure S4b The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3,

A1[$H_N P_N$], A2[$H_N P_N$], A3[$H_N P_N$] and A1[H_N]A3[P_N] predicted with B3LYP/6-31G (d, p).

Figure S4c The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3,

A1[$H_B P_B$], A1[$H_B P_N$], A1[$H_N P_B$] and A1[$H_N P_N$] predicted with B3LYP/6-31G (d, p).

Figure S4d The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3,

A3[$H_B P_B$], A3[$H_B P_N$], A3[$H_N P_B$] and A3[$H_N P_N$] predicted with B3LYP/6-31G (d, p).

Figure S4e The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3,

A1[H_B]A3[P_B], A1[H_B]A3[P_N], A1[H_N]A3[P_B] and A1[H_N]A3[P_N] predicted with B3LYP/6-31G (d, p).

Figure S4f The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3,

A1[H$_B$P$_B$]A2[H$_B$P$_B$]A3[H$_B$P$_B$], A1[H$_B$P$_N$]A2[H$_B$P$_N$]A3[H$_B$P$_N$], A1[H$_N$P$_B$]A2[H$_N$P$_B$]A3[H$_N$P$_B$] and A1[H$_N$P$_N$]A2[H$_N$P$_N$]A3[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4g The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$P$_B$]A2[H$_B$P$_B$], A1[H$_B$P$_N$]A2[H$_B$P$_N$], A1[H$_N$P$_B$]A2[H$_N$P$_B$] and A1[H$_N$P$_N$]A2[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4h The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A2[H$_B$P$_B$]A3[H$_B$P$_B$], A2[H$_B$P$_N$]A3[H$_B$P$_N$], A2[H$_N$P$_B$]A3[H$_N$P$_B$] and A2[H$_N$P$_N$]A3[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4i The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$P$_B$]A3[H$_B$P$_B$], A1[H$_B$P$_N$]A3[H$_B$P$_N$], A1[H$_N$P$_B$]A3[H$_N$P$_B$] and A1[H$_N$P$_N$]A3[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4j The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$]A2[H$_B$P$_B$]A3[P$_B$], A1[H$_B$]A2[H$_N$P$_B$]A3[P$_N$], A1[H$_N$]A2[H$_B$P$_N$]A3[P$_B$] and A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S5 The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$P$_B$], A3[H$_B$P$_N$] and A1[H$_N$]A3[P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S6 Two-dimensional second order NLO spectra predicted with TD-CAM-B3LYP/6-31++G(d, p)-SOS [damping coefficients Γ_m = 0.01 × ε_m/ε_2] of (a) A3[H$_N$P$_N$], (b), (c), (d) A1[H$_N$]A3[P$_N$], and (e) A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] with step size of 0.005 eV. (a) ω_1 scanned from −0.50 eV to 0.50 eV and ω_2 scanned from 2.00 eV to 3.00 eV; (b) ω_1 scanned from −0.50 eV to 0.50 eV and ω_2 scanned from 1.50 eV to 2.50 eV; (c) ω_1 scanned from 0.50 eV to 1.50 eV and ω_2 scanned from 0.50 eV to 1.50 eV; (d) ω_1 scanned from −1.50 eV to −0.50 eV and ω_2 scanned from 1.50 eV to 2.50 eV; (e) ω_1 scanned from −0.50 eV to 0.50 eV and ω_2 scanned from 2.00 eV to 3.00 eV.

Figure S7 Evolution of third-order nonlinear optic properties with electronic spectra of A1A2A3 at specific external fields.

Figure S8 Evolution of third-order nonlinear optic properties with electronic spectra of A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] at specific external fields.

Figure S9 (a) Fine-scanned TDTPA of A1A2A3 and A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] from 1.60 eV to 2.10 eV. (b) Fine-scanned TDTPA of A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] from 0.90 eV to 1.40 eV.

Table S1 The relative energy (ΔE with respect to the most stable isomer ΔE = 0, in eV), the lowest vibrational frequency (LVF, in cm^{-1}), energy gap (E$_{gap}$, in eV) between the HOMO (E$_H$, in eV) and the LUMO (E$_L$, in eV) the static first and second hyperpolarizability (<β_0> and <γ_0>), the <β_0> (in 10^{-30} esu) and <γ_0> (in 10^{-34} esu) per heavy

atom ($<\beta_0>$/N and $<\gamma_0>$/N) of A1A2A3 and its N-doped series of molecules in closed-shell singlet predicted with

B3LYP/6-31G(d, p) and TD-CAM-B3LYP/6-31++G(d, p)-SOS, respectively. The relative electronic energy differences

(ΔE_{OS-CS} and $\Delta E_{T-CS,}$ in kcal/mol) between open-shell singlet (OS) or triplet (T) and closed-shell singlet (CS) (CS is

taken as reference), and spin contamination of open-shell singlet ($<S^2>_{OS}$) obtained at the UB3LYP/6-31G (d, p) level.

Table S2 Major absorption peaks with transition nature in azulene-based molecules (*f* is the oscillator strength in

the arbitrary unit, E is the transition energy in eV unit, λ is the wavelength in nm unit, TNMC to $<\beta_0>$ is the transition

nature of electron excitation with a major contribution to $<\beta_0>$, and $<\beta_0>_{Con}$ is contribution value to $<\beta_0>$ in 10^{-30}

esu).

Table S3 Calculated important parameters of $(\beta_{ijk})_m$ [i, j, k $\in$ (x, y, z)] ($\times 10^{-30}$ esu) of azulene-based molecules. The

$[(\beta_{ijk})_m$ is the first hyperpolarizability tensor of the mth excited state (S_m) with a major contribution to the static

first hyperpolarizability ($<\beta_0>$), m = 0 is the ground state, and m > 0 is the mth excited state].

Table S4 Major electron excitations with transition nature in A1[H_N]A3[P_N], A1[H_N]A2[H_NP_N]A3[P_N] and AG. The *f* is

the oscillator strength, λ is the wavelength, and TNMC to $<\gamma_0>_{3L}$ is the transition nature of electron excitation with

a major contribution to $<\gamma_0>_{3L}$.

Table S5 Calculated important parameters of $(\gamma_{ijk})_m$ ($\times 10^{-34}$ esu) of azulene-based molecules. The $(\gamma_{ijk})_m$ is the

second hyperpolarizability tensor of the mth excited state (S_m) with a major contribution to the static first

hyperpolarizability ($<\beta_0>$), m = 0 is the ground state, and m > 0 is the mth excited state.

Table S6 The strong response and corresponding major electron excitation contribution of the dynamic third-order

nonlinear optic response for A1A2A3.

Table S7 The strong response and corresponding major electron excitation contribution of the dynamic third-order

nonlinear optic response for A1[H_N]A2[H_NP_N]A3[P_N].

Figure S1 The structure of B, N doped nanographenes. H or P in square brackets indicates that the carbon atom at the end of a heptagon (H) or pentagon (P) in azulene of A1A2A3 is replaced by B and N atoms.

Figure S2 The proposed Kekulé structures of all investigated molecules according to bond distance and spin distribution.

(a)

(b)

Figure S3 Evolution of the static first hyperpolarizability ($<\beta_0>$) and the static second hyperpolarizability ($<\gamma_0>$) with the numbers of excited states in A1[H_N]A3[P_N] and A1[H_N]A2[H_NP_N]A3[P_N], respectively.

Figure S4a The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A2[H_BP_B], A2[H_BP_N] and A2[H_NP_N] predicted with B3LYP/6-31G (d, p).

L+5 (-0.41 eV)   L+6 (-0.05 eV)   L+5 (-0.41 eV)   L+5 (-0.87 eV)   L+5 (-0.41 eV)   L+4 (-1.02 eV)

L+4 (-0.97 eV)   L+5 (-0.67 eV)   L+4 (-0.97 eV)   L+4 (-1.32 eV)   L+4 (-0.97 eV)   L+3 (-1.23 eV)

L+3 (-1.19 eV)   L+4 (-0.99 eV)   L+3 (-1.19 eV)   L+3 (-1.46 eV)   L+3 (-1.19 eV)   L+2 (-1.67 eV)

L+2 (-1.84 eV)   L+3 (-1.75 eV)   L+2 (-1.84 eV)   L+2 (-1.98 eV)   L+2 (-1.84 eV)   L+1 (-1.98 eV)

L+1 (-2.34 eV)   L+2 (-2.22 eV)   L+1 (-2.34 eV)   L+1 (-2.08 eV)   L+1 (-2.34 eV)   L (-2.07 eV)

L (-2.73 eV)   L+1 (-2.44 eV)   L (-2.73 eV)   L (-2.39 eV)   L (-2.73 eV)   H (-4.08 eV)

                L (-3.20 eV)

H (-3.91 eV)   H (-3.91 eV)   H (-4.14 eV)   H (-3.91 eV)   H-1 (-4.19 eV)

H-1 (-5.07 eV)   H (-4.63 eV)   H-1 (-5.07 eV)   H-1 (-4.94 eV)   H-1 (-5.07 eV)   H-2 (-5.00 eV)

H-2 (-5.73 eV)   H-1 (-4.92 eV)   H-2 (-5.73 eV)   H-2 (-5.15 eV)   H-2 (-5.73 eV)   H-3 (-6.05 eV)

H-3 (-5.88 eV)   H-2 (-5.64 eV)   H-3 (-5.88 eV)   H-3 (-6.00 eV)   H-3 (-5.88 eV)   H-4 (-6.09 eV)

H-4 (-6.53 eV)   H-3 (-5.71 eV)   H-4 (-6.53 eV)   H-4 (-6.10 eV)   H-4 (-6.53 eV)   H-5 (-6.71 eV)

H-5 (-6.81 eV)   H-4 (-6.05 eV)   H-5 (-6.81 eV)   H-5 (-6.56 eV)   H-5 (-6.81 eV)   H-6 (-7.30 eV)

A1A2A3   A2[$H_B P_B$]   A1A2A3   A2[$H_B P_N$]   A1A2A3   A2[$H_N P_N$]

Figure S4b The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[$H_N P_N$], A2[$H_N P_N$], A3[$H_N P_N$] and A1[H_N]A3[P_N] predicted with B3LYP/6-31G (d, p).

Figure S4c The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$P$_B$], A1[H$_B$P$_N$], A1[H$_N$P$_B$] and A1[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4d The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A3[H$_B$P$_B$], A3[H$_B$P$_N$], A3[H$_N$P$_B$] and A3[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

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Figure S4e The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$]A3[P$_B$], A1[H$_B$]A3[P$_N$], A1[H$_N$]A3[P$_B$] and A1[H$_N$]A3[P$_N$] predicted with B3LYP/6-31G (d, p).

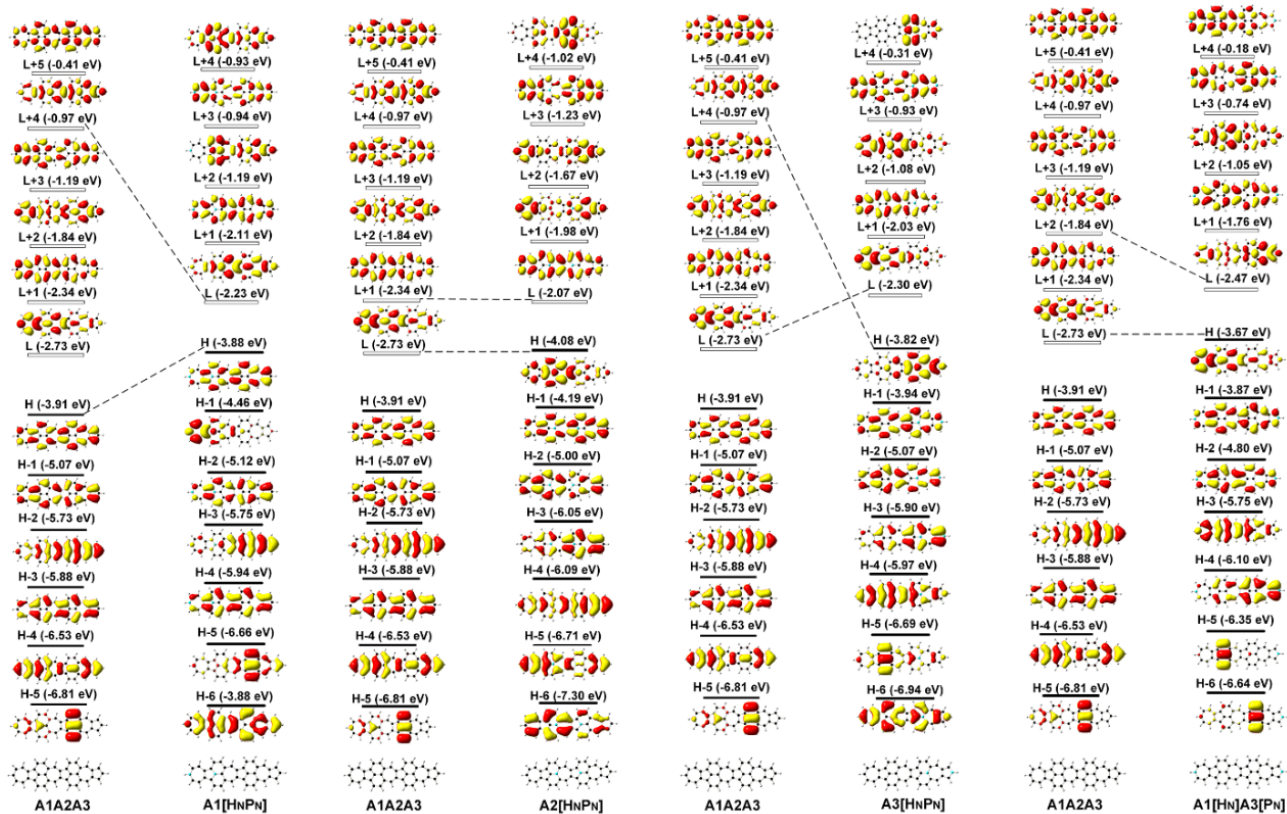**Figure S4f** The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$P$_B$]A2[H$_B$P$_B$]A3[H$_B$P$_B$], A1[H$_B$P$_N$]A2[H$_B$P$_N$]A3[H$_B$P$_N$], A1[H$_N$P$_B$]A2[H$_N$P$_B$]A3[H$_N$P$_B$] and A1[H$_N$P$_N$]A2[H$_N$P$_N$]A3[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4g The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H_BP_B]A2[H_BP_B], A1[H_BP_N]A2[H_BP_N], A1[H_NP_B]A2[H_NP_B] and A1[H_NP_N]A2[H_NP_N] predicted with B3LYP/6-31G (d, p).

Figure S4h The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A2[H_BP_B]A3[H_BP_B], A2[H_BP_N]A3[H_BP_N], A2[H_NP_B]A3[H_NP_B] and A2[H_NP_N]A3[H_NP_N] predicted with B3LYP/6-31G (d, p).
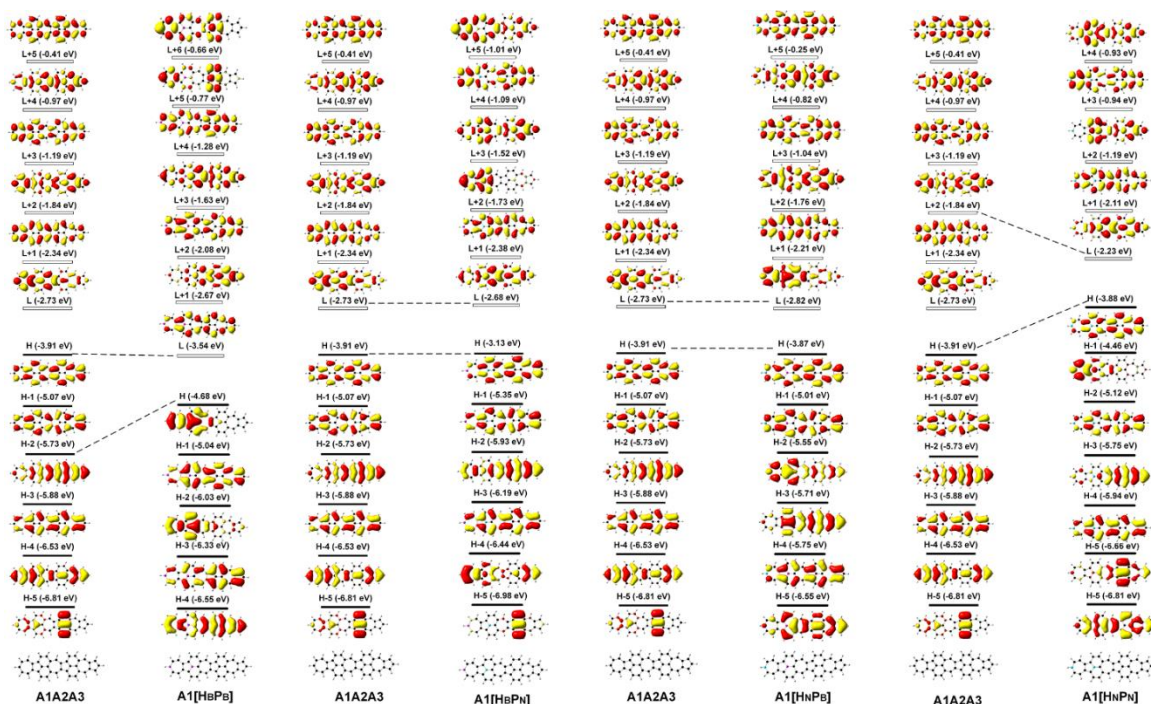
Figure S4i The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$P$_B$]A3[H$_B$P$_B$], A1[H$_B$P$_N$]A3[H$_B$P$_N$], A1[H$_N$P$_B$]A3[H$_N$P$_B$] and A1[H$_N$P$_N$]A3[H$_N$P$_N$] predicted with B3LYP/6-31G (d, p).

Figure S4j The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H$_B$]A2[H$_B$P$_B$]A3[P$_B$], A1[H$_B$]A2[H$_N$P$_B$]A3[P$_N$], A1[H$_N$]A2[H$_B$P$_N$]A3[P$_B$] and A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] predicted with B3LYP/6-31G (d, p).

The following orbital energy labels appear across six columns:

Column 1 (A1[H_B P_B]):
L+5 (-0.77 eV)
L+4 (-1.28 eV)
L+3 (-1.63 eV)
L+2 (-2.08 eV)
L+1 (-2.67 eV)
L (-3.54 eV)
H (-4.68 eV)
H-1 (-5.04 eV)
H-2 (-6.03 eV)
H-3 (-6.33 eV)
H-4 (-6.55 eV)
H-5 (-7.11 eV)

Column 2 (A1A2A3):
L+5 (-0.41 eV)
L+4 (-0.97 eV)
L+3 (-1.19 eV)
L+2 (-1.84 eV)
L+1 (-2.34 eV)
L (-2.73 eV)
H (-3.91 eV)
H-1 (-5.07 eV)
H-2 (-5.73 eV)
H-3 (-5.88 eV)
H-4 (-6.53 eV)
H-5 (-6.81 eV)

Column 3 (A1A2A3):
L+5 (-0.41 eV)
L+4 (-0.97 eV)
L+3 (-1.19 eV)
L+2 (-1.84 eV)
L+1 (-2.34 eV)
L (-2.73 eV)
H (-3.91 eV)
H-1 (-5.07 eV)
H-2 (-5.73 eV)
H-3 (-5.88 eV)
H-4 (-6.53 eV)
H-5 (-6.81 eV)

Column 4 (A3[H_N P_B]):
L+5 (-0.59 eV)
L+4 (-1.26 eV)
L+3 (-1.37 eV)
L+2 (-2.00 eV)
L+1 (-2.43 eV)
L (-2.83 eV)
H (-4.11 eV)
H-1 (-5.07 eV)
H-2 (-5.23 eV)
H-3 (-6.05 eV)
H-4 (-6.56 eV)
H-5 (-7.16 eV)

Column 5 (A1A2A3):
L+5 (-0.41 eV)
L+4 (-0.97 eV)
L+3 (-1.19 eV)
L+2 (-1.84 eV)
L+1 (-2.34 eV)
L (-2.73 eV)
H (-3.91 eV)
H-1 (-5.07 eV)
H-2 (-5.73 eV)
H-3 (-5.88 eV)
H-4 (-6.53 eV)
H-5 (-6.81 eV)

Column 6 (A1[H_N]A3[P_N]):
L+5 (0.21 eV)
L+4 (0.18 eV)
L+3 (-0.74 eV)
L+2 (-1.05 eV)
L+1 (-1.76 eV)
L (-2.47 eV)
H (-3.67 eV)
H-1 (-3.78 eV)
H-2 (-4.80 eV)
H-3 (-5.75 eV)
H-4 (-6.10 eV)
H-5 (-6.35 eV)

Column labels: A1[H_B P_B]   A1A2A3   A1A2A3   A3[H_N P_B]   A1A2A3   A1[H_N]A3[P_N]

Figure S5 The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of A1A2A3, A1[H_B P_B], A3[H_B P_N] and A1[H_N]A3[P_N] predicted with B3LYP/6-31G (d, p).
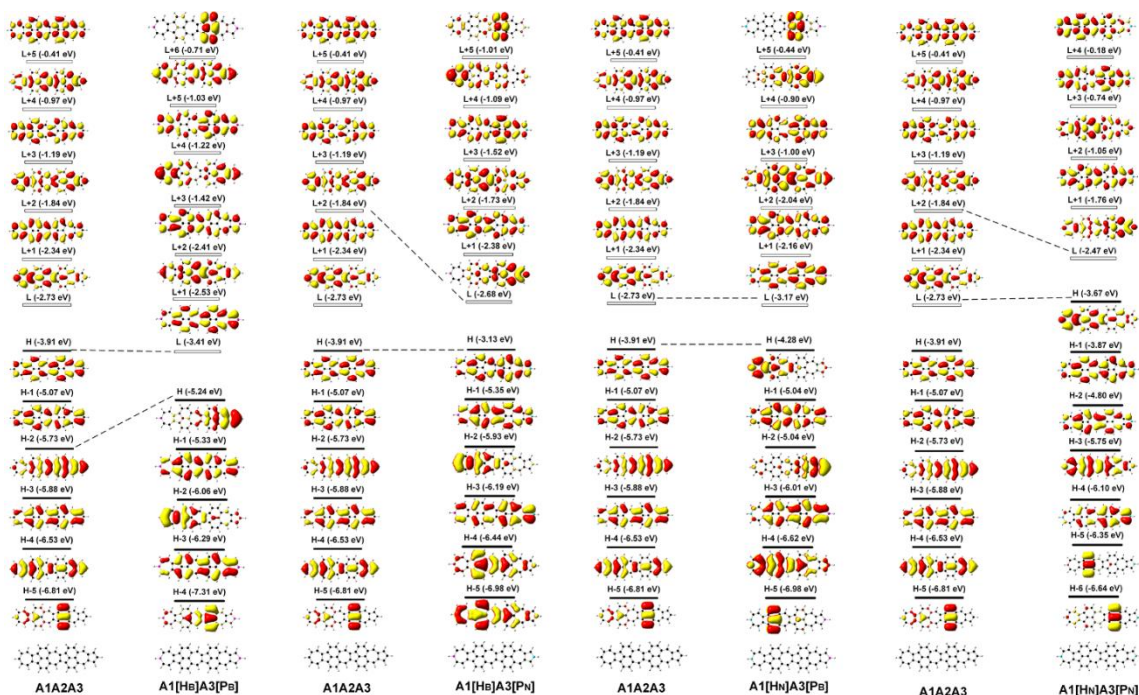
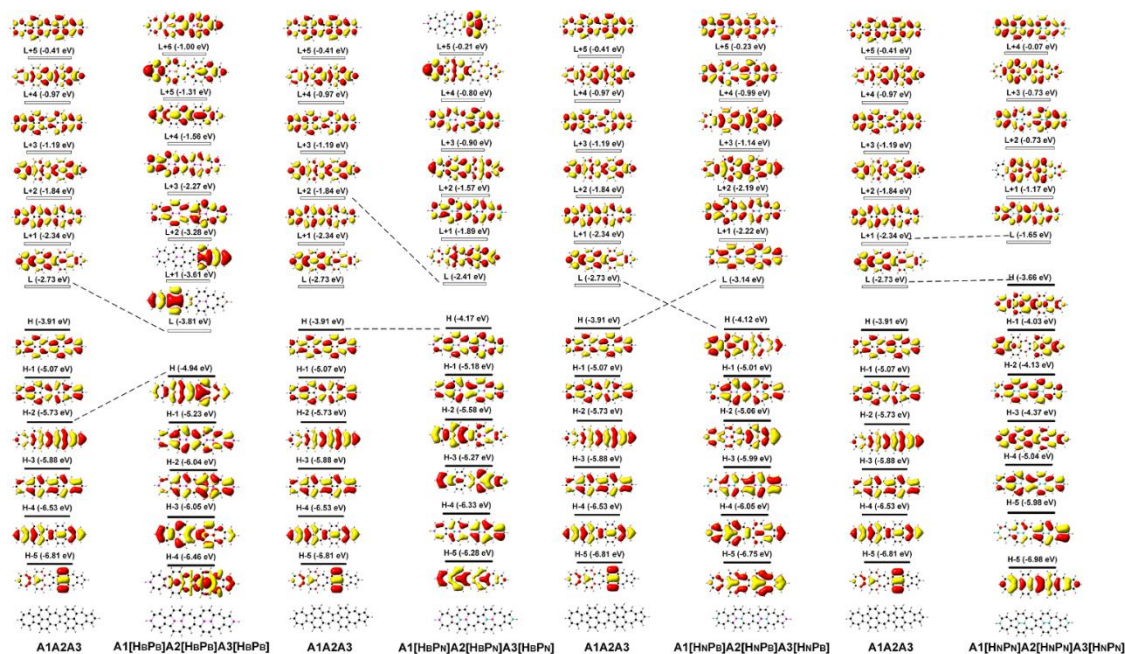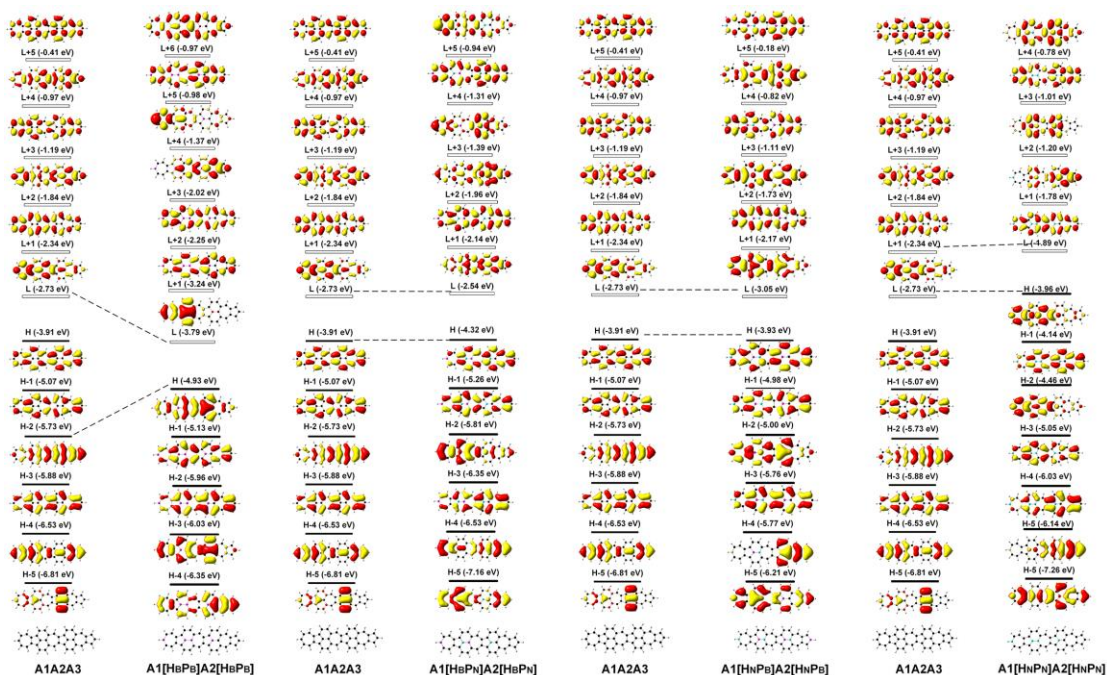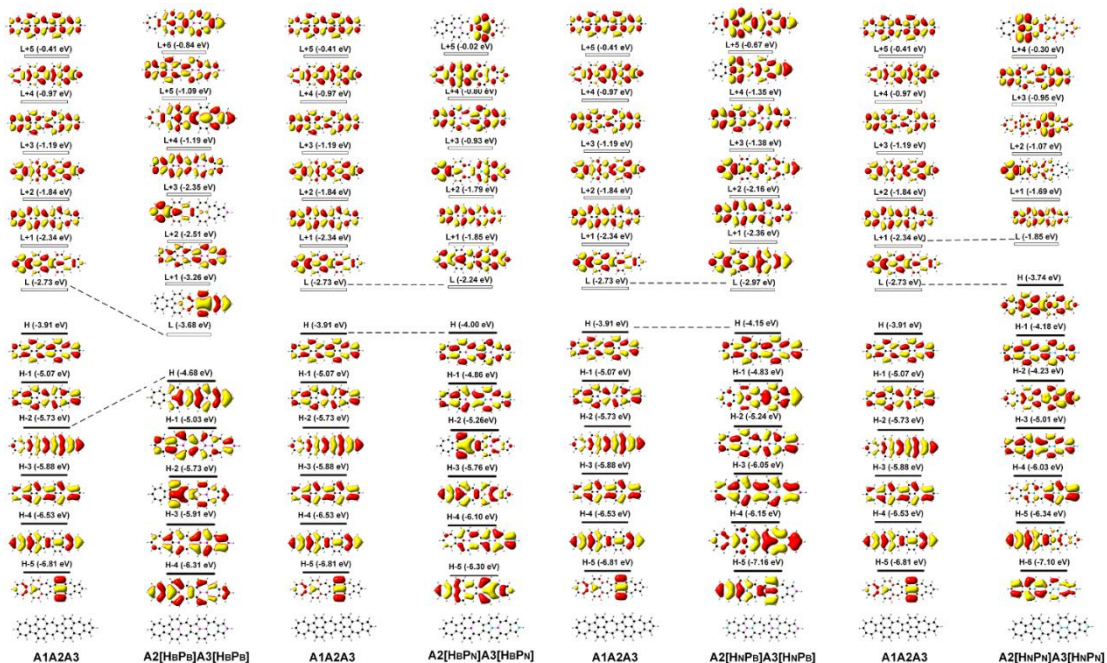**Figure S6** Two-dimensional second order NLO spectra predicted with TD-CAM-B3LYP/6-31++G (d, p)-SOS [damping coefficients $\Gamma_m = 0.01 \times \varepsilon_m/\varepsilon_2$] of (a) A3[$H_N P_N$], (b), (c), (d) A1[$H_N$]A3[$P_N$], and (e) A1[$H_N$]A2[$H_N P_N$]A3[$P_N$] with step size of 0.005 eV. (a) ω_1 scanned from -0.50 eV to 0.50 eV and ω_2 scanned from 2.00 eV to 3.00 eV; (b) ω_1 scanned from -0.50 eV to 0.50 eV and ω_2 scanned from 1.50 eV to 2.50 eV; (c) ω_1 scanned from 0.50 eV to 1.50 eV and ω_2 scanned from 0.50 eV to 1.50 eV; (d) ω_1 scanned from -1.50 eV to -0.50 eV and ω_2 scanned from 1.50 eV to 2.50 eV; (e) ω_1 scanned from -0.50 eV to 0.50 eV and ω_2 scanned from 2.00 eV to 3.00 eV.

TPA: a) TPA at 1.80 eV
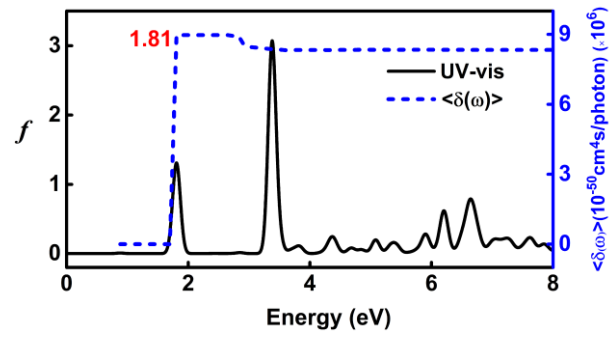
b) TPA at 3.35 eV
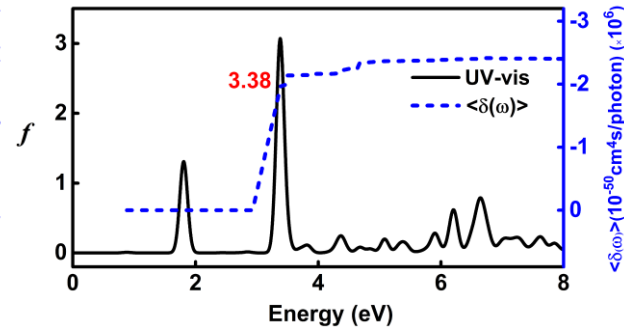
c) TPA at 3.40 eV
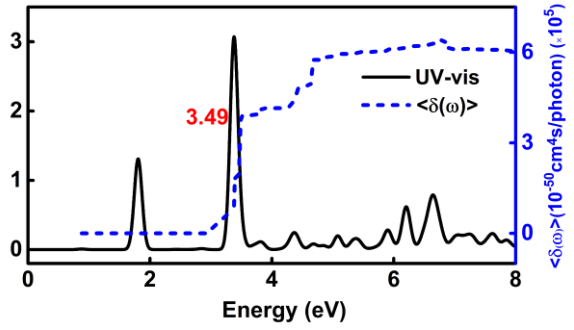
DFWM: a) DFWM at 1.80 eV
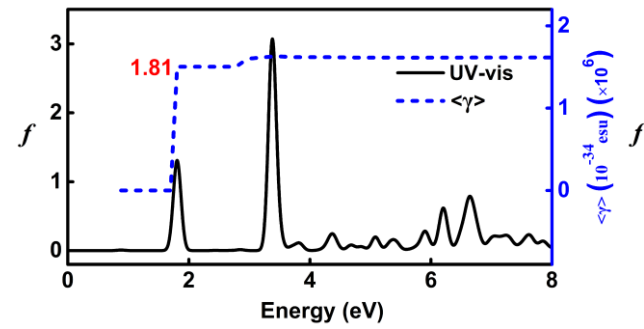
b) DFWM at 3.35 eV
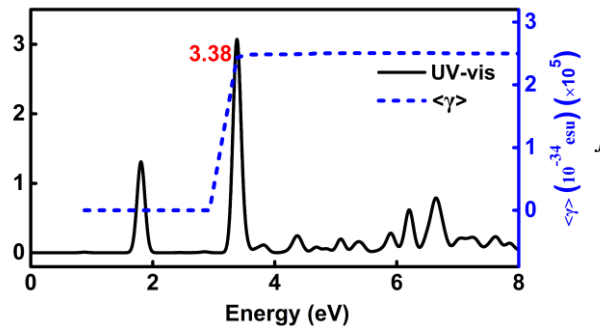
c) DFWM at 3.40 eV
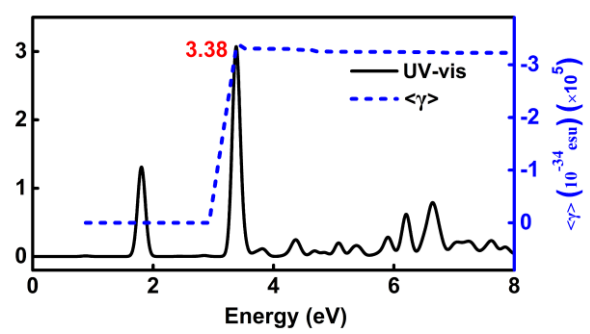
THG: a) THG at 1.75 eV
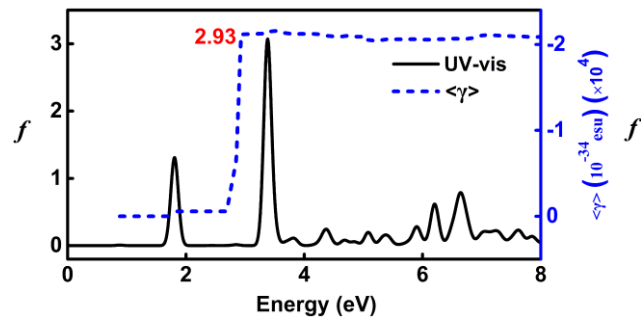
b) THG at 1.80 eV
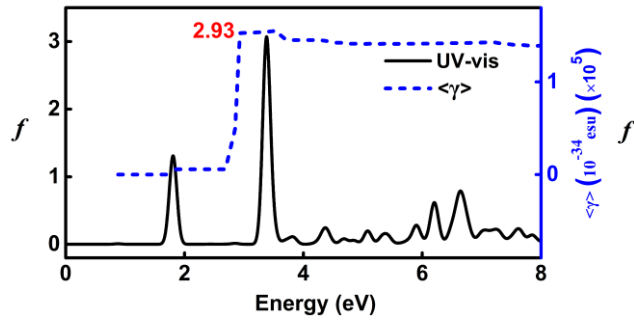
c) THG at 1.85 eV
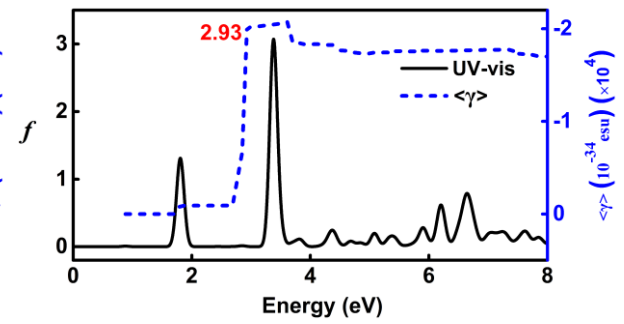
d) THG at 3.40 eV
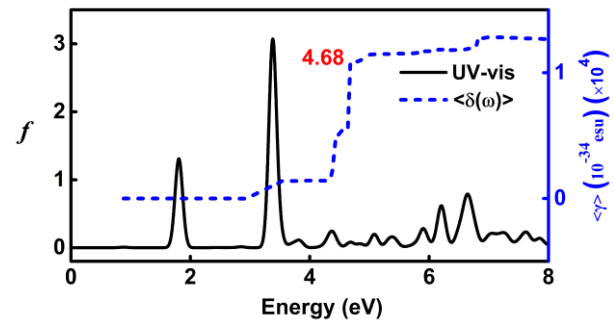
EFISH: a) EFISH at 0.90 eV
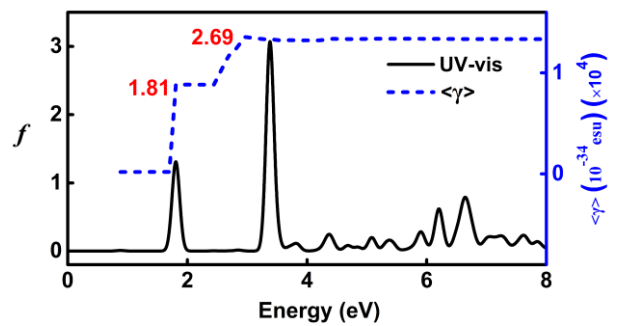
b) EFISH at 1.80 eV
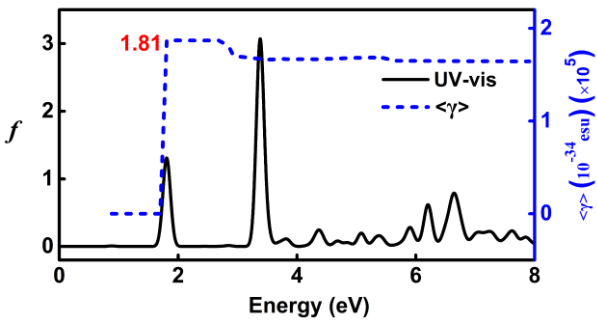
c) EFISH at 3.35 eV
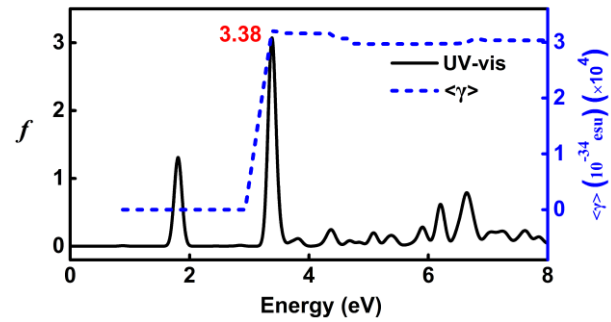
d) EFISH at 3.40 eV
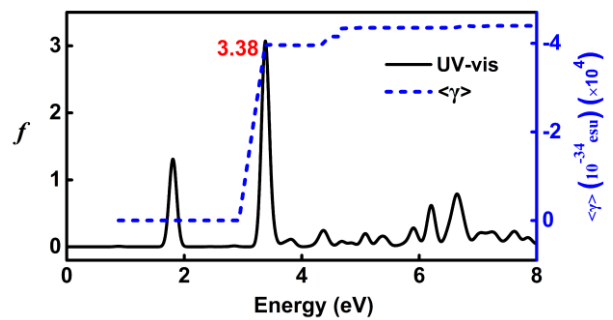
Figure S7 Evolution of third-order nonlinear optic properties with electronic spectra of A1A2A3 at specific external fields.

TPA: a) TPA at 1.15 eV
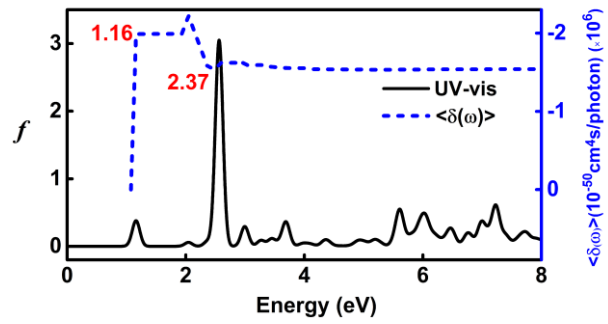
b) TPA at 2.50 eV
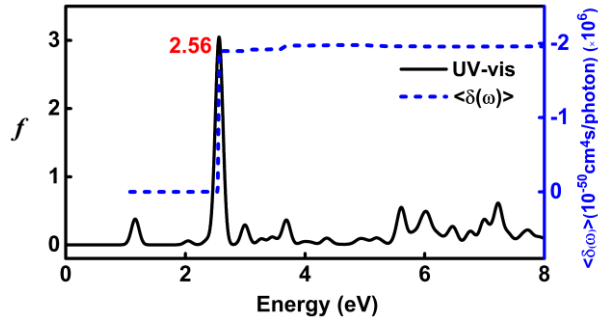
c) TPA at 2.55 eV
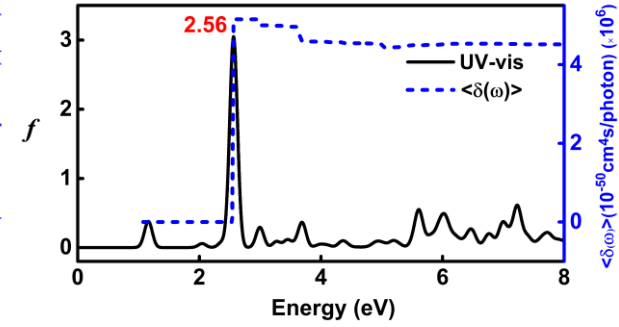
d) TPA at 2.60 eV
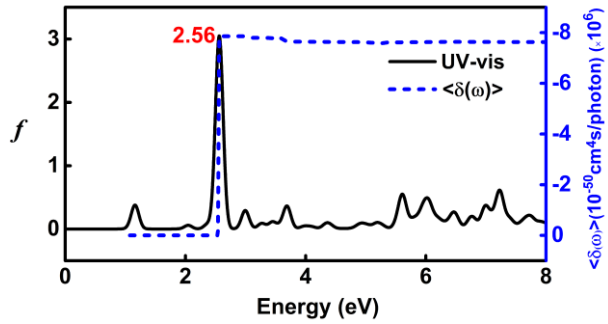
DFWM: a) DFWM at 1.15 eV
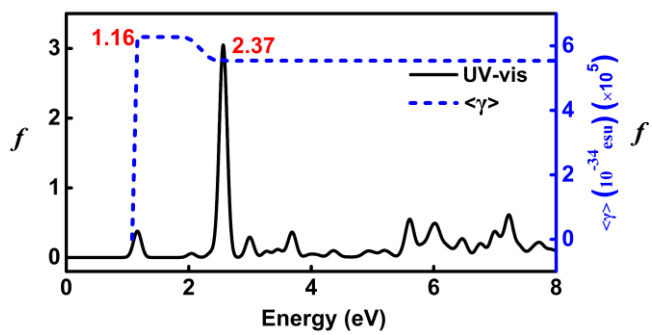
b) DFWM at 2.55 eV
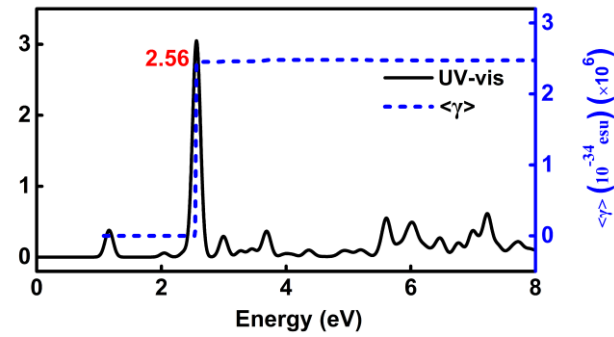
THG: a) THG at 1.05 eV
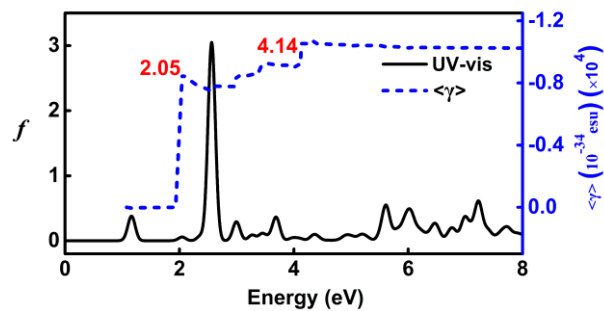
b) THG at 2.55 eV
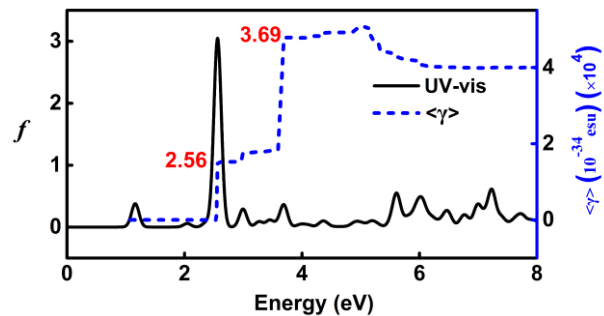
EFISH: a) EFISH at 1.15 eV
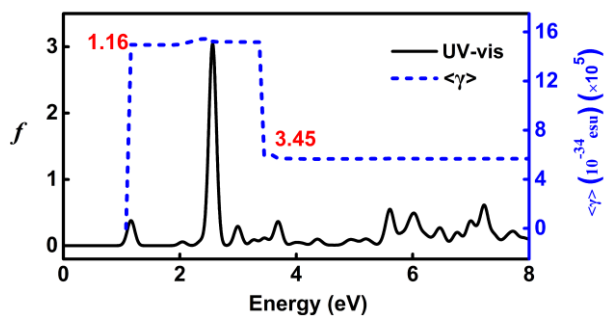
b) EFISH at 2.05 eV
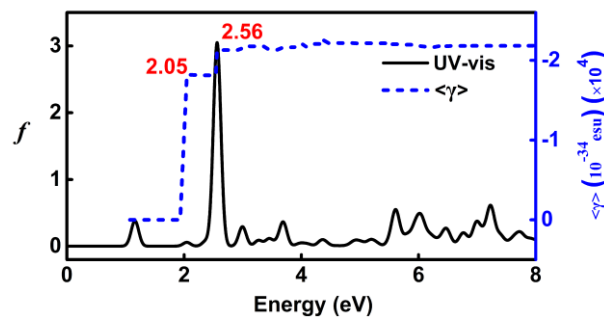
c) EFISH at 2.55 eV
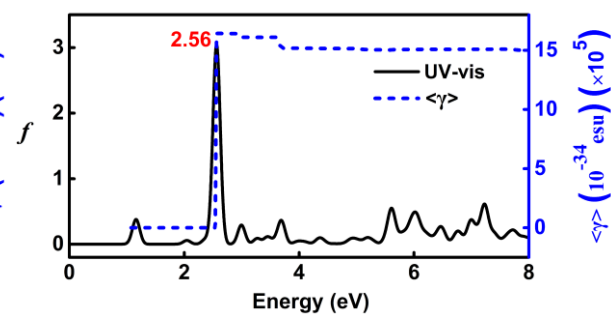
Figure S8 Evolution of third-order nonlinear optic properties with electronic spectra for A1[H_N]A2[H_NP_N]A3[P_N] at specific external fields.
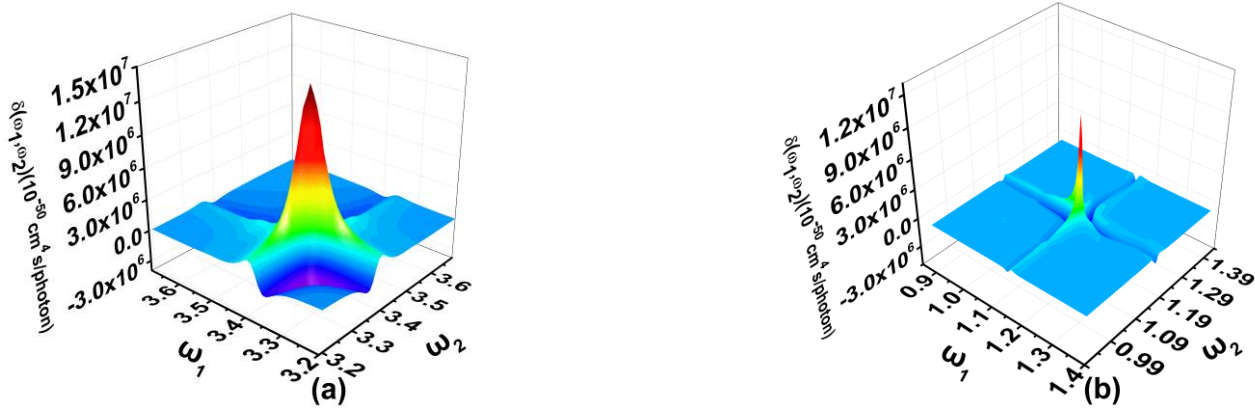
Figure S9 (a) Fine-scanned TDTPA of A1A2A3 and A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] from 3.20 eV to 3.70 eV. (b) Fine-scanned TDTPA of A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$] from 0.90 eV to 1.40 eV.

Table S1 The relative energy (ΔE with respect to the most stable isomer ΔE = 0, in eV), the lowest vibrational frequency (LVF, in cm⁻¹), energy gap (E_gap, in eV) between the HOMO (E_H, in eV) and the LUMO (E_L, in eV), the static first and second hyperpolarizability (<β₀> and <γ₀>), the <β₀> (in 10^{-30} esu) and <γ₀> (in 10^{-34} esu) per heavy atom (<β₀>/N and <γ₀>/N) of A1A2A3 and its N-doped series of molecules in closed-shell singlet predicted with B3LYP/6-31G (d, p) and TD-CAM-B3LYP/6-31++G (d, p)-SOS, respectively. The relative electronic energy differences (ΔE_OS–CS and ΔE_T–CS, in kcal/mol) between open-shell singlet (OS) or triplet (T) and closed-shell singlet (CS) (CS is taken as reference), and spin contamination of open-shell singlet (<S²>_OS) obtained at the UB3LYP/6-31G (d, p) level.

Compounds	ΔE (eV)	LVF (cm⁻¹)	ΔE_OS-CS (Kcal/mol)	ΔE_T-CS (Kcal/mol)	<S²>_OS	E_H (eV)	E_L (eV)	E_gap (eV)	D_g/Debye	<β₀>/(<β₀>/N) (10^{-30} esu)	<γ₀>/(<γ₀>/N) (10^{-30} esu)	<γ₀>_3L/<γ₀>_4L (10^{-34} esu)
A1A2A3	/	16.98	0.00	6.03	0.00	−3.91	−2.73	1.18	6.48	1808.94/47.60	−21.74/−0.57	−34.77/13.03
A1[H_BP_B] (C_2V)	0.95	15.87	0.00	11.13	0.00	−4.68	−3.54	1.13	11.93	1151.11/30.29	−22.37/−0.59	−39.97/17.60
A2[H_BP_B] (C_2V)	0.91	15.12	0.00	8.79	0.00	−4.63	−3.20	1.43	3.42	123.52/3.25	−11.17/−0.03	−28.77/17.60
A1[H_BP_B]A2[H_BP_B] (C_S)	1.24	9.42	−0.71	9.52	0.21	−4.93	−3.79	1.14	3.11	/	/	/
A2[H_BP_B]A3[H_BP_B] (C_S)	1.09	16.57	−2.55	0.41	0.87	−4.71	−3.49	1.22	6.14	/	/	/
A1[H_BP_N] (C_2V)	0.13	16.86	0.00	10.89	0.00	−4.13	−2.68	1.45	0.65	683.83/17.99	−13.08/−0.34	−26.70/13.62
A1[H_NP_B] (C_2V)	1.40	16.85	0.00	1.85	0.00	−3.87	−2.82	1.05	10.66	/	/	/
A2[H_BP_N] (C_2V)	0.29	16.61	0.00	18.71	0.00	−4.14	−2.39	1.75	0.71	1.77/0.05	−4.91/−0.13	−17.70/12.79
A2[H_NP_B] (C_2V)	2.04	14.66	−0.01	3.73	0.00	−3.99	−2.85	1.14	8.7	/	/	/
A1[H_BP_N]A2[H_BP_N] (C_2V)	0.11	16.84	0.00	17.68	0.00	−4.32	−2.54	1.78	6.24	326.51/8.59	−5.03/−0.13	−16.06/11.03
A1[H_NP_B]A2[H_NP_B] (C_2V)	3.14	14.89	−6.12	−4.32	1.21	−3.93	−3.05	0.88	12.65	/	/	/
A2[H_BP_N]A3[H_BP_N] (C_2V)	0.00	16.34	0.00	16.69	0.00	4.00	−2.24	1.76	7.24	90.91/2.39	−4.47/−0.12	−15.70/11.23
A2[H_NP_B]A3[H_NP_B] (C_2V)	3.10	15.56	−1.44	2.81	0.63	−4.15	−2.97	1.18	13.20	/	/	/
A1[H_B]A2[H_NP_B]A3[P_N] (C_S)	3.38	14.52	−0.78	1.26	0.43	−3.92	−2.95	0.97	15.13	/	/	/
A1[H_N]A2[H_BP_N]A3[P_B] (C_S)	3.33	16.56	0.00	−9.14	0.00	−4.02	−3.45	0.58	5.36	/	/	/
A1[H_NP_N] (C_2V)	0.00	17.15	0.00	13.77	0.00	−3.88	−2.23	1.64	8.19	−139.91/−3.68	−6.71/−0.18	−23.66/16.94
A2[H_NP_N] (C_2V)	0.75	14.37	0.00	18.91	0.00	−4.08	−2.07	2.01	2.66	−951.47/−25.04	1.43/0.04	−18.65/20.08
A1[H_NP_N]A2[H_NP_N] (C_2V)	1.47	14.03	0.00	20.53	0.00	−3.96	−1.89	2.07	4.70	−803.74/−21.15	−4.38/−0.12	−11.78/7.40
A2[H_NP_N]A3[H_NP_N] (C_2V)	1.92	13.72	0.00	16.61	0.00	−3.74	−1.85	1.89	3.60	−341.59/−8.99	−2.24/−0.06	−8.26/6.40

Table S2 Major absorption peaks with transition nature in azulene-based molecules (f is the oscillator strength in the arbitrary unit, E is the transition energy in eV unit, λ is the wavelength in nm unit, TNMC to $<\beta_0>$ is the transition nature of electron excitation with a major contribution to $<\beta_0>$, $<\beta_0>_{Con}$ is contribution value to $<\beta_0>$ in 10^{-30} esu).

Compounds	f	E	λ	Transition	TNMC to $<\beta_0>$	$<\beta_0>_{Con}$
A3[$H_N P_N$]	2.9897	2.52	492.90	$S_0 \to S_5$	H−1→L+1 (49.4%) H→L (46.5%)	2498.26
A1[H_N]A3[P_N]	2.3376	2.31	536.03	$S_0 \to S_5$	H−1→L+1 (52.0%) H→L (41.9%)	2706.72
A1[H_N]A2[$H_N P_N$]A3[P_N]	0.3753	1.16	1067.72	$S_0 \to S_2$	H→L (81.2%) H−1→L+1 (17.8%)	1156.25
	3.0497	2.56	483.88	$S_0 \to S_9$	H−1→L+1 (72.9%) H→L (20.4%)	847.17

Table S3 Calculated important parameters of $(\beta_{ijk})_m$ [i, j, k $\in$ (x, y, z)] ($\times 10^{-30}$ esu) of azulene-based molecules. The $(\beta_{ijk})_m$ is the first hyperpolarizability tensor of the mth excited state (S_m) with a major contribution to the static first hyperpolarizability ($<\beta_0>$), m = 0 is the ground state, and m > 0 is the mth excited state.

Structures ($<\beta_0>$)	$(\beta_{zzz})_m$	$(\beta_{YYY})_m$	$(\beta_{xxx})_m$	S_m	E_m	State dipole moment				Transition dipole moment			
						X	Y	Z	tot	X	Y	Z	tot
A3[$H_N P_N$] (3002.80)				S_0		0.00	0.00	−1.40	1.40				
	−2579.90	0.00	0.00	S_5 [$S_0 \to S_5$]	2.52	0.00	0.00	20.16	20.16	0.00	0.00	17.72	17.72
A1[H_N]A3[P_N] (3469.37)				S_0		0.00	0.00	10.35	10.35				
	2899.75	0.00	0.00	S_5 [$S_0 \to S_5$]	2.31	0.00	0.00	−12.86	12.86	0.00	0.00	16.34	16.34
A1[H_N]A2[$H_N P_N$]A3 [P_N] (2106.08)				S_0		0.00	0.00	5.54	5.54				
	1156.25	0.00	0.00	S_2 [$S_0 \to S_2$]	1.16	0.00	0.00	−2.28	2.28	0.00	0.00	−9.24	9.24
	847.17	0.00	0.00	S_9 [$S_0 \to S_9$]	2.56	0.00	0.00	−2.03	2.03	0.00	0.00	17.73	17.73
A1A2A3 (1808.94)				S_0		0.00	0.00	−7.99	7.99				
	−1205.81	0.00	0.00	S_3 [$S_0 \to S_3$]	1.81	0.00	0.00	0.46	0.46	0.00	0.00	14.11	14.11
	−470.71	0.00	0.00	S_8 [$S_0 \to S_8$]	3.38	0.00	0.00	1.59	1.59	0.00	0.00	15.49	15.49

(1) A3[$H_N P_N$]:

$$\beta_{ZZZ}[S_0 \to S_5] = 6 \times \frac{17.72 \times [20.16 - (-1.40)] \times (-17.72)}{2.52^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu = -2492.31 \times 10^{-30} esu$$

(2) A1[H_N]A3[P_N]:

$$\beta_{ZZZ}[S_0 \to S_5] = 6 \times \frac{16.34 \times [(-12.86) - 10.35] \times (-16.34)}{2.31^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu = 2715.07 \times 10^{-30} esu$$

(3) A1[H_N]A2[$H_N P_N$]A3[P_N]:

$$\beta_{ZZZ}[S_0 \to S_2] = 6 \times \frac{(-9.24) \times [(-2.28) - 5.54] \times 9.24}{1.16^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu = 1160.01 \times 10^{-30} esu$$

$$\beta_{ZZZ}[S_0 \to S_9] = 6 \times \frac{17.73 \times [(-2.03) - 5.54] \times (-17.73)}{2.56^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu = 848.91 \times 10^{-30} esu$$

(4) A1A2A3:

$$\beta_{ZZZ}[S_0 \to S_3] = 6 \times \frac{14.11 \times [0.46 - (-7.99)] \times (-14.11)}{1.81^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu = -1200.55 \times 10^{-30} esu$$

$$\beta_{ZZZ}[S_0 \to S_8] = 6 \times \frac{15.49 \times [1.59 - (-7.99)] \times (-15.49)}{3.38^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu = -470.39 \times 10^{-30} esu$$

Table S4 Major electron excitations with transition nature in A1[H_N]A3[P_N], A1[H_N]A2[H_NP_N]A3[P_N] and A1A2A3. The f is the oscillator strength, λ is the wavelength, and TNMC to $\langle\gamma_0\rangle_{3L}$ is the transition nature of electron excitation with a major contribution to $\langle\gamma_0\rangle_{3L}$.

Compounds	f	E	λ	Transition	TNMC to $\langle\gamma_0\rangle_{3L}$	[$\langle\gamma_0\rangle_{3L}$]$_{Con}$
A1[H_N]A3[P_N]	2.34	2.31	536.03	$S_0{\rightarrow}S_5$	H−1→L+1 (52.0%) H→L (41.9%)	−10.67
	1.83	3.27	378.94	$S_0{\rightarrow}S_{10}$	H→L+2 (35.8%) H−3→L (29.6%)	−6.62
A1[H_N]A2[H_NP_N]A3[P_N]	0.3753	1.16	1067.72	$S_0{\rightarrow}S_2$	H→L (81.2%) H−1→L+1 (17.8%)	−9.22
	3.0497	2.56	483.88	$S_0{\rightarrow}S_9$	H−1→L+1 (72.9%) H→L (20.4%)	−35.04
A1A2A3	1.3624	1.81	686.50	$S_0{\rightarrow}S_3$	H→L+1 (91.9%)	−13.46
	3.0711	3.38	367.00	$S_0{\rightarrow}S_8$	H−2→L+1 (71.2%)	−16.09

Table S5 Calculated important parameters of $(\gamma_{ijk})_m$ (× 10^{-34} esu) of azulene-based molecules. The $(\gamma_{ijk})_m$ is the second hyperpolarizability tensor of the mth excited state (S_m) with a major contribution to the static first hyperpolarizability ($\langle\beta_0\rangle$), m = 0 is the ground state, and m > 0 is the mth excited state.

Structures ($\langle\gamma_0\rangle_{3L}$)	$(\gamma_{zzzz})_{3Lm}$ (Contribution)	S_m	E_m	State dipole moment				Transition dipole moment			
				X	Y	Z	tot	X	Y	Z	tot
A1[H_N]A2[H_NP_N] A3[P_N] (−59.80)		S_0		0.00	0.00	5.54	5.54				
		S_1 [$S_0{\rightarrow}S_1$]	1.07	0.00	0.00	6.36	6.36	0.00	1.51	0.00	1.51
	−45.19	S_2 [$S_0{\rightarrow}S_2$]	1.16	0.00	0.00	−2.28	2.28	0.00	0.00	−9.24	9.24
		S_3 [$S_0{\rightarrow}S_3$]	1.25	0.00	0.00	−1.38	1.38	0.00	−0.01	0.00	0.01
		S_4 [$S_0{\rightarrow}S_4$]	1.93	0.00	0.00	0.30	0.30	0.00	−0.48	0.00	0.48
		S_5 [$S_0{\rightarrow}S_5$]	2.05	0.00	0.00	−8.84	8.84	0.00	0.00	−2.74	2.74
		S_6 [$S_0{\rightarrow}S_6$]	2.37	0.00	0.00	−1.01	1.01	0.00	0.00	−2.88	2.88
		S_7 [$S_0{\rightarrow}S_7$]	2.44	0.00	0.00	1.45	1.45	0.00	−0.002	0.00	0.002
		S_8 [$S_0{\rightarrow}S_8$]	2.54	0.00	0.00	3.36	3.36	0.00	−0.56	0.00	0.56
	−174.01	S_9 [$S_0{\rightarrow}S_9$]	2.56	0.00	0.00	−2.03	2.03	0.00	0.00	17.73	17.73
A1A2A3 (−37.30)		S_0		0.00	0.00	−7.99	7.99				
		S_1 [$S_0{\rightarrow}S_1$]	0.88	0.00	0.00	2.64	2.64	0.00	−1.62	0.00	1.62
		S_2 [$S_0{\rightarrow}S_2$]	1.70	0.00	0.00	−1.43	1.43	0.00	−0.27	0.00	0.27
	−65.46	S_3 [$S_0{\rightarrow}S_3$]	1.81	0.00	0.00	0.46	0.46	0.00	0.00	14.11	14.11
		S_4 [$S_0{\rightarrow}S_4$]	2.44	0.00	0.00	−3.71	3.71	0.00	0.57	0.00	0.57
		S_5 [$S_0{\rightarrow}S_5$]	2.69	0.00	0.00	7.93	7.93	0.00	−0.49	0.00	0.49
		S_6 [$S_0{\rightarrow}S_6$]	2.85	0.00	0.00	−1.78	1.78	0.00	0.00	1.17	1.17
		S_7 [$S_0{\rightarrow}S_7$]	2.93	0.00	0.00	−2.39	2.39	0.00	0.00	0.08	0.08
	−79.45	S_8 [$S_0{\rightarrow}S_8$]	3.38	0.00	0.00	1.59	1.59	0.00	0.00	15.49	15.49

1. A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$]:

（1）S$_0 \to$S$_2$：

S$_0 \to$S$_1 \to$S$_0 \to$S$_2 \to$S$_0$;　S$_0 \to$S$_2 \to$S$_0 \to$S$_1 \to$S$_0$; S$_0 \to$S$_2 \to$S$_0 \to$S$_2 \to$S$_0$

$$\gamma_{3L(zzzz)(\text{Contribution})}[S_0 \to S_2] \approx -\frac{24}{6}\frac{r_{01}^z r_{10}^z r_{02}^z r_{20}^z}{E_1 E_2^2} - \frac{24}{6}\frac{r_{02}^z r_{20}^z r_{01}^z r_{10}^z}{E_2 E_1^2} - \frac{24}{6}\frac{r_{02}^z r_{20}^z r_{02}^z r_{20}^z}{E_2^3}$$

$$= \left[-4 \times \frac{0 \times 0 \times (-9.24) \times (9.24)}{1.07 \times 1.16^2} - 4 \times \frac{(-9.24) \times (9.24) \times 0 \times 0}{1.16 \times 1.07^2} - 4 \times \frac{(-9.24) \times (9.24) \times (-9.24) \times (9.24)}{1.16^3}\right]$$

$$\times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3} = -45.43 \times 10^{-34}$$

（2）S$_0 \to$S$_9$：

S$_0 \to$S$_1 \to$S$_0 \to$S$_9 \to$S$_0$;　S$_0 \to$S$_9 \to$S$_0 \to$S$_1 \to$S$_0$;　S$_0 \to$S$_2 \to$S$_0 \to$S$_9 \to$S$_0$; S$_0 \to$S$_9 \to$S$_0 \to$S$_2 \to$S$_0$;

S$_0 \to$S$_3 \to$S$_0 \to$S$_9 \to$S$_0$; S$_0 \to$S$_9 \to$S$_0 \to$S$_3 \to$S$_0$;　S$_0 \to$ S$_4 \to$S$_0 \to$ S$_9 \to$S$_0$; S$_0 \to$ S$_9 \to$S$_0 \to$S$_4 \to$S$_0$;

S$_0 \to$ S$_5 \to$S$_0 \to$ S$_9 \to$S$_0$;　S$_0 \to$S$_9 \to$S$_0 \to$S$_5 \to$S$_0$;　S$_0 \to$S$_6 \to$S$_0 \to$S$_9 \to$S$_0$; S$_0 \to$S$_9 \to$S$_0 \to$S$_6 \to$S$_0$;

S$_0 \to$ S$_7 \to$S$_0 \to$ S$_9 \to$S$_0$;　S$_0 \to$S$_9 \to$S$_0 \to$S$_7 \to$S$_0$;　S$_0 \to$S$_8 \to$S$_0 \to$S$_9 \to$S$_0$; S$_0 \to$S$_9 \to$S$_0 \to$S$_8 \to$S$_0$;

S$_0 \to$S$_9 \to$S$_0 \to$S$_9 \to$S$_0$

$$\gamma_{3L(zzzz)(\text{Contribution})}[S_0 \to S_9] \approx -\frac{24}{6}\frac{r_{01}^z r_{10}^z r_{09}^z r_{90}^z}{E_1 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{01}^z r_{10}^z}{E_9 E_1^2} - \frac{24}{6}\frac{r_{02}^z r_{20}^z r_{09}^z r_{90}^z}{E_2 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{02}^z r_{20}^z}{E_9 E_2^2} - \frac{24}{6}\frac{r_{03}^z r_{30}^z r_{09}^z r_{90}^z}{E_3 E_9^2} -$$

$$\frac{24}{6}\frac{r_{09}^z r_{90}^z r_{03}^z r_{30}^z}{E_9 E_3^2} - \frac{24}{6}\frac{r_{04}^z r_{40}^z r_{09}^z r_{90}^z}{E_4 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{04}^z r_{40}^z}{E_9 E_4^2} - \frac{24}{6}\frac{r_{05}^z r_{50}^z r_{09}^z r_{90}^z}{E_5 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{05}^z r_{50}^z}{E_9 E_5^2} - \frac{24}{6}\frac{r_{06}^z r_{60}^z r_{09}^z r_{90}^z}{E_6 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{06}^z r_{60}^z}{E_9 E_6^2} -$$

$$\frac{24}{6}\frac{r_{07}^z r_{70}^z r_{09}^z r_{90}^z}{E_7 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{07}^z r_{70}^z}{E_9 E_7^2} - \frac{24}{6}\frac{r_{08}^z r_{80}^z r_{09}^z r_{90}^z}{E_8 E_9^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{08}^z r_{80}^z}{E_9 E_8^2} - \frac{24}{6}\frac{r_{09}^z r_{90}^z r_{09}^z r_{90}^z}{E_9^3}$$

$$= \left[-4 \times \frac{0 \times 0 \times (17.73) \times (-17.73)}{1.07 \times 2.56^2} - 4 \times \frac{(17.73) \times (-17.73) \times 0 \times 0}{2.56 \times 1.07^2} - 4 \times \frac{(-9.24) \times (9.24) \times (17.73) \times (-17.73)}{1.16 \times 2.56^2} - 4 \times\right.$$

$$\frac{(17.73) \times (-17.73) \times (-9.24) \times (9.24)}{2.56 \times 1.16^2} - 4 \times \frac{0 \times 0 \times (17.73) \times (-17.73)}{1.25 \times 2.56^2} - 4 \times \frac{(17.73) \times (-17.73) \times 0 \times 0}{1.93 \times 1.07^2} - 4 \times \frac{0 \times 0 \times (17.73) \times (-17.73)}{1.93 \times 2.56^2} - 4 \times$$

$$\frac{(17.73) \times (-17.73) \times 0 \times 0}{1.25 \times 1.07^2} - 4 \times \frac{(-2.74) \times (2.74) \times (17.73) \times (-17.73)}{2.04 \times 2.56^2} - 4 \times \frac{(17.73) \times (-17.73) \times (-2.74) \times (2.74)}{2.56 \times 2.04^2} - 4 \times$$

$$\frac{(-2.88) \times (2.88) \times (17.73) \times (-17.73)}{2.37 \times 2.56^2} - 4 \times \frac{(17.73) \times (-17.73) \times (-2.88) \times (2.88)}{2.56 \times 2.37^2} - 4 \times \frac{0 \times 0 \times (17.73) \times (-17.73)}{2.44 \times 2.56^2} - 4 \times \frac{(17.73) \times (-17.73) \times 0 \times 0}{2.56 \times 2.44^2} -$$

$$\left. 4 \times \frac{0 \times 0 \times (17.73) \times (-17.73)}{2.53 \times 2.56^2} - 4 \times \frac{(17.73) \times (-17.73) \times 0 \times 0}{2.53 \times 1.07^2} - 4 \times \frac{(17.73) \times (-17.73) \times (17.73) \times (-17.73)}{2.56^3}\right] \times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3}$$

$$= [-14121.59 - 31164.88 - 706.10 - 886.09 - 671.48 - 725.31 - 23559.99] \times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3}$$

$$= -174.72 \times 10^{-34}$$

2. A1A2A3:

(1) S$_0 \to$S$_3$：

S$_0 \to$S$_1 \to$S$_0 \to$S$_3 \to$S$_0$;　S$_0 \to$S$_3 \to$S$_0 \to$S$_1 \to$S$_0$;　S$_0 \to$ S$_2 \to$S$_0 \to$S$_3 \to$S$_0$; S$_0 \to$S$_3 \to$S$_0 \to$S$_2 \to$S$_0$;

S$_0 \to$S$_3 \to$S$_0 \to$S$_3 \to$S$_0$

$$\gamma_{3L(zzzz)(\text{Contribution})}[S_0 \to S_3] \approx -\frac{24}{6}\frac{r_{01}^z r_{10}^z r_{03}^z r_{30}^z}{E_1 E_3^2} - \frac{24}{6}\frac{r_{03}^z r_{30}^z r_{01}^z r_{10}^z}{E_3 E_1^2} - \frac{24}{6}\frac{r_{02}^z r_{20}^z r_{03}^z r_{30}^z}{E_2 E_3^2}$$

$$-\frac{24}{6}\frac{r_{03}^z r_{30}^z r_{02}^z r_{20}^z}{E_3 E_2^2} - \frac{24}{6}\frac{r_{03}^z r_{30}^z r_{03}^z r_{30}^z}{E_3^3}$$

$$= \left[-4 \times \frac{0 \times 0 \times (14.11) \times (-14.11)}{0.88 \times 1.81^2} - 4 \times \frac{(14.11) \times (-14.11) \times 0 \times 0}{1.81 \times 0.88^2} - 4 \times \frac{0 \times 0 \times (14.11) \times (-14.11)}{1.70 \times 1.81^2} - 4\right.$$

$$\times \frac{(14.11) \times (-14.11) \times 0 \times 0}{1.81 \times 1.70^2} - 4 \times \frac{(14.11) \times (-14.11) \times (14.11) \times (-14.11)}{1.81^3}\bigg]$$

$$\times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3} = -65.03 \times 10^{-34}$$

（2）$S_0 \rightarrow S_8$：

$S_0 \rightarrow S_1 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$； $S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_1 \rightarrow S_0$； $S_0 \rightarrow S_2 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$；$S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_2 \rightarrow S_0$ ；

$S_0 \rightarrow S_3 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$；$S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_3 \rightarrow S_0$； $S_0 \rightarrow S_4 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$；$S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_4 \rightarrow S_0$；

$S_0 \rightarrow S_5 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$； $S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_5 \rightarrow S_0$； $S_0 \rightarrow S_6 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$；$S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_6 \rightarrow S_0$；

$S_0 \rightarrow S_7 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$； $S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_7 \rightarrow S_0$； $S_0 \rightarrow S_8 \rightarrow S_0 \rightarrow S_8 \rightarrow S_0$

$$\gamma_{3L(zzzz)(\text{Contribution})}[S_0 \rightarrow S_8] \approx -\frac{24}{6}\frac{r_{01}^z r_{10}^z r_{08}^z r_{80}^z}{E_1 E_8^2} - \frac{24}{6}\frac{r_{08}^z r_{80}^z r_{01}^z r_{10}^z}{E_8 E_1^2} - \frac{24}{6}\frac{r_{02}^z r_{20}^z r_{08}^z r_{80}^z}{E_2 E_8^2}$$

$$-\frac{24}{6}\frac{r_{08}^z r_{80}^z r_{08}^z r_{80}^z}{E_8 E_2^2} - \frac{24}{6}\frac{r_{03}^z r_{30}^z r_{08}^z r_{80}^z}{E_3 E_8^2} - \frac{24}{6}\frac{r_{08}^z r_{80}^z r_{03}^z r_{30}^z}{E_8 E_3^2} - \frac{24}{6}\frac{r_{04}^z r_{40}^z r_{08}^z r_{80}^z}{E_4 E_{98}^2}$$

$$-\frac{24}{6}\frac{r_{08}^z r_{80}^z r_{04}^z r_{40}^z}{E_8 E_4^2} - \frac{24}{6}\frac{r_{05}^z r_{50}^z r_{08}^z r_{80}^z}{E_5 E_8^2} - \frac{24}{6}\frac{r_{08}^z r_{80}^z r_{05}^z r_{50}^z}{E_8 E_5^2} - \frac{24}{6}\frac{r_{06}^z r_{60}^z r_{08}^z r_{80}^z}{E_6 E_8^2} - \frac{24}{6}\frac{r_{08}^z r_{80}^z r_{06}^z r_{60}^z}{E_8 E_6^2} - \frac{24}{6}\frac{r_{07}^z r_{70}^z r_{08}^z r_{80}^z}{E_7 E_8^2}$$

$$-\frac{24}{6}\frac{r_{08}^z r_{80}^z r_{07}^z r_{70}^z}{E_8 E_7^2} - \frac{24}{6}\frac{r_{08}^z r_{80}^z r_{08}^z r_{80}^z}{E_8^3}$$

$$= \Big[-4 \times \frac{0\times0\times(15.49)\times(-15.49)}{0.88\times3.38^2} - 4 \times \frac{(15.49)\times(-15.49)\times0\times0}{3.38\times0.88^2} - 4 \times \frac{0\times0\times(15.49)\times(-15.49)}{1.70\times3.38^2} - 4 \times \frac{(15.49)\times(-15.49)\times0\times0}{3.38\times1.70^2} - 4 \times$$
$$\frac{(14.11)\times(-14.11)\times(15.49)\times(-15.49)}{1.81\times3.38^2} - 4 \times \frac{(15.49)\times(-15.49)\times(14.11)\times(-14.11)}{3.38\times1.81^2} - 4 \times \frac{0\times0\times(15.49)\times(-15.49)}{2.44\times3.38^2} - 4 \times$$
$$\frac{(15.49)\times(-15.49)\times0\times0}{3.38\times2.44^2} - 4 \times \frac{0\times0\times(15.49)\times(-15.49)}{2.69\times3.38^2} - 4 \times \frac{(15.49)\times(-15.49)\times0\times0}{3.38\times2.69^2} - 4 \times \frac{(1.17)\times(-1.17)\times(15.49)\times(-15.49)}{2.85\times3.38^2} - 4 \times$$
$$\frac{(15.49)\times(-15.49)\times(1.17)\times(-1.17)}{3.38\times2.85^2} - 4 \times \frac{(0.08)\times(-0.08)\times(15.49)\times(-15.49)}{2.93\times3.38^2} - 4 \times \frac{(15.49)\times(-15.49)\times(0.08)\times(-0.08)}{3.38\times2.93^2} - 4 \times$$
$$\frac{(15.49)\times(-15.49)\times(15.49)\times(-15.49)}{3.38^3} \Big] \times \frac{(10^{-18})^4}{(1.602\times10^{-12})^3}$$

$$= [-9240.70 - 17256.11 - 40.35 - 47.86 - 0.18 - 0.21 - 5963.70] \times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3}$$

$$= -79.17 \times 10^{-34}$$

Table S6 The strong response and corresponding major electron excitations contribution of the dynamic third-order nonlinear optic response for A1A2A3.

processes	External Field/eV (λ/nm)	Responses	Major Electron Excitations Contribution
TPA	1.80 (688.89)	8246230	1.81 eV (685.08 nm) (8970470.13)
δ(−ω; ω, −ω, ω)	3.35 (370.15)	−2422840	3.38 eV (366.86 nm) (−1934184.57)
	3.40 (364.71)	−299153	3.49 eV (355.30 nm) (196126)
DFWM	1.80 (688.89)	1620790	1.81 eV (685.08 nm) (1503379.96)
γ(−ω; ω, −ω, ω)	3.35 (370.15)	248589	3.38 eV (366.86 nm) (242769.94)
	3.40 (364.71)	−323553	3.38 eV (366.86 nm) (−330511.54)
THG	1.75 (708.57)	−20806	2.93 eV (423.21 nm) (−14600.93)
γ(−3ω; ω, ω, ω)	1.80 (688.89)	137721	2.93 eV (423.21 nm) (103364.40)
	1.85 (670.27)	−16890	2.93 eV (423.21 nm) (−13468.28)
	3.40 (364.71)	12744	4.68 eV (264.96 nm) (5491.28)
EFISH	0.90 (1377.78)	13334	1.81 eV (685.08 nm) (8636.552); 2.69 eV (460.97 nm) (2854.15)
γ(−2ω; ω, ω, 0)	1.80 (688.89)	164880	1.81 eV (685.08 nm) (186926.01)
	3.35 (370.15)	30184	3.38 eV (366.86 nm) (31996.19)
	3.40 (364.71)	−44008	3.38 eV (366.86 nm) (−39667.90)

Table S7 The strong response and corresponding major electron excitations contribution of the dynamic third-order nonlinear optic response of A1[H_N]A2[H_NP_N]A3[P_N].

processes	External Field/eV (λ/nm)	Responses	Major Electron Excitations Contribution
TPA	1.15 (1078.26)	−1540630	1.16 eV (1068.96 nm) (−1988440); 2.37 eV (523.21 nm) (659830)
	2.50 (496)	−1952420	2.56 eV (484.38 nm) (−1896602.722)
δ(−ω; ω, −ω, ω)	2.55 (486.27)	4266100	2.56 eV (484.38 nm) (5148370.36)
	2.60 (476.92)	−7657630	2.60 eV (476.92 nm) (−7859635.83)
DFWM	1.15 (1078.26)	548686	1.16 eV (1068.96 nm) (627263.91); 2.37 eV (523.21 nm) (−60384)
γ(−ω; ω, −ω, ω)	2.55 (486.27)	2467150	2.56 eV (484.38 nm) (2451555.32)
THG	1.05 (1180.95)	−10249	2.05 eV (604.88 nm) (−8535.56); 4.14 eV(299.52 nm) (−1374.66)
γ(−3ω; ω, ω, ω)	2.55 (486.27)	39561	2.56 eV (484.38 nm) (15228.58); 3.69 eV (336.04 nm) (29654.30)
EFISH	1.15 (1078.26)	55719	1.16 eV (1068.96 nm) (149783.01); 3.45 eV (359.42 nm) (−92064.70)
γ(−2ω; ω, ω, 0)	2.05 (604.88)	−21656	2.05 eV (604.88 nm) (−18189.62); 2.56 eV (484.38 nm) (−3165.80)
	2.55 (486.27)	149427	2.56 eV (484.38 nm) (−164192.85)

Cartesian coordinates of all molecules optimized with b3lyp/6-31G(d,p)

A1A2A3

C	0	0	-9.187777
C	0	1.265996	-8.595756
C	0	1.589678	-7.23148
C	0	-1.265996	-8.595756
C	0	0.749116	-6.127958
C	0	-1.589678	-7.23148
C	0	-0.749116	-6.127958
H	0	0	-10.276295
H	0	2.109709	-9.280405
H	0	2.655422	-7.00769
H	0	-2.109709	-9.280405
H	0	-2.655422	-7.00769
C	0	1.165553	-4.766228
C	0	0	-3.950521
C	0	-1.165553	-4.766228
C	0	0	-2.532055
C	0	-1.305082	-1.910542
C	0	1.305082	-1.910542
C	0	-1.580366	-0.518412
C	0	1.580366	-0.518412
C	0	-0.74355	0.575092
H	0	-2.642683	-0.279472
C	0	0.74355	0.575092
H	0	2.642683	-0.279472
C	0	-1.163845	1.943244
C	0	1.163845	1.943244
C	0	0	2.759477
C	0	-2.429854	-4.132841
H	0	-3.353322	-4.704177
C	0	-2.468447	-2.761666
H	0	-3.434671	-2.265396
C	0	2.468447	-2.761666
H	0	3.434671	-2.265396
C	0	2.429854	-4.132841
H	0	3.353322	-4.704177
C	0	0	4.178768
C	0	-1.306075	4.800517
C	0	-1.585021	6.187263
C	0	1.306075	4.800517
C	0	-0.744681	7.285435
C	0	1.585021	6.187263
C	0	0.744681	7.285435
H	0	-2.646903	6.43105
H	0	2.646903	6.43105
C	0	-1.148431	8.638495
C	0	0	9.444565
C	0	1.148431	8.638495
C	0	2.426537	2.573474
C	0	2.46902	3.944852
H	0	3.349235	2.00036
H	0	3.436075	4.439408
C	0	-2.426537	2.573474
C	0	-2.46902	3.944852
H	0	-3.349235	2.00036
H	0	-3.436075	4.439408
H	0	2.176091	8.981712
H	0	0	10.52892
H	0	-2.176091	8.981712

A3[H_BP_B]

C	0	0	-9.13239766
C	0	1.265996	-8.54037666
C	0	1.589678	-7.17610066
C	0	-1.265996	-8.54037666
C	0	0.749116	-6.07257866
C	0	-1.589678	-7.17610066
C	0	-0.749116	-6.07257866
H	0	0	-10.22091566
H	0	2.109709	-9.22502566
H	0	2.655422	-6.95231066
H	0	-2.109709	-9.22502566
H	0	-2.655422	-6.95231066
C	0	1.165553	-4.71084866
C	0	0	-3.89514166
C	0	-1.165553	-4.71084866
C	0	0	-2.47667566
C	0	-1.305082	-1.85516266
C	0	1.305082	-1.85516266
C	0	-1.580366	-0.46303266
C	0	1.580366	-0.46303266
C	0	-0.74355	0.63047134
H	0	-2.642683	-0.22409266
C	0	0.74355	0.63047134
H	0	2.642683	-0.22409266
C	0	-1.163845	1.99862334
C	0	1.163845	1.99862334
C	0	0	2.81485634
C	0	-2.429854	-4.07746166
H	0	-3.353322	-4.64879766
C	0	-2.468447	-2.70628666
H	0	-3.434671	-2.21001666
C	0	2.468447	-2.70628666
H	0	3.434671	-2.21001666
C	0	2.429854	-4.07746166
H	0	3.353322	-4.64879766
C	0	-1.306075	4.85589634
C	0	-1.585021	6.24264234
C	0	1.306075	4.85589634
C	0	-0.744681	7.34081434
C	0	1.585021	6.24264234
C	0	0.744681	7.34081434
H	0	-2.646903	6.48642934
H	0	2.646903	6.48642934
C	0	-1.148431	8.69387434
C	0	1.148431	8.69387434
C	0	2.426537	2.62885334
C	0	2.46902	4.00023134
H	0	3.349235	2.05573934
H	0	3.436075	4.49478734
C	0	-2.426537	2.62885334
C	0	-2.46902	4.00023134
H	0	-3.349235	2.05573934
H	0	-3.436075	4.49478734
H	0	2.176091	9.03709134
H	0	0	10.58429934
H	0	-2.176091	9.03709134
B	0	0	9.49994434
B	0	0	4.23414734

A3[H_NP_N]

A3[H_BP_N]

C	0	0	-9.24227039	C	0	0	-9.20901011
C	0	1.265996	-8.65024939	C	0	1.265996	-8.61698911
C	0	1.589678	-7.28597339	C	0	1.589678	-7.25271311
C	0	-1.265996	-8.65024939	C	0	-1.265996	-8.61698911
C	0	0.749116	-6.18245139	C	0	0.749116	-6.14919111
C	0	-1.589678	-7.28597339	C	0	-1.589678	-7.25271311
C	0	-0.749116	-6.18245139	C	0	-0.749116	-6.14919111
H	0	0	-10.33078839	H	0	0	-10.29752811
H	0	2.109709	-9.33489839	H	0	2.109709	-9.30163811
H	0	2.655422	-7.06218339	H	0	2.655422	-7.02892311
H	0	-2.109709	-9.33489839	H	0	-2.109709	-9.30163811
H	0	-2.655422	-7.06218339	H	0	-2.655422	-7.02892311
C	0	1.165553	-4.82072139	C	0	1.165553	-4.78746111
C	0	0	-4.00501439	C	0	0	-3.97175411
C	0	-1.165553	-4.82072139	C	0	-1.165553	-4.78746111
C	0	0	-2.58654839	C	0	0	-2.55328811
C	0	-1.305082	-1.96503539	C	0	-1.305082	-1.93177511
C	0	1.305082	-1.96503539	C	0	1.305082	-1.93177511
C	0	-1.580366	-0.57290539	C	0	-1.580366	-0.53964511
C	0	1.580366	-0.57290539	C	0	1.580366	-0.53964511
C	0	-0.74355	0.52059861	C	0	-0.74355	0.55385889
H	0	-2.642683	-0.33396539	H	0	-2.642683	-0.30070511
C	0	0.74355	0.52059861	C	0	0.74355	0.55385889
H	0	2.642683	-0.33396539	H	0	2.642683	-0.30070511
C	0	-1.163845	1.88875061	C	0	-1.163845	1.92201089
C	0	1.163845	1.88875061	C	0	1.163845	1.92201089
C	0	0	2.70498361	C	0	0	2.73824389
C	0	-2.429854	-4.18733439	C	0	-2.429854	-4.15407411
H	0	-3.353322	-4.75867039	H	0	-3.353322	-4.72541011
C	0	-2.468447	-2.81615939	C	0	-2.468447	-2.78289911
H	0	-3.434671	-2.31988939	H	0	-3.434671	-2.28662911
C	0	2.468447	-2.81615939	C	0	2.468447	-2.78289911
H	0	3.434671	-2.31988939	H	0	3.434671	-2.28662911
C	0	2.429854	-4.18733439	C	0	2.429854	-4.15407411
H	0	3.353322	-4.75867039	H	0	3.353322	-4.72541011
C	0	-1.306075	4.74602361	C	0	-1.306075	4.77928389
C	0	-1.585021	6.13276961	C	0	-1.585021	6.16602989
C	0	1.306075	4.74602361	C	0	1.306075	4.77928389
C	0	-0.744681	7.23094161	C	0	-0.744681	7.26420189
C	0	1.585021	6.13276961	C	0	1.585021	6.16602989
C	0	0.744681	7.23094161	C	0	0.744681	7.26420189
H	0	-2.646903	6.37655661	H	0	-2.646903	6.40981689
H	0	2.646903	6.37655661	H	0	2.646903	6.40981689
C	0	-1.148431	8.58400161	C	0	-1.148431	8.61726189
C	0	1.148431	8.58400161	C	0	1.148431	8.61726189
C	0	2.426537	2.51898061	C	0	2.426537	2.55224089
C	0	2.46902	3.89035861	C	0	2.46902	3.92361889
H	0	3.349235	1.94586661	H	0	3.349235	1.97912689
H	0	3.436075	4.38491461	H	0	3.436075	4.41817489
C	0	-2.426537	2.51898061	C	0	-2.426537	2.55224089
C	0	-2.46902	3.89035861	C	0	-2.46902	3.92361889
H	0	-3.349235	1.94586661	H	0	-3.349235	1.97912689
H	0	-3.436075	4.38491461	H	0	-3.436075	4.41817489
H	0	2.176091	8.92721861	H	0	2.176091	8.96047889
H	0	0	10.47442661	H	0	0	10.50768689
H	0	-2.176091	8.92721861	H	0	-2.176091	8.96047889
N	0	0	9.39007161	N	0	0	9.42333189
N	0	0	4.12427461	B	0	0	4.15753489

		A3[$H_N P_B$]				A1[H_B]A3[P_B]	
C	0	0	-9.16654401	C	0	1.265996	-8.59471221
C	0	1.265996	-8.57452301	C	0	1.589678	-7.23043621
C	0	1.589678	-7.21024701	C	0	-1.265996	-8.59471221
C	0	-1.265996	-8.57452301	C	0	0.749116	-6.12691421

C	0	0.749116	-6.10672501	C	0	-1.589678	-7.23043621
C	0	-1.589678	-7.21024701	C	0	-0.749116	-6.12691421
C	0	-0.749116	-6.10672501	H	0	0	-10.27525121
H	0	0	-10.25506201	H	0	2.109709	-9.27936121
H	0	2.109709	-9.25917201	H	0	2.655422	-7.00664621
H	0	2.655422	-6.98645701	H	0	-2.109709	-9.27936121
H	0	-2.109709	-9.25917201	H	0	-2.655422	-7.00664621
H	0	-2.655422	-6.98645701	C	0	1.165553	-4.76518421
C	0	1.165553	-4.74499501	C	0	0	-3.94947721
C	0	0	-3.92928801	C	0	-1.165553	-4.76518421
C	0	-1.165553	-4.74499501	C	0	0	-2.53101121
C	0	0	-2.51082201	C	0	-1.305082	-1.90949821
C	0	-1.305082	-1.88930901	C	0	1.305082	-1.90949821
C	0	1.305082	-1.88930901	C	0	-1.580366	-0.51736821
C	0	-1.580366	-0.49717901	C	0	1.580366	-0.51736821
C	0	1.580366	-0.49717901	C	0	-0.74355	0.57613579
C	0	-0.74355	0.59632499	H	0	-2.642683	-0.27842821
H	0	-2.642683	-0.25823901	C	0	0.74355	0.57613579
C	0	0.74355	0.59632499	H	0	2.642683	-0.27842821
H	0	2.642683	-0.25823901	C	0	-1.163845	1.94428779
C	0	-1.163845	1.96447699	C	0	1.163845	1.94428779
C	0	1.163845	1.96447699	C	0	0	2.76052079
C	0	0	2.78070999	C	0	-2.429854	-4.13179721
C	0	-2.429854	-4.11160801	H	0	-3.353322	-4.70313321
H	0	-3.353322	-4.68294401	C	0	-2.468447	-2.76062221
C	0	-2.468447	-2.74043301	H	0	-3.434671	-2.26435221
H	0	-3.434671	-2.24416301	C	0	2.468447	-2.76062221
C	0	2.468447	-2.74043301	H	0	3.434671	-2.26435221
H	0	3.434671	-2.24416301	C	0	2.429854	-4.13179721
C	0	2.429854	-4.11160801	H	0	3.353322	-4.70313321
H	0	3.353322	-4.68294401	C	0	0	4.17981179
C	0	-1.306075	4.82174999	C	0	-1.306075	4.80156079
C	0	-1.585021	6.20849599	C	0	-1.585021	6.18830679
C	0	1.306075	4.82174999	C	0	1.306075	4.80156079
C	0	-0.744681	7.30666799	C	0	-0.744681	7.28647879
C	0	1.585021	6.20849599	C	0	1.585021	6.18830679
C	0	0.744681	7.30666799	C	0	0.744681	7.28647879
H	0	-2.646903	6.45228299	H	0	-2.646903	6.43209379
H	0	2.646903	6.45228299	H	0	2.646903	6.43209379
C	0	-1.148431	8.65972799	C	0	-1.148431	8.63953879
C	0	1.148431	8.65972799	C	0	1.148431	8.63953879
C	0	2.426537	2.59470699	C	0	2.426537	2.57451779
C	0	2.46902	3.96608499	C	0	2.46902	3.94589579
H	0	3.349235	2.02159299	H	0	3.349235	2.00140379
H	0	3.436075	4.46064099	H	0	3.436075	4.44045179
C	0	-2.426537	2.59470699	C	0	-2.426537	2.57451779
C	0	-2.46902	3.96608499	C	0	-2.46902	3.94589579
H	0	-3.349235	2.02159299	H	0	-3.349235	2.00140379
H	0	-3.436075	4.46064099	H	0	-3.436075	4.44045179
H	0	2.176091	9.00294499	H	0	2.176091	8.98275579
H	0	0	10.55015299	H	0	0	10.52996379
H	0	-2.176091	9.00294499	H	0	-2.176091	8.98275579
B	0	0	9.46579799	B	0	0	9.44560879
N	0	0	4.20000099	B	0	0	-9.18673321

$A1[H_N]A3[P_N]$				$A1[H_B]A3[P_N]$			
C	0	1.265996	-8.59678321	C	0	1.265996	-8.67088647
C	0	1.589678	-7.23250721	C	0	1.589678	-7.30661047
C	0	-1.265996	-8.59678321	C	0	-1.265996	-8.67088647
C	0	0.749116	-6.12898521	C	0	0.749116	-6.20308847
C	0	-1.589678	-7.23250721	C	0	-1.589678	-7.30661047
C	0	-0.749116	-6.12898521	C	0	-0.749116	-6.20308847
H	0	0	-10.27732221	H	0	0	-10.35142547
H	0	2.109709	-9.28143221	H	0	2.109709	-9.35553547

H	0	2.655422	-7.00871721	H	0	2.655422	-7.08282047
H	0	-2.109709	-9.28143221	H	0	-2.109709	-9.35553547
H	0	-2.655422	-7.00871721	H	0	-2.655422	-7.08282047
C	0	1.165553	-4.76725521	C	0	1.165553	-4.84135847
C	0	0	-3.95154821	C	0	0	-4.02565147
C	0	-1.165553	-4.76725521	C	0	-1.165553	-4.84135847
C	0	0	-2.53308221	C	0	0	-2.60718547
C	0	-1.305082	-1.91156921	C	0	-1.305082	-1.98567247
C	0	1.305082	-1.91156921	C	0	1.305082	-1.98567247
C	0	-1.580366	-0.51943921	C	0	-1.580366	-0.59354247
C	0	1.580366	-0.51943921	C	0	1.580366	-0.59354247
C	0	-0.74355	0.57406479	C	0	-0.74355	0.49996153
H	0	-2.642683	-0.28049921	H	0	-2.642683	-0.35460247
C	0	0.74355	0.57406479	C	0	0.74355	0.49996153
H	0	2.642683	-0.28049921	H	0	2.642683	-0.35460247
C	0	-1.163845	1.94221679	C	0	-1.163845	1.86811353
C	0	1.163845	1.94221679	C	0	1.163845	1.86811353
C	0	0	2.75844979	C	0	0	2.68434653
C	0	-2.429854	-4.13386821	C	0	-2.429854	-4.20797147
H	0	-3.353322	-4.70520421	H	0	-3.353322	-4.77930747
C	0	-2.468447	-2.76269321	C	0	-2.468447	-2.83679647
H	0	-3.434671	-2.26642321	H	0	-3.434671	-2.34052647
C	0	2.468447	-2.76269321	C	0	2.468447	-2.83679647
H	0	3.434671	-2.26642321	H	0	3.434671	-2.34052647
C	0	2.429854	-4.13386821	C	0	2.429854	-4.20797147
H	0	3.353322	-4.70520421	H	0	3.353322	-4.77930747
C	0	0	4.17774079	C	0	0	4.10363753
C	0	-1.306075	4.79948979	C	0	-1.306075	4.72538653
C	0	-1.585021	6.18623579	C	0	-1.585021	6.11213253
C	0	1.306075	4.79948979	C	0	1.306075	4.72538653
C	0	-0.744681	7.28440779	C	0	-0.744681	7.21030453
C	0	1.585021	6.18623579	C	0	1.585021	6.11213253
C	0	0.744681	7.28440779	C	0	0.744681	7.21030453
H	0	-2.646903	6.43002279	H	0	-2.646903	6.35591953
H	0	2.646903	6.43002279	H	0	2.646903	6.35591953
C	0	-1.148431	8.63746779	C	0	-1.148431	8.56336453
C	0	1.148431	8.63746779	C	0	1.148431	8.56336453
C	0	2.426537	2.57244679	C	0	2.426537	2.49834353
C	0	2.46902	3.94382479	C	0	2.46902	3.86972153
H	0	3.349235	1.99933279	H	0	3.349235	1.92522953
H	0	3.436075	4.43838079	H	0	3.436075	4.36427753
C	0	-2.426537	2.57244679	C	0	-2.426537	2.49834353
C	0	-2.46902	3.94382479	C	0	-2.46902	3.86972153
H	0	-3.349235	1.99933279	H	0	-3.349235	1.92522953
H	0	-3.436075	4.43838079	H	0	-3.436075	4.36427753
H	0	2.176091	8.98068479	H	0	2.176091	8.90658153
H	0	0	10.52789279	H	0	0	10.45378953
H	0	-2.176091	8.98068479	H	0	-2.176091	8.90658153
N	0	0	-9.18880421	B	0	0	-9.26290747
N	0	0	9.44353779	N	0	0	9.36943453

		A1[H$_N$]A3[P$_B$]				A1[H$_B$P$_B$]A3[H$_B$P$_B$]	
C	0	1.265996	-8.52062565	C	0	1.265996	-8.59376821
C	0	1.589678	-7.15634965	C	0	1.589678	-7.22949221
C	0	-1.265996	-8.52062565	C	0	-1.265996	-8.59376821
C	0	0.749116	-6.05282765	C	0	0.749116	-6.12597021
C	0	-1.589678	-7.15634965	C	0	-1.589678	-7.22949221
C	0	-0.749116	-6.05282765	C	0	-0.749116	-6.12597021
H	0	0	-10.20116465	H	0	0	-10.27430721
H	0	2.109709	-9.20527465	H	0	2.109709	-9.27841721
H	0	2.655422	-6.93255965	H	0	2.655422	-7.00570221
H	0	-2.109709	-9.20527465	H	0	-2.109709	-9.27841721
H	0	-2.655422	-6.93255965	H	0	-2.655422	-7.00570221
C	0	1.165553	-4.69109765	C	0	1.165553	-4.76424021

Atom		x	y	Atom		x	y
C	0	0	-3.87539065	C	0	-1.165553	-4.76424021
C	0	-1.165553	-4.69109765	C	0	-1.305082	-1.90855421
C	0	0	-2.45692465	C	0	1.305082	-1.90855421
C	0	-1.305082	-1.83541165	C	0	-1.580366	-0.51642421
C	0	1.305082	-1.83541165	C	0	1.580366	-0.51642421
C	0	-1.580366	-0.44328165	C	0	-0.74355	0.57707979
C	0	1.580366	-0.44328165	H	0	-2.642683	-0.27748421
C	0	-0.74355	0.65022235	C	0	0.74355	0.57707979
H	0	-2.642683	-0.20434165	H	0	2.642683	-0.27748421
C	0	0.74355	0.65022235	C	0	-1.163845	1.94523179
H	0	2.642683	-0.20434165	C	0	1.163845	1.94523179
C	0	-1.163845	2.01837435	C	0	-2.429854	-4.13085321
C	0	1.163845	2.01837435	H	0	-3.353322	-4.70218921
C	0	0	2.83460735	C	0	-2.468447	-2.75967821
C	0	-2.429854	-4.05771065	H	0	-3.434671	-2.26340821
H	0	-3.353322	-4.62904665	C	0	2.468447	-2.75967821
C	0	-2.468447	-2.68653565	H	0	3.434671	-2.26340821
H	0	-3.434671	-2.19026565	C	0	2.429854	-4.13085321
C	0	2.468447	-2.68653565	H	0	3.353322	-4.70218921
H	0	3.434671	-2.19026565	C	0	-1.306075	4.80250479
C	0	2.429854	-4.05771065	C	0	-1.585021	6.18925079
H	0	3.353322	-4.62904665	C	0	1.306075	4.80250479
C	0	0	4.25389835	C	0	-0.744681	7.28742279
C	0	-1.306075	4.87564735	C	0	1.585021	6.18925079
C	0	-1.585021	6.26239335	C	0	0.744681	7.28742279
C	0	1.306075	4.87564735	H	0	-2.646903	6.43303779
C	0	-0.744681	7.36056535	H	0	2.646903	6.43303779
C	0	1.585021	6.26239335	C	0	-1.148431	8.64048279
C	0	0.744681	7.36056535	C	0	1.148431	8.64048279
H	0	-2.646903	6.50618035	C	0	2.426537	2.57546179
H	0	2.646903	6.50618035	C	0	2.46902	3.94683979
C	0	-1.148431	8.71362535	H	0	3.349235	2.00234779
C	0	1.148431	8.71362535	H	0	3.436075	4.44139579
C	0	2.426537	2.64860435	C	0	-2.426537	2.57546179
C	0	2.46902	4.01998235	C	0	-2.46902	3.94683979
H	0	3.349235	2.07549035	H	0	-3.349235	2.00234779
H	0	3.436075	4.51453835	H	0	-3.436075	4.44139579
C	0	-2.426537	2.64860435	H	0	2.176091	8.98369979
C	0	-2.46902	4.01998235	H	0	0	10.53090779
H	0	-3.349235	2.07549035	H	0	-2.176091	8.98369979
H	0	-3.436075	4.51453835	B	0	0	-9.18578921
H	0	2.176091	9.05684235	B	0	0	-3.94853321
H	0	0	10.60405035	C	0	0	-2.53006721
H	0	-2.176091	9.05684235	C	0	0	2.76146479
N	0	0	-9.11264665	B	0	0	4.18075579
B	0	0	9.51969535	B	0	0	9.44655279

$A1[H_N P_N]A3[H_N P_N]$				$A1[H_B P_N]A3[H_B P_N]$			
C	0	1.260969	-8.56685391	C	0	1.265996	-8.63810708
C	0	1.591273	-7.25766291	C	0	1.589678	-7.27383108
C	0	-1.260969	-8.56685391	C	0	-1.265996	-8.63810708
C	0	0.708707	-6.10458891	C	0	0.749116	-6.17030908
C	0	-1.591273	-7.25766291	C	0	-1.589678	-7.27383108
C	0	-0.708707	-6.10458891	C	0	-0.749116	-6.17030908
H	0	0	-10.16740391	H	0	0	-10.31864608
H	0	2.056954	-9.30507391	H	0	2.109709	-9.32275608
H	0	2.65772	-7.05300391	H	0	2.655422	-7.05004108
H	0	-2.056954	-9.30507391	H	0	-2.109709	-9.32275608
H	0	-2.65772	-7.05300391	H	0	-2.655422	-7.05004108
C	0	1.151847	-4.75342491	C	0	1.165553	-4.80857908
C	0	-1.151847	-4.75342491	C	0	-1.165553	-4.80857908
C	0	-1.282645	-1.89681891	C	0	-1.305082	-1.95289308
C	0	1.282645	-1.89681891	C	0	1.305082	-1.95289308

C	0	-1.546067	-0.52901191	C	0	-1.580366	-0.56076308
C	0	1.546067	-0.52901191	C	0	1.580366	-0.56076308
C	0	-0.717908	0.60407909	C	0	-0.74355	0.53274092
H	0	-2.61049	-0.31811491	H	0	-2.642683	-0.32182308
C	0	0.717908	0.60407909	C	0	0.74355	0.53274092
H	0	2.61049	-0.31811491	H	0	2.642683	-0.32182308
C	0	-1.136157	1.94321009	C	0	-1.163845	1.90089292
C	0	1.136157	1.94321009	C	0	1.163845	1.90089292
C	0	-2.409477	-4.12108891	C	0	-2.429854	-4.17519208
H	0	-3.336578	-4.68620391	H	0	-3.353322	-4.74652808
C	0	-2.438447	-2.75271691	C	0	-2.468447	-2.80401708
H	0	-3.392791	-2.23926891	H	0	-3.434671	-2.30774708
C	0	2.438447	-2.75271691	C	0	2.468447	-2.80401708
H	0	3.392791	-2.23926891	H	0	3.434671	-2.30774708
C	0	2.409477	-4.12108891	C	0	2.429854	-4.17519208
H	0	3.336578	-4.68620391	H	0	3.353322	-4.74652808
C	0	-1.314593	4.79386109	C	0	-1.306075	4.75816592
C	0	-1.587139	6.15013409	C	0	-1.585021	6.14491192
C	0	1.314593	4.79386109	C	0	1.306075	4.75816592
C	0	-0.722008	7.28434809	C	0	-0.744681	7.24308392
C	0	1.587139	6.15013409	C	0	1.585021	6.14491192
C	0	0.722008	7.28434809	C	0	0.744681	7.24308392
H	0	-2.646871	6.39562709	H	0	-2.646903	6.38869892
H	0	2.646871	6.39562709	H	0	2.646903	6.38869892
C	0	-1.124814	8.61291709	C	0	-1.148431	8.59614392
C	0	1.124814	8.61291709	C	0	1.148431	8.59614392
C	0	2.401894	2.56854609	C	0	2.426537	2.53112292
C	0	2.477813	3.92275609	C	0	2.46902	3.90250092
H	0	3.296785	1.95622609	H	0	3.349235	1.95800892
H	0	3.449572	4.40578909	H	0	3.436075	4.39705692
C	0	-2.401894	2.56854609	C	0	-2.426537	2.53112292
C	0	-2.477813	3.92275609	C	0	-2.46902	3.90250092
H	0	-3.296785	1.95622609	H	0	-3.349235	1.95800892
H	0	-3.449572	4.40578909	H	0	-3.436075	4.39705692
H	0	2.115366	9.04260009	H	0	2.176091	8.93936092
H	0	0	10.40873009	H	0	0	10.48656892
H	0	-2.115366	9.04260009	H	0	-2.176091	8.93936092
N	0	0	-9.16141091	B	0	0	-9.23012808
N	0	0	9.40198809	N	0	0	-3.99287208
N	0	0	-3.92222691	C	0	0	2.71712592
N	0	0	4.14034409	C	0	0	-2.57440608
C	0	0	-2.54326091	B	0	0	4.13641692
C	0	0	2.77300209	N	0	0	9.40221392

A1[H_NP_B]A3[H_NP_B]				A1[H_B]A2[H_BP_B]A3[P_B]			
C	0	1.265996	-8.55340504	C	-1.259729	0	-8.63105269
C	0	1.589678	-7.18912904	C	-1.59234	0	-7.32501569
C	0	-1.265996	-8.55340504	C	1.259729	0	-8.63105269
C	0	0.749116	-6.08560704	C	-0.700322	0	-6.17246769
C	0	-1.589678	-7.18912904	C	1.59234	0	-7.32501569
C	0	-0.749116	-6.08560704	C	0.700322	0	-6.17246769
H	0	0	-10.23394404	H	0	0	-10.23380269
H	0	2.109709	-9.23805404	H	-2.056657	0	-9.36808869
H	0	2.655422	-6.96533904	H	-2.657372	0	-7.11749969
H	0	-2.109709	-9.23805404	H	2.056657	0	-9.36808869
H	0	-2.655422	-6.96533904	H	2.657372	0	-7.11749969
C	0	1.165553	-4.72387704	C	-1.151214	0	-4.81000669
C	0	-1.165553	-4.72387704	C	0	0	-3.97910669
C	0	-1.305082	-1.86819104	C	1.151214	0	-4.81000669
C	0	1.305082	-1.86819104	C	1.275312	0	-1.96196069
C	0	-1.580366	-0.47606104	C	-1.275312	0	-1.96196069
C	0	1.580366	-0.47606104	C	1.530405	0	-0.57021669
C	0	-0.74355	0.61744296	C	-1.530405	0	-0.57021669

Atom	X	Y	Z	Atom	X	Y	Z
H	0	-2.642683	-0.23712104	C	0.739693	0	0.56123631
C	0	0.74355	0.61744296	H	2.597382	0	-0.36773469
H	0	2.642683	-0.23712104	C	-0.739693	0	0.56123631
C	0	-1.163845	1.98559496	H	-2.597382	0	-0.36773469
C	0	1.163845	1.98559496	C	1.219407	0	1.92900331
C	0	-2.429854	-4.09049004	C	-1.219407	0	1.92900331
H	0	-3.353322	-4.66182604	C	2.396423	0	-4.18302169
C	0	-2.468447	-2.71931504	H	3.32674	0	-4.74191769
H	0	-3.434671	-2.22304504	C	2.42006	0	-2.80048169
C	0	2.468447	-2.71931504	H	3.374614	0	-2.28894269
H	0	3.434671	-2.22304504	C	-2.42006	0	-2.80048169
C	0	2.429854	-4.09049004	H	-3.374614	0	-2.28894269
H	0	3.353322	-4.66182604	C	-2.396423	0	-4.18302169
C	0	-1.306075	4.84286796	H	-3.32674	0	-4.74191769
C	0	-1.585021	6.22961396	C	0	0	4.28707731
C	0	1.306075	4.84286796	C	1.306783	0	4.87006331
C	0	-0.744681	7.32778596	C	1.603732	0	6.27844731
C	0	1.585021	6.22961396	C	-1.306783	0	4.87006331
C	0	0.744681	7.32778596	C	0.747695	0	7.35511531
H	0	-2.646903	6.47340096	C	-1.603732	0	6.27844731
H	0	2.646903	6.47340096	C	-0.747695	0	7.35511531
C	0	-1.148431	8.68084596	H	2.663681	0	6.53112431
C	0	1.148431	8.68084596	H	-2.663681	0	6.53112431
C	0	2.426537	2.61582496	C	1.184404	0	8.71324131
C	0	2.46902	3.98720296	C	-1.184404	0	8.71324131
H	0	3.349235	2.04271096	C	-2.44928	0	2.59011231
H	0	3.436075	4.48175896	C	-2.448939	0	3.99948631
C	0	-2.426537	2.61582496	H	-3.415978	0	2.08431731
C	0	-2.46902	3.98720296	H	-3.42025	0	4.48954031
H	0	-3.349235	2.04271096	C	2.44928	0	2.59011231
H	0	-3.436075	4.48175896	C	2.448939	0	3.99948631
H	0	2.176091	9.02406296	H	3.415978	0	2.08431731
H	0	0	10.57127096	H	3.42025	0	4.48954031
H	0	-2.176091	9.02406296	H	-2.254151	0	8.91825931
N	0	0	-9.14542604	H	2.254151	0	8.91825931
B	0	0	-3.90817004	H	0	0	10.85649331
C	0	0	-2.48970404	B	0	0	2.80052131
C	0	0	2.80182796	B	0	0	9.66269231
N	0	0	4.22111896	B	0	0	-9.22768169
B	0	0	9.48691596	B	0	0	-2.60721469

A1[H_B]A2[H_NP_B]A3[P_N]				A1[H_N]A2[H_BP_N]A3[P_B]			
C	8.38948515	-0.10992736	1.38843829	C	8.27311317	0.05084598	1.29366775
C	7.11986433	0.15100192	1.7436043	C	6.95765543	0.18946422	1.61425849
C	8.38948515	-0.10992736	-1.38843829	C	8.27311317	0.05084598	-1.29366775
C	6.05676194	0.10997581	0.7882559	C	5.92733319	0.14740218	0.75778516
C	7.11986433	0.15100192	-1.7436043	C	6.95765543	0.18946422	-1.61425849
C	6.05676194	0.10997581	-0.7882559	C	5.92733319	0.14740218	-0.75778516
H	8.77811547	-2.07313785	0	H	9.80631893	0.03912481	0
H	9.22442809	0.18460098	1.98929998	H	8.96232542	0.24489006	2.08874394
H	6.90069646	0.40007076	2.76087561	H	6.72406177	0.34555565	2.64690294
H	9.22442809	0.18460098	-1.98929998	H	8.96232542	0.24489006	-2.08874394
H	6.90069646	0.40007076	-2.76087561	H	6.72406177	0.34555565	-2.64690294
C	4.70175574	0.09473718	1.1394608	C	4.57377429	0.1152284	1.12161947
C	3.91175366	0.08460144	0	C	3.838699	0.0973216	0
C	4.70175574	0.09473718	-1.1394608	C	4.57377429	0.1152284	-1.12161947
C	1.97429631	0.06156023	-1.36364225	C	1.76181707	0.04716592	-1.47868338
C	1.97429631	0.06156023	1.36364225	C	1.76181707	0.04716592	1.47868338
C	0.60368017	0.04421159	-1.67431284	C	0.38616646	0.01295234	-1.73940206
C	0.60368017	0.04421159	1.67431284	C	0.38616646	0.01295234	1.73940206
C	-0.45719142	0.03111973	-0.77715789	C	-0.63934504	0.00005063	-0.77354041
H	0.3498318	0.04085015	-2.71376356	H	0.08651701	-0.00477556	-2.76630935
C	-0.45719142	0.03111973	0.77715789	C	-0.63934504	0.00005063	0.77354041
H	0.3498318	0.04085015	2.71376356	H	0.08651701	-0.00477556	2.76630935

C	-1.80832352	0.01470453	-1.18279754	C	-1.99854381	-0.06395598	-1.10986389
C	-1.80832352	0.01470453	1.18279754	C	-1.99854381	-0.06395598	1.10986389
C	4.15795055	0.09011581	-2.40722931	C	4.03679553	0.10327019	-2.37949374
H	4.78151419	0.09940634	-3.27671582	H	4.68691069	0.12018962	-3.22907813
C	2.80865997	0.07320187	-2.51381346	C	2.66637918	0.0695019	-2.57226604
H	2.36052515	0.06851764	-3.48544193	H	2.27948792	0.06017501	-3.57004717
C	2.80865997	0.07320187	2.51381346	C	2.66637918	0.0695019	2.57226604
H	2.36052515	0.06851764	3.48544193	H	2.27948792	0.06017501	3.57004717
C	4.15795055	0.09011581	2.40722931	C	4.03679553	0.10327019	2.37949374
H	4.78151419	0.09940634	3.27671582	H	4.68691069	0.12018962	3.22907813
C	-4.04840812	-0.01127535	0	C	-4.13761141	-0.0848866	0
C	-4.67180171	-0.01841931	-1.41687287	C	-4.74097755	-0.34031925	-1.39459763
C	-6.04381637	-0.03363408	-1.70273966	C	-6.07463315	-0.06883476	-1.72455842
C	-4.67180171	-0.01841931	1.41687287	C	-4.74097755	-0.34031925	1.39459763
C	-7.08181925	-0.04463954	-0.76212138	C	-7.08912673	0.26146898	-0.80840961
C	-6.04381637	-0.03363408	1.70273966	C	-6.07463315	-0.06883476	1.72455842
C	-7.08181925	-0.04463954	0.76212138	C	-7.08912673	0.26146898	0.80840961
H	-6.32444185	-0.037085	-2.73528633	H	-6.34427561	-0.11712387	-2.75899829
H	-6.32444185	-0.037085	2.73528633	H	-6.34427561	-0.11712387	2.75899829
C	-8.43445773	-0.05894492	-1.1136307	C	-8.36960871	0.71003413	-1.23753111
C	-8.43445773	-0.05894492	1.1136307	C	-8.36960871	0.71003413	1.23753111
C	-2.39820543	0.00735212	2.44706242	C	-2.51526676	-0.60829894	2.29977998
C	-3.78353938	-0.00869305	2.55336956	C	-3.9081635	-0.78987956	2.4274263
H	-1.78931461	0.01404556	3.32689	H	-1.85756618	-0.89585558	3.09321405
H	-4.21529944	-0.01408147	3.53237493	H	-4.32204763	-1.22887973	3.31086096
C	-2.39820543	0.00735212	-2.44706242	C	-2.51526676	-0.60829894	-2.29977998
C	-3.78353938	-0.00869305	-2.55336956	C	-3.9081635	-0.78987956	-2.4274263
H	-1.78931461	0.01404556	-3.32689	H	-1.85756618	-0.89585558	-3.09321405
H	-4.21529944	-0.01408147	-3.53237493	H	-4.32204763	-1.22887973	-3.31086096
H	-8.8092559	-0.06291805	2.11582838	H	-8.63154816	1.20558492	2.14913229
H	-8.8092559	-0.06291805	-2.11582838	H	-8.63154816	1.20558492	-2.14913229
H	-10.19746348	-0.07747329	0	N	8.88914571	-0.35944055	0
B	-2.61950984	0.00524785	0	H	-10.34075439	-0.23094771	0
N	2.61881226	0.06904366	0	B	-9.30312241	0.33077692	0
N	-9.19752669	-0.0669659	0	N	-2.81913426	0.45251871	0
B	8.56617293	-0.91232494	0	B	2.44345647	0.06382067	0

	A1[H$_N$]A2[H$_N$P$_N$]A3[P$_N$]				**A1[H$_B$P$_B$]A2[H$_B$P$_B$]A3[H$_B$P$_B$]**		
C	0	1.265996	-8.59767753	C	0	1.265996	-8.59281202
C	0	1.589678	-7.23340153	C	0	1.589678	-7.22853602
C	0	-1.265996	-8.59767753	C	0	-1.265996	-8.59281202
C	0	0.749116	-6.12987953	C	0	0.749116	-6.12501402
C	0	-1.589678	-7.23340153	C	0	-1.589678	-7.22853602
C	0	-0.749116	-6.12987953	C	0	-0.749116	-6.12501402
H	0	0	-10.27821653	H	0	0	-10.27335102
H	0	2.109709	-9.28232653	H	0	2.109709	-9.27746102
H	0	2.655422	-7.00961153	H	0	2.655422	-7.00474602
H	0	-2.109709	-9.28232653	H	0	-2.109709	-9.27746102
H	0	-2.655422	-7.00961153	H	0	-2.655422	-7.00474602
C	0	1.165553	-4.76814953	C	0	1.165553	-4.76328402
C	0	0	-3.95244253	C	0	-1.165553	-4.76328402
C	0	-1.165553	-4.76814953	C	0	-1.305082	-1.90759802
C	0	-1.305082	-1.91246353	C	0	1.305082	-1.90759802
C	0	1.305082	-1.91246353	C	0	-1.580366	-0.51546802
C	0	-1.580366	-0.52033353	C	0	1.580366	-0.51546802
C	0	1.580366	-0.52033353	C	0	-0.74355	0.57803598
C	0	-0.74355	0.57317047	H	0	-2.642683	-0.27652802
H	0	-2.642683	-0.28139353	C	0	0.74355	0.57803598
C	0	0.74355	0.57317047	H	0	2.642683	-0.27652802
H	0	2.642683	-0.28139353	C	0	-1.163845	1.94618798
C	0	-1.163845	1.94132247	C	0	1.163845	1.94618798
C	0	1.163845	1.94132247	C	0	-2.429854	-4.12989702
C	0	-2.429854	-4.13476253	H	0	-3.353322	-4.70123302

H	0	-3.353322	-4.70609853	C	0	-2.468447	-2.75872202
C	0	-2.468447	-2.76358753	H	0	-3.434671	-2.26245202
H	0	-3.434671	-2.26731753	C	0	2.468447	-2.75872202
C	0	2.468447	-2.76358753	H	0	3.434671	-2.26245202
H	0	3.434671	-2.26731753	C	0	2.429854	-4.12989702
C	0	2.429854	-4.13476253	H	0	3.353322	-4.70123302
H	0	3.353322	-4.70609853	C	0	-1.306075	4.80346098
C	0	0	4.17684647	C	0	-1.585021	6.19020698
C	0	-1.306075	4.79859547	C	0	1.306075	4.80346098
C	0	-1.585021	6.18534147	C	0	-0.744681	7.28837898
C	0	1.306075	4.79859547	C	0	1.585021	6.19020698
C	0	-0.744681	7.28351347	C	0	0.744681	7.28837898
C	0	1.585021	6.18534147	H	0	-2.646903	6.43399398
C	0	0.744681	7.28351347	H	0	2.646903	6.43399398
H	0	-2.646903	6.42912847	C	0	-1.148431	8.64143898
H	0	2.646903	6.42912847	C	0	1.148431	8.64143898
C	0	-1.148431	8.63657347	C	0	2.426537	2.57641798
C	0	1.148431	8.63657347	C	0	2.46902	3.94779598
C	0	2.426537	2.57155247	H	0	3.349235	2.00330398
C	0	2.46902	3.94293047	H	0	3.436075	4.44235198
H	0	3.349235	1.99843847	C	0	-2.426537	2.57641798
H	0	3.436075	4.43748647	C	0	-2.46902	3.94779598
C	0	-2.426537	2.57155247	H	0	-3.349235	2.00330398
C	0	-2.46902	3.94293047	H	0	-3.436075	4.44235198
H	0	-3.349235	1.99843847	H	0	2.176091	8.98465598
H	0	-3.436075	4.43748647	H	0	0	10.53186398
H	0	2.176091	8.97979047	H	0	-2.176091	8.98465598
H	0	0	10.52699847	B	0	0	9.44750898
H	0	-2.176091	8.97979047	B	0	0	4.18171198
N	0	0	-9.18969853	B	0	0	2.76242098
N	0	0	9.44264347	B	0	0	-2.52911102
N	0	0	2.75755547	B	0	0	-3.94757702
N	0	0	-2.53397653	B	0	0	-9.18483302

A1[H_BP_N]A2[H_BP_N]A3[H_BP_N]				A1[H_NP_B]A2[H_NP_B]A3[H_NP_B]			
C	0	1.265996	-8.6594439	C	0	1.265996	-8.53206822
C	0	1.589678	-7.2951679	C	0	1.589678	-7.16779222
C	0	-1.265996	-8.6594439	C	0	-1.265996	-8.53206822
C	0	0.749116	-6.1916459	C	0	0.749116	-6.06427022
C	0	-1.589678	-7.2951679	C	0	-1.589678	-7.16779222
C	0	-0.749116	-6.1916459	C	0	-0.749116	-6.06427022
H	0	0	-10.3399829	H	0	0	-10.21260722
H	0	2.109709	-9.3440929	H	0	2.109709	-9.21671722
H	0	2.655422	-7.0713779	H	0	2.655422	-6.94400222
H	0	-2.109709	-9.3440929	H	0	-2.109709	-9.21671722
H	0	-2.655422	-7.0713779	H	0	-2.655422	-6.94400222
C	0	1.165553	-4.8299159	C	0	1.165553	-4.70254022
C	0	-1.165553	-4.8299159	C	0	-1.165553	-4.70254022
C	0	-1.305082	-1.9742299	C	0	-1.305082	-1.84685422
C	0	1.305082	-1.9742299	C	0	1.305082	-1.84685422
C	0	-1.580366	-0.5820999	C	0	-1.580366	-0.45472422
C	0	1.580366	-0.5820999	C	0	1.580366	-0.45472422
C	0	-0.74355	0.5114041	C	0	-0.74355	0.63877978
H	0	-2.642683	-0.3431599	H	0	-2.642683	-0.21578422
C	0	0.74355	0.5114041	C	0	0.74355	0.63877978
H	0	2.642683	-0.3431599	H	0	2.642683	-0.21578422
C	0	-1.163845	1.8795561	C	0	-1.163845	2.00693178
C	0	1.163845	1.8795561	C	0	1.163845	2.00693178
C	0	-2.429854	-4.1965289	C	0	-2.429854	-4.06915322
H	0	-3.353322	-4.7678649	H	0	-3.353322	-4.64048922
C	0	-2.468447	-2.8253539	C	0	-2.468447	-2.69797822
H	0	-3.434671	-2.3290839	H	0	-3.434671	-2.20170822
C	0	2.468447	-2.8253539	C	0	2.468447	-2.69797822
H	0	3.434671	-2.3290839	H	0	3.434671	-2.20170822

C	0	2.429854	-4.1965289	C	0	2.429854	-4.06915322
H	0	3.353322	-4.7678649	H	0	3.353322	-4.64048922
C	0	-1.306075	4.7368291	C	0	-1.306075	4.86420478
C	0	-1.585021	6.1235751	C	0	-1.585021	6.25095078
C	0	1.306075	4.7368291	C	0	1.306075	4.86420478
C	0	-0.744681	7.2217471	C	0	-0.744681	7.34912278
C	0	1.585021	6.1235751	C	0	1.585021	6.25095078
C	0	0.744681	7.2217471	C	0	0.744681	7.34912278
H	0	-2.646903	6.3673621	H	0	-2.646903	6.49473778
H	0	2.646903	6.3673621	H	0	2.646903	6.49473778
C	0	-1.148431	8.5748071	C	0	-1.148431	8.70218278
C	0	1.148431	8.5748071	C	0	1.148431	8.70218278
C	0	2.426537	2.5097861	C	0	2.426537	2.63716178
C	0	2.46902	3.8811641	C	0	2.46902	4.00853978
H	0	3.349235	1.9366721	H	0	3.349235	2.06404778
H	0	3.436075	4.3757201	H	0	3.436075	4.50309578
C	0	-2.426537	2.5097861	C	0	-2.426537	2.63716178
C	0	-2.46902	3.8811641	C	0	-2.46902	4.00853978
H	0	-3.349235	1.9366721	H	0	-3.349235	2.06404778
H	0	-3.436075	4.3757201	H	0	-3.436075	4.50309578
H	0	2.176091	8.9180241	H	0	2.176091	9.04539978
H	0	0	10.4652321	H	0	0	10.59260778
H	0	-2.176091	8.9180241	H	0	-2.176091	9.04539978
N	0	0	9.3808771	B	0	0	9.50825278
N	0	0	2.6957891	B	0	0	2.82316478
N	0	0	-4.0142089	B	0	0	-3.88683322
B	0	0	4.1150801	N	0	0	4.24245578
B	0	0	-2.5957429	N	0	0	-2.46836722
B	0	0	-9.2514649	N	0	0	-9.12408922

	A1[HNPN]A2[HNPN]A3[HNPN]				A2[HBPB]		
C	0	1.265996	-8.59856101	C	0	1.265996	-8.59483158
C	0	1.589678	-7.23428501	C	0	1.589678	-7.23055558
C	0	-1.265996	-8.59856101	C	0	-1.265996	-8.59483158
C	0	0.749116	-6.13076301	C	0	0.749116	-6.12703358
C	0	-1.589678	-7.23428501	C	0	-1.589678	-7.23055558
C	0	-0.749116	-6.13076301	C	0	-0.749116	-6.12703358
H	0	0	-10.27910001	H	0	0	-10.27537058
H	0	2.109709	-9.28321001	H	0	2.109709	-9.27948058
H	0	2.655422	-7.01049501	H	0	2.655422	-7.00676558
H	0	-2.109709	-9.28321001	H	0	-2.109709	-9.27948058
H	0	-2.655422	-7.01049501	H	0	-2.655422	-7.00676558
C	0	1.165553	-4.76903301	C	0	1.165553	-4.76530358
C	0	-1.165553	-4.76903301	C	0	0	-3.94959658
C	0	-1.305082	-1.91334701	C	0	-1.165553	-4.76530358
C	0	1.305082	-1.91334701	C	0	-1.305082	-1.90961758
C	0	-1.580366	-0.52121701	C	0	1.305082	-1.90961758
C	0	1.580366	-0.52121701	C	0	-1.580366	-0.51748758
C	0	-0.74355	0.57228699	C	0	1.580366	-0.51748758
H	0	-2.642683	-0.28227701	C	0	-0.74355	0.57601642
C	0	0.74355	0.57228699	H	0	-2.642683	-0.27854758
H	0	2.642683	-0.28227701	C	0	0.74355	0.57601642
C	0	-1.163845	1.94043899	H	0	2.642683	-0.27854758
C	0	1.163845	1.94043899	C	0	-1.163845	1.94416842
C	0	-2.429854	-4.13564601	C	0	1.163845	1.94416842
H	0	-3.353322	-4.70698201	C	0	-2.429854	-4.13191658
C	0	-2.468447	-2.76447101	H	0	-3.353322	-4.70325258
H	0	-3.434671	-2.26820101	C	0	-2.468447	-2.76074158
C	0	2.468447	-2.76447101	H	0	-3.434671	-2.26447158
H	0	3.434671	-2.26820101	C	0	2.468447	-2.76074158
C	0	2.429854	-4.13564601	H	0	3.434671	-2.26447158
H	0	3.353322	-4.70698201	C	0	2.429854	-4.13191658
C	0	-1.306075	4.79771199	H	0	3.353322	-4.70325258
C	0	-1.585021	6.18445799	C	0	0	4.17969242

C	0	1.306075	4.79771199	C	0	-1.306075	4.80144142
C	0	-0.744681	7.28262999	C	0	-1.585021	6.18818742
C	0	1.585021	6.18445799	C	0	1.306075	4.80144142
C	0	0.744681	7.28262999	C	0	-0.744681	7.28635942
H	0	-2.646903	6.42824499	C	0	1.585021	6.18818742
H	0	2.646903	6.42824499	C	0	0.744681	7.28635942
C	0	-1.148431	8.63568999	H	0	-2.646903	6.43197442
C	0	1.148431	8.63568999	H	0	2.646903	6.43197442
C	0	2.426537	2.57066899	C	0	-1.148431	8.63941942
C	0	2.46902	3.94204699	C	0	1.148431	8.63941942
H	0	3.349235	1.99755499	C	0	2.426537	2.57439842
H	0	3.436075	4.43660299	C	0	2.46902	3.94577642
C	0	-2.426537	2.57066899	H	0	3.349235	2.00128442
C	0	-2.46902	3.94204699	H	0	3.436075	4.44033242
H	0	-3.349235	1.99755499	C	0	-2.426537	2.57439842
H	0	-3.436075	4.43660299	C	0	-2.46902	3.94577642
H	0	2.176091	8.97890699	H	0	-3.349235	2.00128442
H	0	0	10.52611499	H	0	-3.436075	4.44033242
H	0	-2.176091	8.97890699	H	0	2.176091	8.98263642
N	0	0	9.44175999	H	0	0	10.52984442
N	0	0	4.17596299	H	0	-2.176091	8.98263642
N	0	0	2.75667199	C	0	0	9.44548942
N	0	0	-2.53486001	C	0	0	-9.18685258
N	0	0	-3.95332601	B	0	0	2.76040142
N	0	0	-9.19058201	B	0	0	-2.53113058

A2[H$_B$P$_N$]				A2[H$_N$P$_B$]			
C	0	1.265996	-8.61709288	C	0	1.265996	-8.57441924
C	0	1.589678	-7.25281688	C	0	1.589678	-7.21014324
C	0	-1.265996	-8.61709288	C	0	-1.265996	-8.57441924
C	0	0.749116	-6.14929488	C	0	0.749116	-6.10662124
C	0	-1.589678	-7.25281688	C	0	-1.589678	-7.21014324
C	0	-0.749116	-6.14929488	C	0	-0.749116	-6.10662124
H	0	0	-10.29763188	H	0	0	-10.25495824
H	0	2.109709	-9.30174188	H	0	2.109709	-9.25906824
H	0	2.655422	-7.02902688	H	0	2.655422	-6.98635324
H	0	-2.109709	-9.30174188	H	0	-2.109709	-9.25906824
H	0	-2.655422	-7.02902688	H	0	-2.655422	-6.98635324
C	0	1.165553	-4.78756488	C	0	1.165553	-4.74489124
C	0	0	-3.97185788	C	0	0	-3.92918424
C	0	-1.165553	-4.78756488	C	0	-1.165553	-4.74489124
C	0	-1.305082	-1.93187888	C	0	-1.305082	-1.88920524
C	0	1.305082	-1.93187888	C	0	1.305082	-1.88920524
C	0	-1.580366	-0.53974888	C	0	-1.580366	-0.49707524
C	0	1.580366	-0.53974888	C	0	1.580366	-0.49707524
C	0	-0.74355	0.55375512	C	0	-0.74355	0.59642876
H	0	-2.642683	-0.30080888	H	0	-2.642683	-0.25813524
C	0	0.74355	0.55375512	C	0	0.74355	0.59642876
H	0	2.642683	-0.30080888	H	0	2.642683	-0.25813524
C	0	-1.163845	1.92190712	C	0	-1.163845	1.96458076
C	0	1.163845	1.92190712	C	0	1.163845	1.96458076
C	0	-2.429854	-4.15417788	C	0	-2.429854	-4.11150424
H	0	-3.353322	-4.72551388	H	0	-3.353322	-4.68284024
C	0	-2.468447	-2.78300288	C	0	-2.468447	-2.74032924
H	0	-3.434671	-2.28673288	H	0	-3.434671	-2.24405924
C	0	2.468447	-2.78300288	C	0	2.468447	-2.74032924
H	0	3.434671	-2.28673288	H	0	3.434671	-2.24405924
C	0	2.429854	-4.15417788	C	0	2.429854	-4.11150424
H	0	3.353322	-4.72551388	H	0	3.353322	-4.68284024
C	0	0	4.15743112	C	0	0	4.20010476
C	0	-1.306075	4.77918012	C	0	-1.306075	4.82185376
C	0	-1.585021	6.16592612	C	0	-1.585021	6.20859976
C	0	1.306075	4.77918012	C	0	1.306075	4.82185376

C	0	-0.744681	7.26409812	C	0	-0.744681	7.30677176
C	0	1.585021	6.16592612	C	0	1.585021	6.20859976
C	0	0.744681	7.26409812	C	0	0.744681	7.30677176
H	0	-2.646903	6.40971312	H	0	-2.646903	6.45238676
H	0	2.646903	6.40971312	H	0	2.646903	6.45238676
C	0	-1.148431	8.61715812	C	0	-1.148431	8.65983176
C	0	1.148431	8.61715812	C	0	1.148431	8.65983176
C	0	2.426537	2.55213712	C	0	2.426537	2.59481076
C	0	2.46902	3.92351512	C	0	2.46902	3.96618876
H	0	3.349235	1.97902312	H	0	3.349235	2.02169676
H	0	3.436075	4.41807112	H	0	3.436075	4.46074476
C	0	-2.426537	2.55213712	C	0	-2.426537	2.59481076
C	0	-2.46902	3.92351512	C	0	-2.46902	3.96618876
H	0	-3.349235	1.97902312	H	0	-3.349235	2.02169676
H	0	-3.436075	4.41807112	H	0	-3.436075	4.46074476
H	0	2.176091	8.96037512	H	0	2.176091	9.00304876
H	0	0	10.50758312	H	0	0	10.55025676
H	0	-2.176091	8.96037512	H	0	-2.176091	9.00304876
C	0	0	9.42322812	C	0	0	9.46590176
C	0	0	-9.20911388	C	0	0	-9.16644024
N	0	0	2.73814012	B	0	0	2.78081376
B	0	0	-2.55339188	N	0	0	-2.51071824

A2[H$_N$P$_N$]				A1[H$_B$P$_B$]			
C	0	1.265996	-8.59666575	C	0	0	-9.13239766
C	0	1.589678	-7.23238975	C	0	1.265996	-8.54037666
C	0	-1.265996	-8.59666575	C	0	1.589678	-7.17610066
C	0	0.749116	-6.12886775	C	0	-1.265996	-8.54037666
C	0	-1.589678	-7.23238975	C	0	0.749116	-6.07257866
C	0	-0.749116	-6.12886775	C	0	-1.589678	-7.17610066
H	0	0	-10.27720475	C	0	-0.749116	-6.07257866
H	0	2.109709	-9.28131475	H	0	0	-10.22091566
H	0	2.655422	-7.00859975	H	0	2.109709	-9.22502566
H	0	-2.109709	-9.28131475	H	0	2.655422	-6.95231066
H	0	-2.655422	-7.00859975	H	0	-2.109709	-9.22502566
C	0	1.165553	-4.76713775	H	0	-2.655422	-6.95231066
C	0	0	-3.95143075	C	0	1.165553	-4.71084866
C	0	-1.165553	-4.76713775	C	0	0	-3.89514166
C	0	-1.305082	-1.91145175	C	0	-1.165553	-4.71084866
C	0	1.305082	-1.91145175	C	0	0	-2.47667566
C	0	-1.580366	-0.51932175	C	0	-1.305082	-1.85516266
C	0	1.580366	-0.51932175	C	0	1.305082	-1.85516266
C	0	-0.74355	0.57418225	C	0	-1.580366	-0.46303266
H	0	-2.642683	-0.28038175	C	0	1.580366	-0.46303266
C	0	0.74355	0.57418225	C	0	-0.74355	0.63047134
H	0	2.642683	-0.28038175	H	0	-2.642683	-0.22409266
C	0	-1.163845	1.94233425	C	0	0.74355	0.63047134
C	0	1.163845	1.94233425	H	0	2.642683	-0.22409266
C	0	-2.429854	-4.13375075	C	0	-1.163845	1.99862334
H	0	-3.353322	-4.70508675	C	0	1.163845	1.99862334
C	0	-2.468447	-2.76257575	C	0	0	2.81485634
H	0	-3.434671	-2.26630575	C	0	-2.429854	-4.07746166
C	0	2.468447	-2.76257575	H	0	-3.353322	-4.64879766
H	0	3.434671	-2.26630575	C	0	-2.468447	-2.70628666
C	0	2.429854	-4.13375075	H	0	-3.434671	-2.21001666
H	0	3.353322	-4.70508675	C	0	2.468447	-2.70628666
C	0	0	4.17785825	H	0	3.434671	-2.21001666
C	0	-1.306075	4.79960725	C	0	2.429854	-4.07746166
C	0	-1.585021	6.18635325	H	0	3.353322	-4.64879766
C	0	1.306075	4.79960725	C	0	-1.306075	4.85589634
C	0	-0.744681	7.28452525	C	0	-1.585021	6.24264234
C	0	1.585021	6.18635325	C	0	1.306075	4.85589634
C	0	0.744681	7.28452525	C	0	-0.744681	7.34081434
H	0	-2.646903	6.43014025	C	0	1.585021	6.24264234

H	0	2.646903	6.43014025	C	0	0.744681	7.34081434
C	0	-1.148431	8.63758525	H	0	-2.646903	6.48642934
C	0	1.148431	8.63758525	H	0	2.646903	6.48642934
C	0	2.426537	2.57256425	C	0	-1.148431	8.69387434
C	0	2.46902	3.94394225	C	0	1.148431	8.69387434
H	0	3.349235	1.99945025	C	0	2.426537	2.62885334
H	0	3.436075	4.43849825	C	0	2.46902	4.00023134
C	0	-2.426537	2.57256425	H	0	3.349235	2.05573934
C	0	-2.46902	3.94394225	H	0	3.436075	4.49478734
H	0	-3.349235	1.99945025	C	0	-2.426537	2.62885334
H	0	-3.436075	4.43849825	C	0	-2.46902	4.00023134
H	0	2.176091	8.98080225	H	0	-3.349235	2.05573934
H	0	0	10.52801025	H	0	-3.436075	4.49478734
H	0	-2.176091	8.98080225	H	0	2.176091	9.03709134
C	0	0	9.44365525	H	0	0	10.58429934
C	0	0	-9.18868675	H	0	-2.176091	9.03709134
N	0	0	2.75856725	B	0	0	9.49994434
N	0	0	-2.53296475	B	0	0	4.23414734

	A1[H$_B$P$_N$]				A1[H$_N$P$_B$]		
C	0	1.265996	-8.61687403	C	0	1.265996	-8.57463809
C	0	1.589678	-7.25259803	C	0	1.589678	-7.21036209
C	0	-1.265996	-8.61687403	C	0	-1.265996	-8.57463809
C	0	0.749116	-6.14907603	C	0	0.749116	-6.10684009
C	0	-1.589678	-7.25259803	C	0	-1.589678	-7.21036209
C	0	-0.749116	-6.14907603	C	0	-0.749116	-6.10684009
H	0	0	-10.29741303	H	0	0	-10.25517709
H	0	2.109709	-9.30152303	H	0	2.109709	-9.25928709
H	0	2.655422	-7.02880803	H	0	2.655422	-6.98657209
H	0	-2.109709	-9.30152303	H	0	-2.109709	-9.25928709
H	0	-2.655422	-7.02880803	H	0	-2.655422	-6.98657209
C	0	1.165553	-4.78734603	C	0	1.165553	-4.74511009
C	0	-1.165553	-4.78734603	C	0	-1.165553	-4.74511009
C	0	0	-2.55317303	C	0	0	-2.51093709
C	0	-1.305082	-1.93166003	C	0	-1.305082	-1.88942409
C	0	1.305082	-1.93166003	C	0	1.305082	-1.88942409
C	0	-1.580366	-0.53953003	C	0	-1.580366	-0.49729409
C	0	1.580366	-0.53953003	C	0	1.580366	-0.49729409
C	0	-0.74355	0.55397397	C	0	-0.74355	0.59620991
H	0	-2.642683	-0.30059003	H	0	-2.642683	-0.25835409
C	0	0.74355	0.55397397	C	0	0.74355	0.59620991
H	0	2.642683	-0.30059003	H	0	2.642683	-0.25835409
C	0	-1.163845	1.92212597	C	0	-1.163845	1.96436191
C	0	1.163845	1.92212597	C	0	1.163845	1.96436191
C	0	0	2.73835897	C	0	0	2.78059491
C	0	-2.429854	-4.15395903	C	0	-2.429854	-4.11172309
H	0	-3.353322	-4.72529503	H	0	-3.353322	-4.68305909
C	0	-2.468447	-2.78278403	C	0	-2.468447	-2.74054809
H	0	-3.434671	-2.28651403	H	0	-3.434671	-2.24427809
C	0	2.468447	-2.78278403	C	0	2.468447	-2.74054809
H	0	3.434671	-2.28651403	H	0	3.434671	-2.24427809
C	0	2.429854	-4.15395903	C	0	2.429854	-4.11172309
H	0	3.353322	-4.72529503	H	0	3.353322	-4.68305909
C	0	-1.306075	4.77939897	C	0	-1.306075	4.82163491
C	0	-1.585021	6.16614497	C	0	-1.585021	6.20838091
C	0	1.306075	4.77939897	C	0	1.306075	4.82163491
C	0	-0.744681	7.26431697	C	0	-0.744681	7.30655291
C	0	1.585021	6.16614497	C	0	1.585021	6.20838091
C	0	0.744681	7.26431697	C	0	0.744681	7.30655291
H	0	-2.646903	6.40993197	H	0	-2.646903	6.45216791
H	0	2.646903	6.40993197	H	0	2.646903	6.45216791
C	0	-1.148431	8.61737697	C	0	-1.148431	8.65961291
C	0	1.148431	8.61737697	C	0	1.148431	8.65961291
C	0	2.426537	2.55235597	C	0	2.426537	2.59459191

C	0	2.46902	3.92373397	C	0	2.46902	3.96596991
H	0	3.349235	1.97924197	H	0	3.349235	2.02147791
H	0	3.436075	4.41828997	H	0	3.436075	4.46052591
C	0	-2.426537	2.55235597	C	0	-2.426537	2.59459191
C	0	-2.46902	3.92373397	C	0	-2.46902	3.96596991
H	0	-3.349235	1.97924197	H	0	-3.349235	2.02147791
H	0	-3.436075	4.41828997	H	0	-3.436075	4.46052591
H	0	2.176091	8.96059397	H	0	2.176091	9.00282991
H	0	0	10.50780197	H	0	0	10.55003791
H	0	-2.176091	8.96059397	H	0	-2.176091	9.00282991
N	0	0	-3.97163903	B	0	0	-3.92940309
B	0	0	-9.20889503	N	0	0	-9.16665909
C	0	0	9.42344697	C	0	0	9.46568291
C	0	0	4.15764997	C	0	0	4.19988591

		A1[H_NP_N]				A1[H_BP_B]A2[H_BP_B]	
C	0	1.265996	-8.65024939	C	0	1.265996	-8.64866949
C	0	1.589678	-7.28597339	C	0	1.589678	-7.28439349
C	0	-1.265996	-8.65024939	C	0	-1.265996	-8.64866949
C	0	0.749116	-6.18245139	C	0	0.749116	-6.18087149
C	0	-1.589678	-7.28597339	C	0	-1.589678	-7.28439349
C	0	-0.749116	-6.18245139	C	0	-0.749116	-6.18087149
H	0	0	-10.33078839	H	0	0	-10.32920849
H	0	2.109709	-9.33489839	H	0	2.109709	-9.33331849
H	0	2.655422	-7.06218339	H	0	2.655422	-7.06060349
H	0	-2.109709	-9.33489839	H	0	-2.109709	-9.33331849
H	0	-2.655422	-7.06218339	H	0	-2.655422	-7.06060349
C	0	1.165553	-4.82072139	C	0	1.165553	-4.81914149
C	0	-1.165553	-4.82072139	C	0	-1.165553	-4.81914149
C	0	0	-2.58654839	C	0	-1.305082	-1.96345549
C	0	-1.305082	-1.96503539	C	0	1.305082	-1.96345549
C	0	1.305082	-1.96503539	C	0	-1.580366	-0.57132549
C	0	-1.580366	-0.57290539	C	0	1.580366	-0.57132549
C	0	1.580366	-0.57290539	C	0	-0.74355	0.52217851
C	0	-0.74355	0.52059861	H	0	-2.642683	-0.33238549
H	0	-2.642683	-0.33396539	C	0	0.74355	0.52217851
C	0	0.74355	0.52059861	H	0	2.642683	-0.33238549
H	0	2.642683	-0.33396539	C	0	-1.163845	1.89033051
C	0	-1.163845	1.88875061	C	0	1.163845	1.89033051
C	0	1.163845	1.88875061	C	0	-2.429854	-4.18575449
C	0	0	2.70498361	H	0	-3.353322	-4.75709049
C	0	-2.429854	-4.18733439	C	0	-2.468447	-2.81457949
H	0	-3.353322	-4.75867039	H	0	-3.434671	-2.31830949
C	0	-2.468447	-2.81615939	C	0	2.468447	-2.81457949
H	0	-3.434671	-2.31988939	H	0	3.434671	-2.31830949
C	0	2.468447	-2.81615939	C	0	2.429854	-4.18575449
H	0	3.434671	-2.31988939	H	0	3.353322	-4.75709049
C	0	2.429854	-4.18733439	C	0	0	4.12585451
H	0	3.353322	-4.75867039	C	0	-1.306075	4.74760351
C	0	-1.306075	4.74602361	C	0	-1.585021	6.13434951
C	0	-1.585021	6.13276961	C	0	1.306075	4.74760351
C	0	1.306075	4.74602361	C	0	-0.744681	7.23252151
C	0	-0.744681	7.23094161	C	0	1.585021	6.13434951
C	0	1.585021	6.13276961	C	0	0.744681	7.23252151
C	0	0.744681	7.23094161	H	0	-2.646903	6.37813651
H	0	-2.646903	6.37655661	H	0	2.646903	6.37813651
H	0	2.646903	6.37655661	C	0	-1.148431	8.58558151
C	0	-1.148431	8.58400161	C	0	0	9.39165151
C	0	1.148431	8.58400161	C	0	1.148431	8.58558151
C	0	2.426537	2.51898061	C	0	2.426537	2.52056051
C	0	2.46902	3.89035861	C	0	2.46902	3.89193851
H	0	3.349235	1.94586661	H	0	3.349235	1.94744651
H	0	3.436075	4.38491461	H	0	3.436075	4.38649451
C	0	-2.426537	2.51898061	C	0	-2.426537	2.52056051

C	0	-2.46902	3.89035861	C	0	-2.46902	3.89193851
H	0	-3.349235	1.94586661	H	0	-3.349235	1.94744651
H	0	-3.436075	4.38491461	H	0	-3.436075	4.38649451
H	0	2.176091	8.92721861	H	0	2.176091	8.92879851
H	0	0	10.47442661	H	0	0	10.47600651
H	0	-2.176091	8.92721861	H	0	-2.176091	8.92879851
N	0	0	-4.00501439	B	0	0	-9.24069049
N	0	0	-9.24227039	B	0	0	-4.00343449
C	0	0	9.39007161	B	0	0	-2.58496849
C	0	0	4.12427461	B	0	0	2.70656351

	A1[H_BP_N]A2[H_BP_N]				**A1[H_NP_B]A2[H_NP_B]**		
C	0	1.265996	-8.63821085	C	0	1.265996	-8.55330127
C	0	1.589678	-7.27393485	C	0	1.589678	-7.18902527
C	0	-1.265996	-8.63821085	C	0	-1.265996	-8.55330127
C	0	0.749116	-6.17041285	C	0	0.749116	-6.08550327
C	0	-1.589678	-7.27393485	C	0	-1.589678	-7.18902527
C	0	-0.749116	-6.17041285	C	0	-0.749116	-6.08550327
H	0	0	-10.31874985	H	0	0	-10.23384027
H	0	2.109709	-9.32285985	H	0	2.109709	-9.23795027
H	0	2.655422	-7.05014485	H	0	2.655422	-6.96523527
H	0	-2.109709	-9.32285985	H	0	-2.109709	-9.23795027
H	0	-2.655422	-7.05014485	H	0	-2.655422	-6.96523527
C	0	1.165553	-4.80868285	C	0	1.165553	-4.72377327
C	0	-1.165553	-4.80868285	C	0	-1.165553	-4.72377327
C	0	-1.305082	-1.95299685	C	0	-1.305082	-1.86808727
C	0	1.305082	-1.95299685	C	0	1.305082	-1.86808727
C	0	-1.580366	-0.56086685	C	0	-1.580366	-0.47595727
C	0	1.580366	-0.56086685	C	0	1.580366	-0.47595727
C	0	-0.74355	0.53263715	C	0	-0.74355	0.61754673
H	0	-2.642683	-0.32192685	H	0	-2.642683	-0.23701727
C	0	0.74355	0.53263715	C	0	0.74355	0.61754673
H	0	2.642683	-0.32192685	H	0	2.642683	-0.23701727
C	0	-1.163845	1.90078915	C	0	-1.163845	1.98569873
C	0	1.163845	1.90078915	C	0	1.163845	1.98569873
C	0	-2.429854	-4.17529585	C	0	-2.429854	-4.09038627
H	0	-3.353322	-4.74663185	H	0	-3.353322	-4.66172227
C	0	-2.468447	-2.80412085	C	0	-2.468447	-2.71921127
H	0	-3.434671	-2.30785085	H	0	-3.434671	-2.22294127
C	0	2.468447	-2.80412085	C	0	2.468447	-2.71921127
H	0	3.434671	-2.30785085	H	0	3.434671	-2.22294127
C	0	2.429854	-4.17529585	C	0	2.429854	-4.09038627
H	0	3.353322	-4.74663185	H	0	3.353322	-4.66172227
C	0	0	4.13631315	C	0	0	4.22122273
C	0	-1.306075	4.75806215	C	0	-1.306075	4.84297173
C	0	-1.585021	6.14480815	C	0	-1.585021	6.22971773
C	0	1.306075	4.75806215	C	0	1.306075	4.84297173
C	0	-0.744681	7.24298015	C	0	-0.744681	7.32788973
C	0	1.585021	6.14480815	C	0	1.585021	6.22971773
C	0	0.744681	7.24298015	C	0	0.744681	7.32788973
H	0	-2.646903	6.38859515	H	0	-2.646903	6.47350473
H	0	2.646903	6.38859515	H	0	2.646903	6.47350473
C	0	-1.148431	8.59604015	C	0	-1.148431	8.68094973
C	0	0	9.40211015	C	0	0	9.48701973
C	0	1.148431	8.59604015	C	0	1.148431	8.68094973
C	0	2.426537	2.53101915	C	0	2.426537	2.61592873
C	0	2.46902	3.90239715	C	0	2.46902	3.98730673
H	0	3.349235	1.95790515	H	0	3.349235	2.04281473
H	0	3.436075	4.39695315	H	0	3.436075	4.48186273
C	0	-2.426537	2.53101915	C	0	-2.426537	2.61592873
C	0	-2.46902	3.90239715	C	0	-2.46902	3.98730673
H	0	-3.349235	1.95790515	H	0	-3.349235	2.04281473
H	0	-3.436075	4.39695315	H	0	-3.436075	4.48186273
H	0	2.176091	8.93925715	H	0	2.176091	9.02416673

H	0	0	10.48646515	H	0	0	10.57137473
H	0	-2.176091	8.93925715	H	0	-2.176091	9.02416673
B	0	0	-9.23023185	N	0	0	-9.14532227
B	0	0	-2.57450985	N	0	0	-2.48960027
N	0	0	-3.99297585	B	0	0	-3.90806627
N	0	0	2.71702215	B	0	0	2.80193173

A1[H$_N$P$_N$]A2[H$_N$P$_N$]				A2[H$_B$P$_B$]A3[H$_B$P$_B$]			
C	0	1.265996	-8.54452242	C	0	1.265996	-8.53899067
C	0	1.589678	-7.18024642	C	0	1.589678	-7.17471467
C	0	-1.265996	-8.54452242	C	0	-1.265996	-8.53899067
C	0	0.749116	-6.07672442	C	0	0.749116	-6.07119267
C	0	-1.589678	-7.18024642	C	0	-1.589678	-7.17471467
C	0	-0.749116	-6.07672442	C	0	-0.749116	-6.07119267
H	0	0	-10.22506142	H	0	0	-10.21952967
H	0	2.109709	-9.22917142	H	0	2.109709	-9.22363967
H	0	2.655422	-6.95645642	H	0	2.655422	-6.95092467
H	0	-2.109709	-9.22917142	H	0	-2.109709	-9.22363967
H	0	-2.655422	-6.95645642	H	0	-2.655422	-6.95092467
C	0	1.165553	-4.71499442	C	0	1.165553	-4.70946267
C	0	-1.165553	-4.71499442	C	0	-1.165553	-4.70946267
C	0	-1.305082	-1.85930842	C	0	-1.305082	-1.85377667
C	0	1.305082	-1.85930842	C	0	1.305082	-1.85377667
C	0	-1.580366	-0.46717842	C	0	-1.580366	-0.46164667
C	0	1.580366	-0.46717842	C	0	1.580366	-0.46164667
C	0	-0.74355	0.62632558	C	0	-0.74355	0.63185733
H	0	-2.642683	-0.22823842	H	0	-2.642683	-0.22270667
C	0	0.74355	0.62632558	C	0	0.74355	0.63185733
H	0	2.642683	-0.22823842	H	0	2.642683	-0.22270667
C	0	-1.163845	1.99447758	C	0	-1.163845	2.00000933
C	0	1.163845	1.99447758	C	0	1.163845	2.00000933
C	0	-2.429854	-4.08160742	C	0	-2.429854	-4.07607567
H	0	-3.353322	-4.65294342	H	0	-3.353322	-4.64741167
C	0	-2.468447	-2.71043242	C	0	-2.468447	-2.70490067
H	0	-3.434671	-2.21416242	H	0	-3.434671	-2.20863067
C	0	2.468447	-2.71043242	C	0	2.468447	-2.70490067
H	0	3.434671	-2.21416242	H	0	3.434671	-2.20863067
C	0	2.429854	-4.08160742	C	0	2.429854	-4.07607567
H	0	3.353322	-4.65294342	H	0	3.353322	-4.64741167
C	0	0	4.23000158	C	0	-1.306075	4.85728233
C	0	-1.306075	4.85175058	C	0	-1.585021	6.24402833
C	0	-1.585021	6.23849658	C	0	1.306075	4.85728233
C	0	1.306075	4.85175058	C	0	-0.744681	7.34220033
C	0	-0.744681	7.33666858	C	0	1.585021	6.24402833
C	0	1.585021	6.23849658	C	0	0.744681	7.34220033
C	0	0.744681	7.33666858	H	0	-2.646903	6.48781533
H	0	-2.646903	6.48228358	H	0	2.646903	6.48781533
H	0	2.646903	6.48228358	C	0	-1.148431	8.69526033
C	0	-1.148431	8.68972858	C	0	1.148431	8.69526033
C	0	0	9.49579858	C	0	2.426537	2.63023933
C	0	1.148431	8.68972858	C	0	2.46902	4.00161733
C	0	2.426537	2.62470758	H	0	3.349235	2.05712533
C	0	2.46902	3.99608558	H	0	3.436075	4.49617333
H	0	3.349235	2.05159358	C	0	-2.426537	2.63023933
H	0	3.436075	4.49064158	C	0	-2.46902	4.00161733
C	0	-2.426537	2.62470758	H	0	-3.349235	2.05712533
C	0	-2.46902	3.99608558	H	0	-3.436075	4.49617333
H	0	-3.349235	2.05159358	H	0	2.176091	9.03847733
H	0	-3.436075	4.49064158	H	0	0	10.58568533
H	0	2.176091	9.03294558	H	0	-2.176091	9.03847733
H	0	0	10.58015358	B	0	0	-2.47528967
H	0	-2.176091	9.03294558	B	0	0	2.81624233

N	0	0	-9.13654342	C	0	0	-3.89375567
N	0	0	-3.89928742	C	0	0	-9.13101167
N	0	0	-2.48082142	B	0	0	9.50133033
N	0	0	2.81071058	B	0	0	4.23553333
		A2[H$_B$P$_N$]A3[H$_B$P$_N$]				**A2[H$_N$P$_B$]A3[H$_N$P$_B$]**	
C	0	1.265996	-8.63832594	C	0	1.265996	-8.55340504
C	0	1.589678	-7.27404994	C	0	1.589678	-7.18912904
C	0	-1.265996	-8.63832594	C	0	-1.265996	-8.55340504
C	0	0.749116	-6.17052794	C	0	0.749116	-6.08560704
C	0	-1.589678	-7.27404994	C	0	-1.589678	-7.18912904
C	0	-0.749116	-6.17052794	C	0	-0.749116	-6.08560704
H	0	0	-10.31886494	H	0	0	-10.23394404
H	0	2.109709	-9.32297494	H	0	2.109709	-9.23805404
H	0	2.655422	-7.05025994	H	0	2.655422	-6.96533904
H	0	-2.109709	-9.32297494	H	0	-2.109709	-9.23805404
H	0	-2.655422	-7.05025994	H	0	-2.655422	-6.96533904
C	0	1.165553	-4.80879794	C	0	1.165553	-4.72387704
C	0	-1.165553	-4.80879794	C	0	-1.165553	-4.72387704
C	0	-1.305082	-1.95311194	C	0	-1.305082	-1.86819104
C	0	1.305082	-1.95311194	C	0	1.305082	-1.86819104
C	0	-1.580366	-0.56098194	C	0	-1.580366	-0.47606104
C	0	1.580366	-0.56098194	C	0	1.580366	-0.47606104
C	0	-0.74355	0.53252206	C	0	-0.74355	0.61744296
H	0	-2.642683	-0.32204194	H	0	-2.642683	-0.23712104
C	0	0.74355	0.53252206	C	0	0.74355	0.61744296
H	0	2.642683	-0.32204194	H	0	2.642683	-0.23712104
C	0	-1.163845	1.90067406	C	0	-1.163845	1.98559496
C	0	1.163845	1.90067406	C	0	1.163845	1.98559496
C	0	-2.429854	-4.17541094	C	0	-2.429854	-4.09049004
H	0	-3.353322	-4.74674694	H	0	-3.353322	-4.66182604
C	0	-2.468447	-2.80423594	C	0	-2.468447	-2.71931504
H	0	-3.434671	-2.30796594	H	0	-3.434671	-2.22304504
C	0	2.468447	-2.80423594	C	0	2.468447	-2.71931504
H	0	3.434671	-2.30796594	H	0	3.434671	-2.22304504
C	0	2.429854	-4.17541094	C	0	2.429854	-4.09049004
H	0	3.353322	-4.74674694	H	0	3.353322	-4.66182604
C	0	-1.306075	4.75794706	C	0	-1.306075	4.84286796
C	0	-1.585021	6.14469306	C	0	-1.585021	6.22961396
C	0	1.306075	4.75794706	C	0	1.306075	4.84286796
C	0	-0.744681	7.24286506	C	0	-0.744681	7.32778596
C	0	1.585021	6.14469306	C	0	1.585021	6.22961396
C	0	0.744681	7.24286506	C	0	0.744681	7.32778596
H	0	-2.646903	6.38848006	H	0	-2.646903	6.47340096
H	0	2.646903	6.38848006	H	0	2.646903	6.47340096
C	0	-1.148431	8.59592506	C	0	-1.148431	8.68084596
C	0	1.148431	8.59592506	C	0	1.148431	8.68084596
C	0	2.426537	2.53090406	C	0	2.426537	2.61582496
C	0	2.46902	3.90228206	C	0	2.46902	3.98720296
H	0	3.349235	1.95779006	H	0	3.349235	2.04271096
H	0	3.436075	4.39683806	H	0	3.436075	4.48175896
C	0	-2.426537	2.53090406	C	0	-2.426537	2.61582496
C	0	-2.46902	3.90228206	C	0	-2.46902	3.98720296
H	0	-3.349235	1.95779006	H	0	-3.349235	2.04271096
H	0	-3.436075	4.39683806	H	0	-3.436075	4.48175896
H	0	2.176091	8.93914206	H	0	2.176091	9.02406296
H	0	0	10.48635006	H	0	0	10.57127096
H	0	-2.176091	8.93914206	H	0	-2.176091	9.02406296
B	0	0	-2.57462494	N	0	0	-9.14542604
N	0	0	2.71690706	B	0	0	-3.90817004
C	0	0	-3.99309094	C	0	0	-2.48970404
C	0	0	-9.23034694	C	0	0	2.80182796
B	0	0	4.13619806	N	0	0	4.22111896

N	0	0	9.40199506	B	0	0	9.48691596
	A2[H_NP_N]A3[H_NP_N]				**A1[H_BP_B]A3[H_BP_B]**		
C	0	1.260969	-8.56685391	C	0	1.265996	-8.59376821
C	0	1.591273	-7.25766291	C	0	1.589678	-7.22949221
C	0	-1.260969	-8.56685391	C	0	-1.265996	-8.59376821
C	0	0.708707	-6.10458891	C	0	0.749116	-6.12597021
C	0	-1.591273	-7.25766291	C	0	-1.589678	-7.22949221
C	0	-0.708707	-6.10458891	C	0	-0.749116	-6.12597021
H	0	0	-10.16740391	H	0	0	-10.27430721
H	0	2.056954	-9.30507391	H	0	2.109709	-9.27841721
H	0	2.65772	-7.05300391	H	0	2.655422	-7.00570221
H	0	-2.056954	-9.30507391	H	0	-2.109709	-9.27841721
H	0	-2.65772	-7.05300391	H	0	-2.655422	-7.00570221
C	0	1.151847	-4.75342491	C	0	1.165553	-4.76424021
C	0	-1.151847	-4.75342491	C	0	-1.165553	-4.76424021
C	0	-1.282645	-1.89681891	C	0	-1.305082	-1.90855421
C	0	1.282645	-1.89681891	C	0	1.305082	-1.90855421
C	0	-1.546067	-0.52901191	C	0	-1.580366	-0.51642421
C	0	1.546067	-0.52901191	C	0	1.580366	-0.51642421
C	0	-0.717908	0.60407909	C	0	-0.74355	0.57707979
H	0	-2.61049	-0.31811491	H	0	-2.642683	-0.27748421
C	0	0.717908	0.60407909	C	0	0.74355	0.57707979
H	0	2.61049	-0.31811491	H	0	2.642683	-0.27748421
C	0	-1.136157	1.94321009	C	0	-1.163845	1.94523179
C	0	1.136157	1.94321009	C	0	1.163845	1.94523179
C	0	-2.409477	-4.12108891	C	0	-2.429854	-4.13085321
H	0	-3.336578	-4.68620391	H	0	-3.353322	-4.70218921
C	0	-2.438447	-2.75271691	C	0	-2.468447	-2.75967821
H	0	-3.392791	-2.23926891	H	0	-3.434671	-2.26340821
C	0	2.438447	-2.75271691	C	0	2.468447	-2.75967821
H	0	3.392791	-2.23926891	H	0	3.434671	-2.26340821
C	0	2.409477	-4.12108891	C	0	2.429854	-4.13085321
H	0	3.336578	-4.68620391	H	0	3.353322	-4.70218921
C	0	-1.314593	4.79386109	C	0	-1.306075	4.80250479
C	0	-1.587139	6.15013409	C	0	-1.585021	6.18925079
C	0	1.314593	4.79386109	C	0	1.306075	4.80250479
C	0	-0.722008	7.28434809	C	0	-0.744681	7.28742279
C	0	1.587139	6.15013409	C	0	1.585021	6.18925079
C	0	0.722008	7.28434809	C	0	0.744681	7.28742279
H	0	-2.646871	6.39562709	H	0	-2.646903	6.43303779
H	0	2.646871	6.39562709	H	0	2.646903	6.43303779
C	0	-1.124814	8.61291709	C	0	-1.148431	8.64048279
C	0	1.124814	8.61291709	C	0	1.148431	8.64048279
C	0	2.401894	2.56854609	C	0	2.426537	2.57546179
C	0	2.477813	3.92275609	C	0	2.46902	3.94683979
H	0	3.296785	1.95622609	H	0	3.349235	2.00234779
H	0	3.449572	4.40578909	H	0	3.436075	4.44139579
C	0	-2.401894	2.56854609	C	0	-2.426537	2.57546179
C	0	-2.477813	3.92275609	C	0	-2.46902	3.94683979
H	0	-3.296785	1.95622609	H	0	-3.349235	2.00234779
H	0	-3.449572	4.40578909	H	0	-3.436075	4.44139579
H	0	2.115366	9.04260009	H	0	2.176091	8.98369979
H	0	0	10.40873009	H	0	0	10.53090779
H	0	-2.115366	9.04260009	H	0	-2.176091	8.98369979
N	0	0	-9.16141091	B	0	0	-9.18578921
N	0	0	9.40198809	B	0	0	-3.94853321
N	0	0	-3.92222691	C	0	0	-2.53006721
N	0	0	4.14034409	C	0	0	2.76146479
C	0	0	-2.54326091	B	0	0	4.18075579
C	0	0	2.77300209	B	0	0	9.44655279
	A1[H_BP_N]A3[H_BP_N]				**A1[H_NP_B]A3[H_NP_B]**		

C	0	1.265996	-8.63810708	C	0	1.265996	-8.55340504
C	0	1.589678	-7.27383108	C	0	1.589678	-7.18912904
C	0	-1.265996	-8.63810708	C	0	-1.265996	-8.55340504
C	0	0.749116	-6.17030908	C	0	0.749116	-6.08560704
C	0	-1.589678	-7.27383108	C	0	-1.589678	-7.18912904
C	0	-0.749116	-6.17030908	C	0	-0.749116	-6.08560704
H	0	0	-10.31864608	H	0	0	-10.23394404
H	0	2.109709	-9.32275608	H	0	2.109709	-9.23805404
H	0	2.655422	-7.05004108	H	0	2.655422	-6.96533904
H	0	-2.109709	-9.32275608	H	0	-2.109709	-9.23805404
H	0	-2.655422	-7.05004108	H	0	-2.655422	-6.96533904
C	0	1.165553	-4.80857908	C	0	1.165553	-4.72387704
C	0	-1.165553	-4.80857908	C	0	-1.165553	-4.72387704
C	0	-1.305082	-1.95289308	C	0	-1.305082	-1.86819104
C	0	1.305082	-1.95289308	C	0	1.305082	-1.86819104
C	0	-1.580366	-0.56076308	C	0	-1.580366	-0.47606104
C	0	1.580366	-0.56076308	C	0	1.580366	-0.47606104
C	0	-0.74355	0.53274092	C	0	-0.74355	0.61744296
H	0	-2.642683	-0.32182308	H	0	-2.642683	-0.23712104
C	0	0.74355	0.53274092	C	0	0.74355	0.61744296
H	0	2.642683	-0.32182308	H	0	2.642683	-0.23712104
C	0	-1.163845	1.90089292	C	0	-1.163845	1.98559496
C	0	1.163845	1.90089292	C	0	1.163845	1.98559496
C	0	-2.429854	-4.17519208	C	0	-2.429854	-4.09049004
H	0	-3.353322	-4.74652808	H	0	-3.353322	-4.66182604
C	0	-2.468447	-2.80401708	C	0	-2.468447	-2.71931504
H	0	-3.434671	-2.30774708	H	0	-3.434671	-2.22304504
C	0	2.468447	-2.80401708	C	0	2.468447	-2.71931504
H	0	3.434671	-2.30774708	H	0	3.434671	-2.22304504
C	0	2.429854	-4.17519208	C	0	2.429854	-4.09049004
H	0	3.353322	-4.74652808	H	0	3.353322	-4.66182604
C	0	-1.306075	4.75816592	C	0	-1.306075	4.84286796
C	0	-1.585021	6.14491192	C	0	-1.585021	6.22961396
C	0	1.306075	4.75816592	C	0	1.306075	4.84286796
C	0	-0.744681	7.24308392	C	0	-0.744681	7.32778596
C	0	1.585021	6.14491192	C	0	1.585021	6.22961396
C	0	0.744681	7.24308392	C	0	0.744681	7.32778596
H	0	-2.646903	6.38869892	H	0	-2.646903	6.47340096
H	0	2.646903	6.38869892	H	0	2.646903	6.47340096
C	0	-1.148431	8.59614392	C	0	-1.148431	8.68084596
C	0	1.148431	8.59614392	C	0	1.148431	8.68084596
C	0	2.426537	2.53112292	C	0	2.426537	2.61582496
C	0	2.46902	3.90250092	C	0	2.46902	3.98720296
H	0	3.349235	1.95800892	H	0	3.349235	2.04271096
H	0	3.436075	4.39705692	H	0	3.436075	4.48175896
C	0	-2.426537	2.53112292	C	0	-2.426537	2.61582496
C	0	-2.46902	3.90250092	C	0	-2.46902	3.98720296
H	0	-3.349235	1.95800892	H	0	-3.349235	2.04271096
H	0	-3.436075	4.39705692	H	0	-3.436075	4.48175896
H	0	2.176091	8.93936092	H	0	2.176091	9.02406296
H	0	0	10.48656892	H	0	0	10.57127096
H	0	-2.176091	8.93936092	H	0	-2.176091	9.02406296
B	0	0	-9.23012808	N	0	0	-9.14542604
N	0	0	-3.99287208	B	0	0	-3.90817004
C	0	0	2.71712592	C	0	0	-2.48970404
C	0	0	-2.57440608	C	0	0	2.80182796
B	0	0	4.13641692	N	0	0	4.22111896
N	0	0	9.40221392	B	0	0	9.48691596

A1[$H_N P_N$]A3[$H_N P_N$]

C	0	1.260969	-8.56685391
C	0	1.591273	-7.25766291
C	0	-1.260969	-8.56685391

C	0	0.708707	-6.10458891
C	0	-1.591273	-7.25766291
C	0	-0.708707	-6.10458891
H	0	0	-10.16740391
H	0	2.056954	-9.30507391
H	0	2.65772	-7.05300391
H	0	-2.056954	-9.30507391
H	0	-2.65772	-7.05300391
C	0	1.151847	-4.75342491
C	0	-1.151847	-4.75342491
C	0	-1.282645	-1.89681891
C	0	1.282645	-1.89681891
C	0	-1.546067	-0.52901191
C	0	1.546067	-0.52901191
C	0	-0.717908	0.60407909
H	0	-2.61049	-0.31811491
C	0	0.717908	0.60407909
H	0	2.61049	-0.31811491
C	0	-1.136157	1.94321009
C	0	1.136157	1.94321009
C	0	-2.409477	-4.12108891
H	0	-3.336578	-4.68620391
C	0	-2.438447	-2.75271691
H	0	-3.392791	-2.23926891
C	0	2.438447	-2.75271691
H	0	3.392791	-2.23926891
C	0	2.409477	-4.12108891
H	0	3.336578	-4.68620391
C	0	-1.314593	4.79386109
C	0	-1.587139	6.15013409
C	0	1.314593	4.79386109
C	0	-0.722008	7.28434809
C	0	1.587139	6.15013409
C	0	0.722008	7.28434809
H	0	-2.646871	6.39562709
H	0	2.646871	6.39562709
C	0	-1.124814	8.61291709
C	0	1.124814	8.61291709
C	0	2.401894	2.56854609
C	0	2.477813	3.92275609
H	0	3.296785	1.95622609
H	0	3.449572	4.40578909
C	0	-2.401894	2.56854609
C	0	-2.477813	3.92275609
H	0	-3.296785	1.95622609
H	0	-3.449572	4.40578909
H	0	2.115366	9.04260009
H	0	0	10.40873009
H	0	-2.115366	9.04260009
N	0	0	-9.16141091
N	0	0	9.40198809
N	0	0	-3.92222691
N	0	0	4.14034409
C	0	0	-2.54326091
C	0	0	2.77300209