Supporting information

Megamerger of porphyrin (phthalocyanine) with azulene based graphene nanosheet for high-performance nonlinear optical materials

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Supporting Information list:

Figure S1 Structures of porphyrin and phthalocyanine derivatives. A: azulene; P: porphyrin; P_N: N-substituted porphyrin; Pc: phthalocyanine; Pc_N: N-substituted phthalocyanine, M = Mg, Ni, Zn; Atoms in black are carbon and in blue are nitrogen.

Figure S2 Evolution of the static first hyperpolarizability ($<\beta_0>$) and the static second hyperpolarizability ($<\gamma_0>$) with the numbers of excited states in P_N-A-A and P_N-3A-A, respectively.

Figure S3 The frontier molecular orbitals (H: HOMO; L: LUMO) correlation and energy diagrams of P-3A and P_N-3A predicted with B3LYP/6-31G (d, p).

Figure S4 Evolution of the static first hyperpolarizability ($<\beta_0>$) (in 10^{-30} esu) with the electron excitation in M-P-mA, M-P_N-mA-N, M-P_N-mA-A and M-Pc-mA-N predicted by using CAM-B3LYP/6–31++G (d, p).

Figure S5 The two-dimensional second order nonlinear optical spectra (in 10^{-30} esu) of (a) P_N-3A-A, (b) Mg-P_N-3A-A and (c) Ni-P_N-3A-A scanned up to 7.00 eV with a step size of 0.05 eV by using TD-CAM-B3LYP/6–31++G (d, p) and the sum-over-states model.

Figure S6 The 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) and (b) P_N-3A-A, (c) Mg-P_N-3A-A, (d) and (e) Ni-P_N-3A-A with step size of 0.005 eV .

Figure S7 The evolution of third order nonlinear optic properties with electron excitations of P_N-3A-A at

specific external fields.

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Figure S11 (a) Fine-scanned TDTPA of P_N-3A-A from 1.11 eV to 2.10 eV; (b)Fine-scanned TDTPA of Mg-P_N-3A-A from 1.15 eV to 1.45 eV; (c)Fine-scanned TDTPA of Ni-P_N-3A-A from 1.15 eV to 1.45 eV.

Table S1 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 ($<\beta_0>$ and $<\gamma_0>$), the $<\beta_0>$ (in 10^{-30} esu) and $<\gamma_0>$ (in 10^{-34} esu) per heavy atom ($<\beta_0>$/N and $<\gamma_0>$/N) of porphyrin derivatives 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 electronic spectra absorption peaks with transition nature in P_N-3A-A, Mg-P_N-3A-A and Ni-P-3A-A (*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 unit).

Table S3 Calculated important parameters of $(\beta_{ijk})_m$ [i, j, k∈(x, y, z)] ($\times10^{-30}$ esu) of P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. 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 P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. *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 Important parameters of $(\gamma_{ijk})_m$ ($\times10^{-34}$ esu) of P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. 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 ($<\gamma_0>$), m = 0 is the ground state, and m > 0 is the mth excited state. (γxxxx represents γ

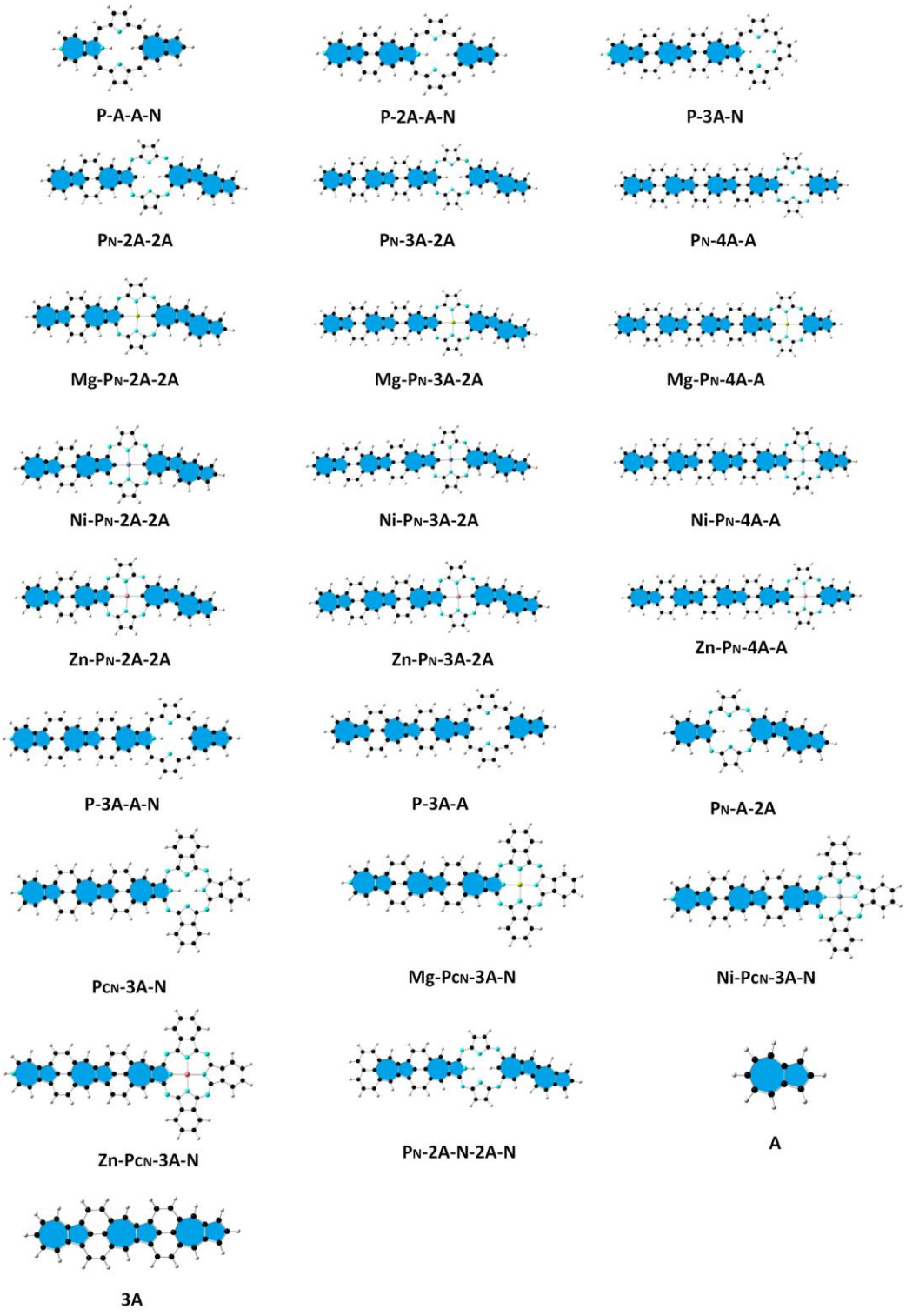
along the X direction, γ_{YYYY} represents γ along the Y direction)

Table S6 Important parameters of $(\gamma_{ijk})_m$ ($\times 10^{-34}$ esu) of P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. The $(\gamma_{ijk})_m$ is the second hyperpolarizability tensor of the m_{th} excited state (S_m) with a major contribution to the static first hyperpolarizability ($<\gamma_0>$), m = 0 is the ground state, and m > 0 is the mth excited state. (γxxxx represents γ along the X direction, γ_{YYYY} represents γ along the Y direction)

Table S7 The strong response and corresponding major electron excitation contribution of the dynamic third order nonlinear optic process for P_N-3A-A. TPA is in 10^{-50} cm^4·s/photon. DFWM, THG and EFISH are in 10^{-34} esu.

Table S8 The strong response and corresponding major electron excitation contribution of the dynamic third order nonlinear optic process for Mg-P_N-3A-A. TPA is in 10^{-50} cm^4·s/photon. DFWM, THG and EFISH are in 10^{-34} esu.

Table S9 The strong response and corresponding major electron excitation contribution of the dynamic third order nonlinear optic process for Ni-P_N-3A-A. TPA is in 10^{-50} cm^4·s/photon. DFWM, THG and EFISH are in 10^{-34} esu.



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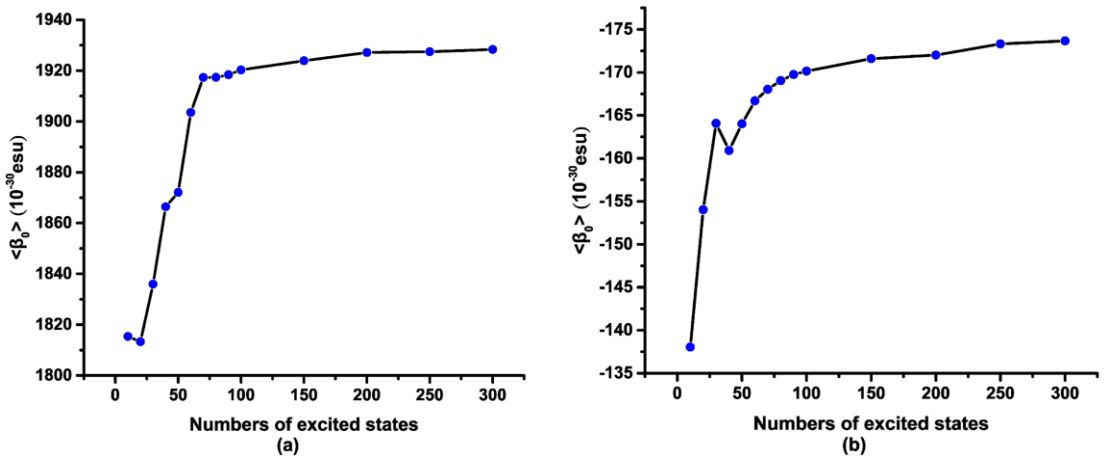
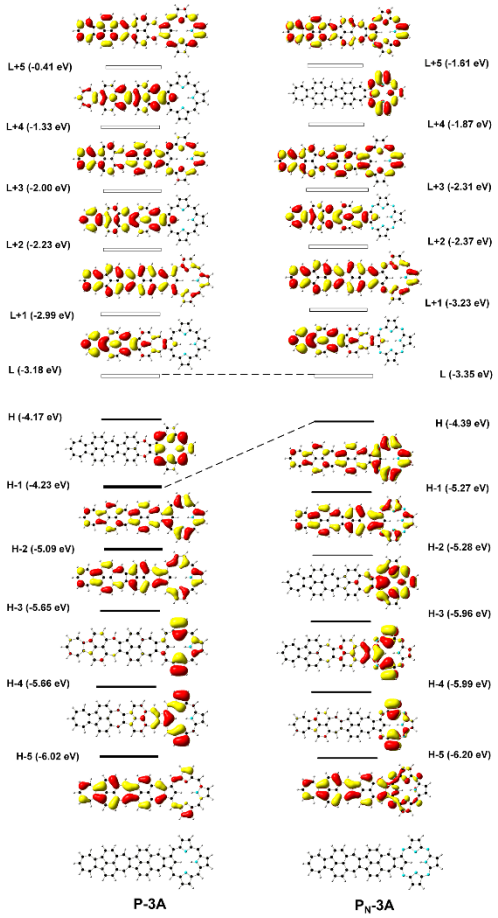


Figure S2 Evolution of the static first hyperpolarizability (<β_0>) and the static second hyperpolarizability (<γ_0>) with the numbers of excited states in P_N-A-A and P_N-3A-A, respectively.



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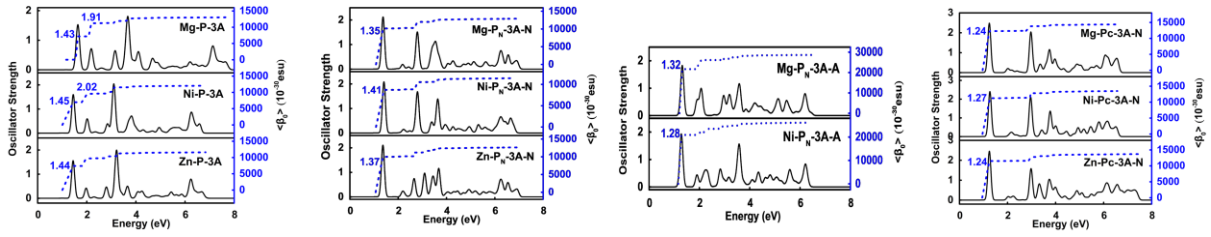

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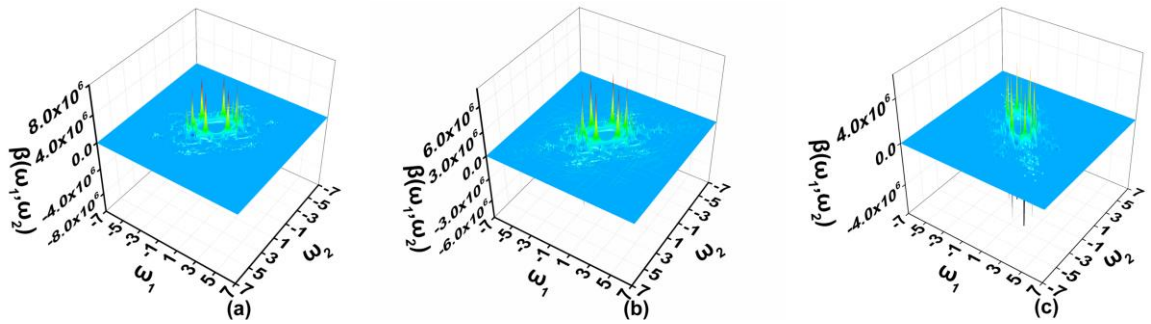

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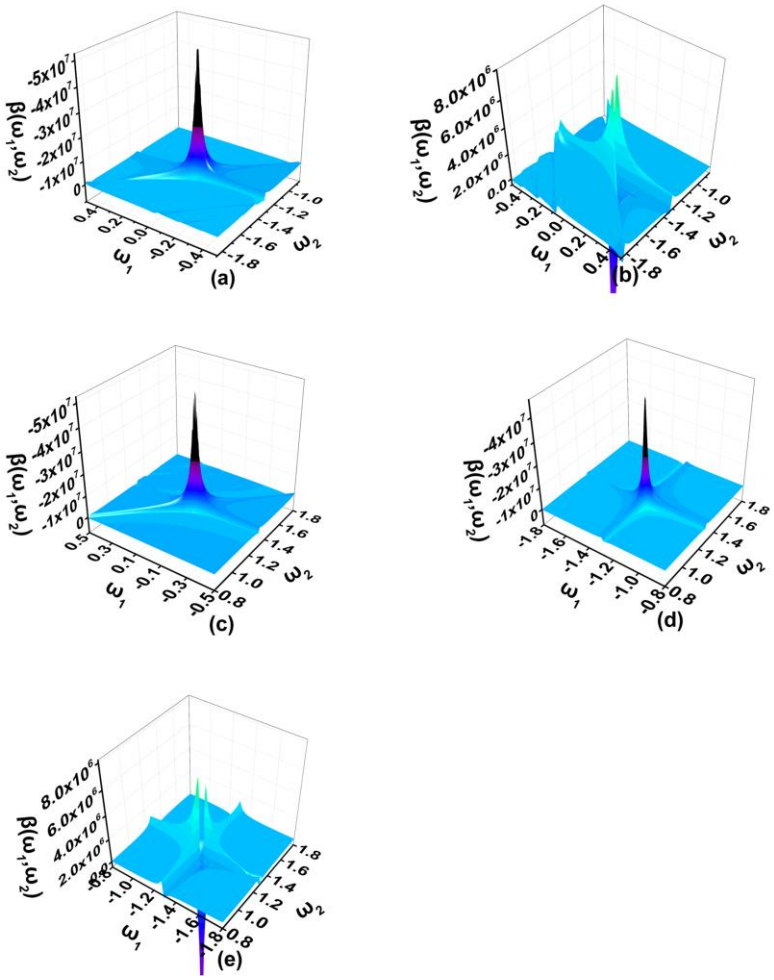

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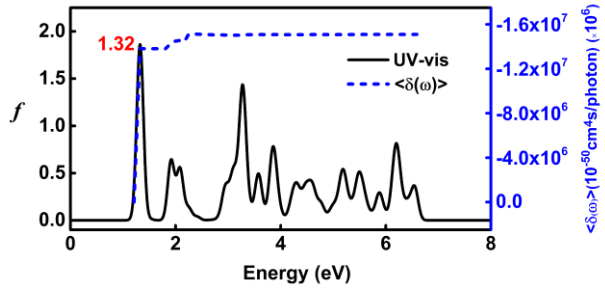
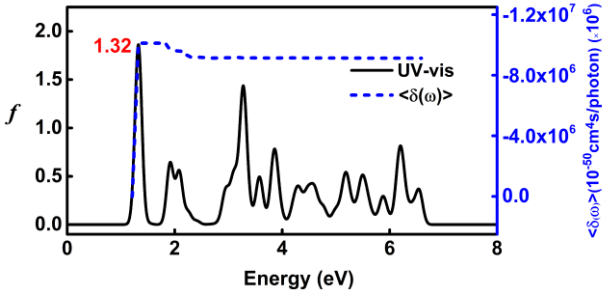
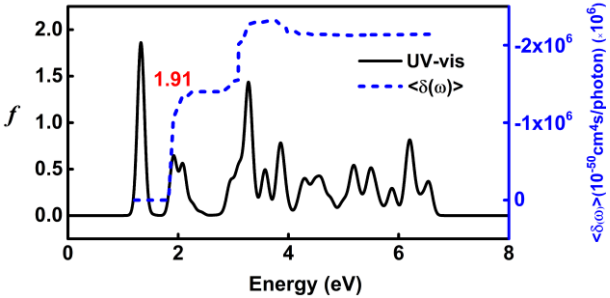
TPA: a) TPA −1.30 eV



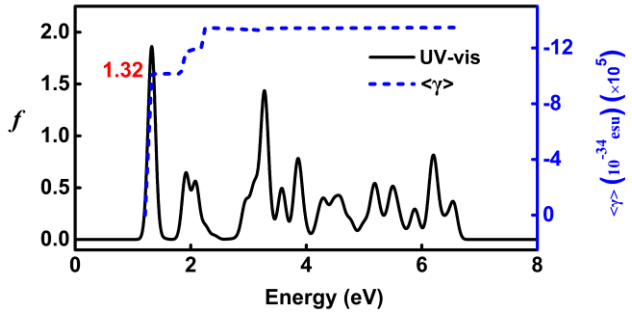
b) TPA −1.35 eV



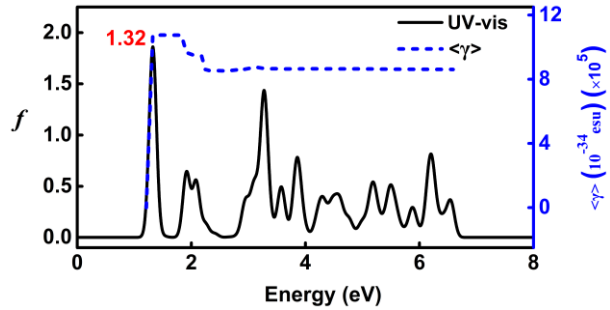
c) TPA −3.40 eV



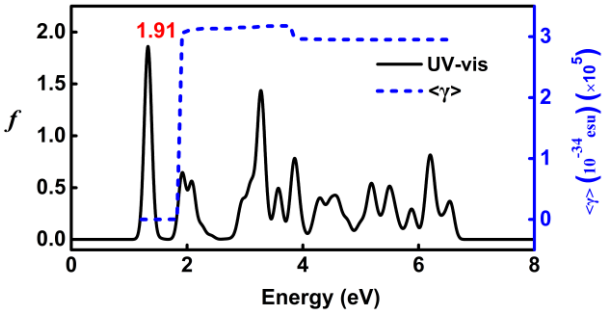
DFWM: a) DFWM −1.30 eV



b) DFWM −1.35 eV



c) DFWM −1.90 eV



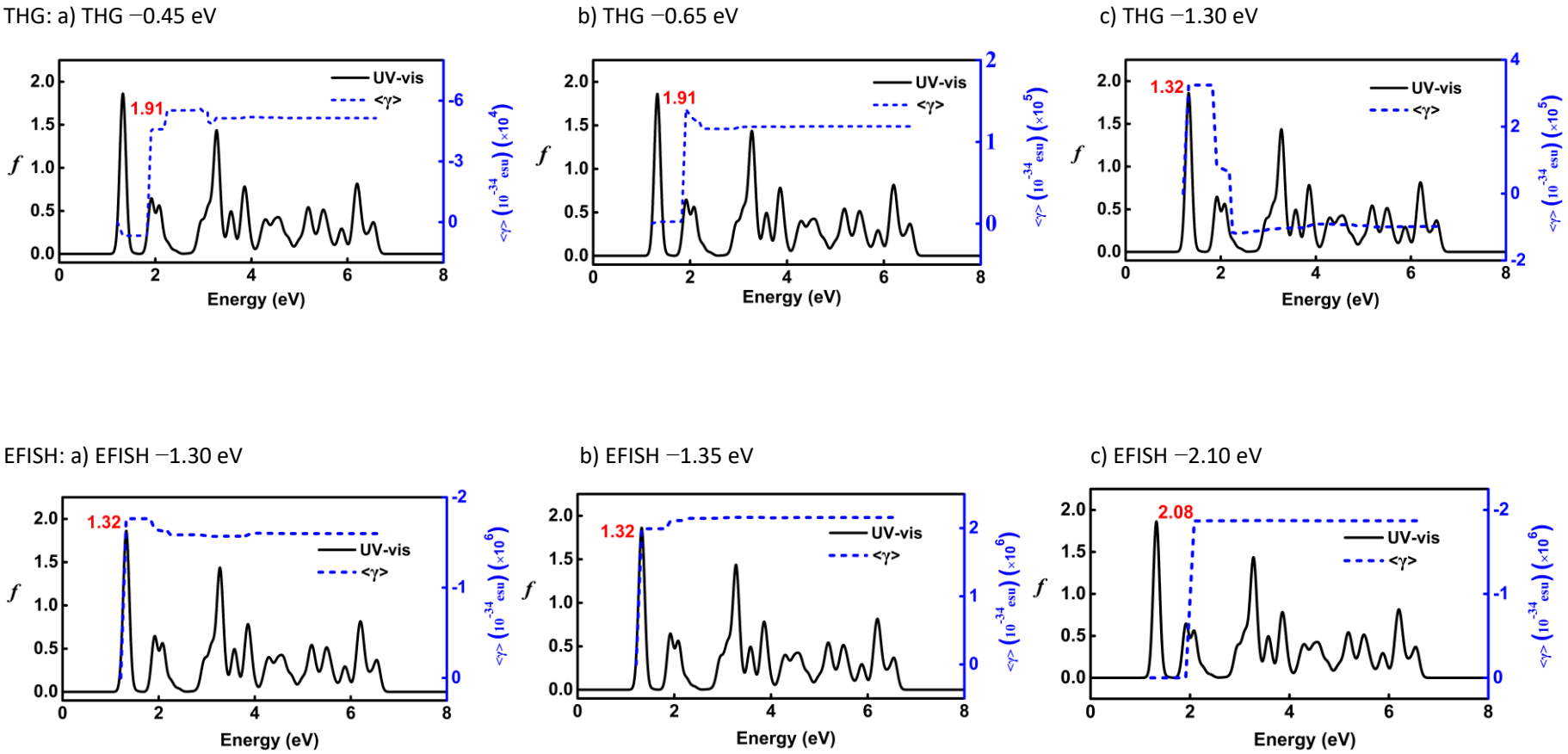
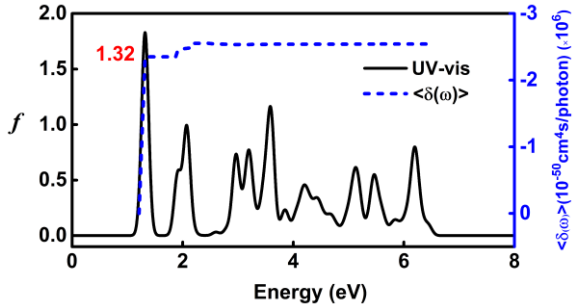
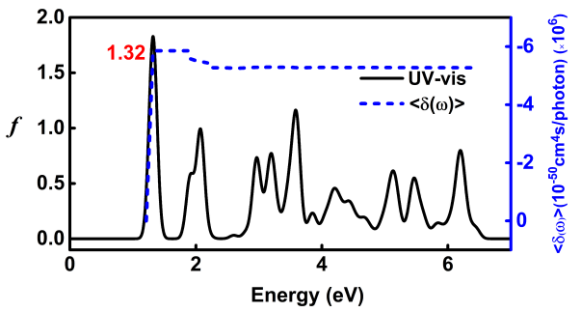


Figure S7 The evolution of third order nonlinear optic properties with electron excitations of P_N-3A-A at specific external fields.

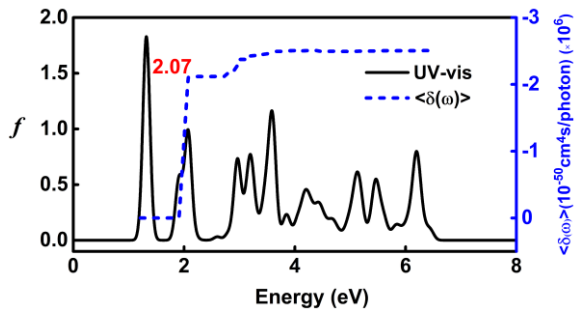
TPA: a) TPA −1.30 eV



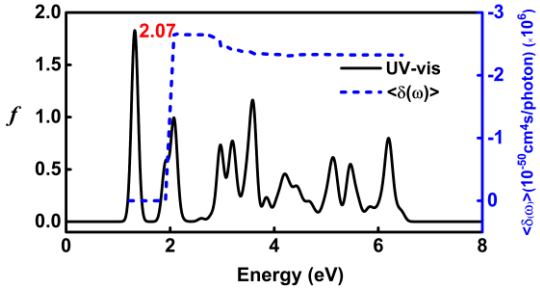
b) TPA −1.35 eV



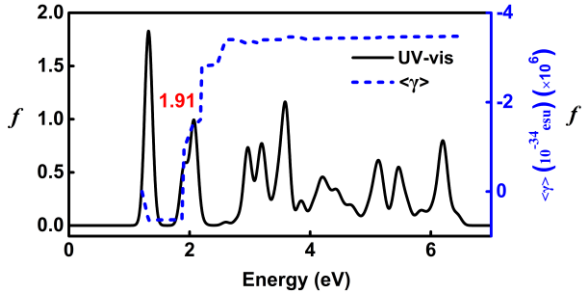
c) TPA −2.05 eV



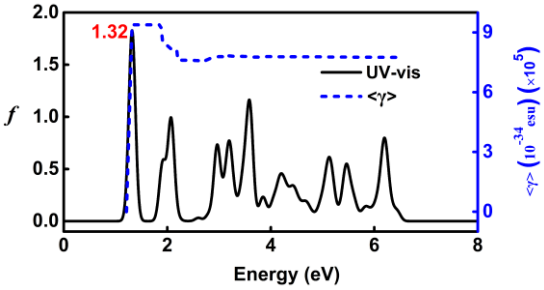
d) TPA −2.10 eV



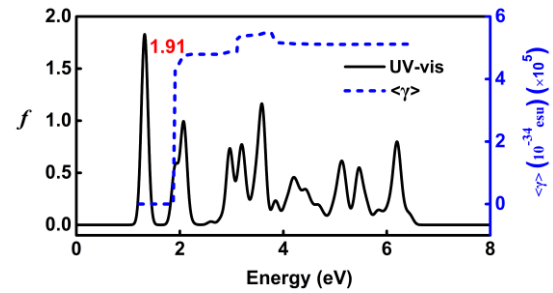
DFWM: a) DFWM −1.16 eV

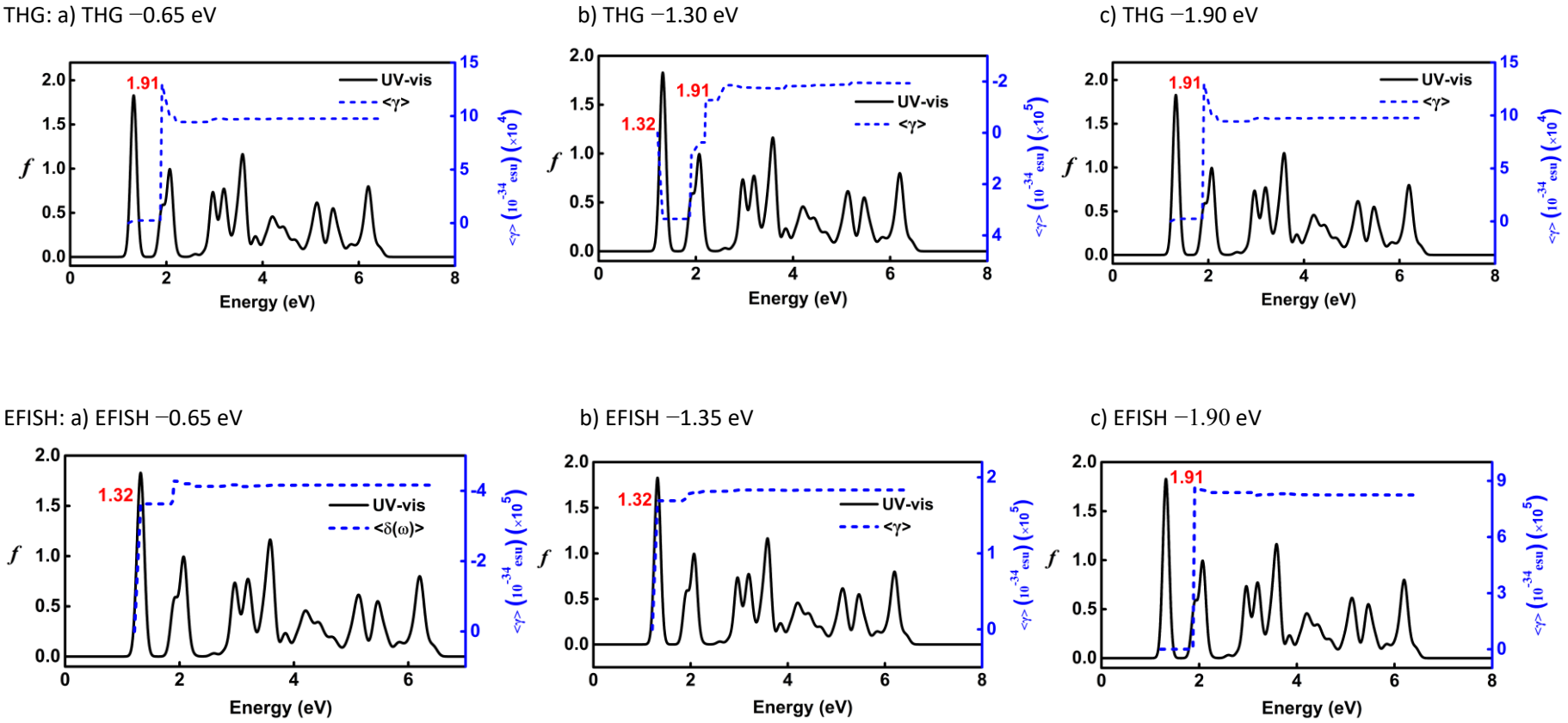


b) DFWM −1.32 eV



c) DFWM −1.91 eV





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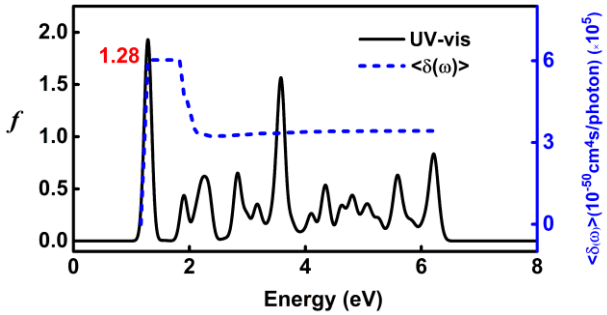
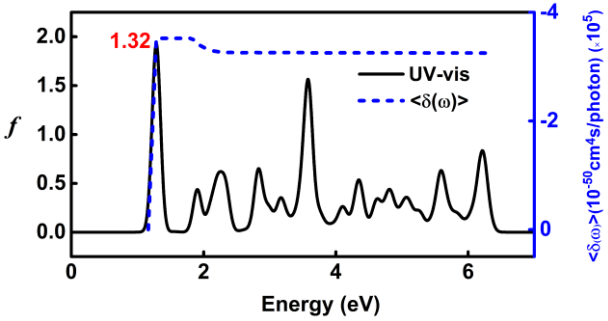
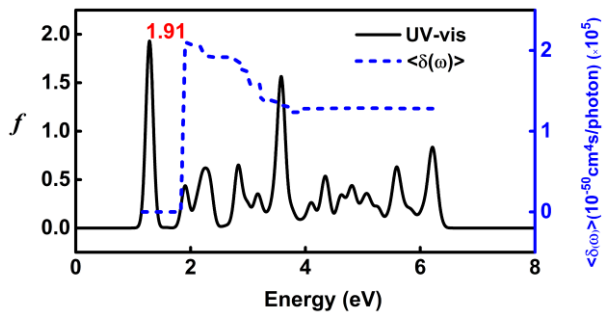
TPA: a) TPA –1.20 eV



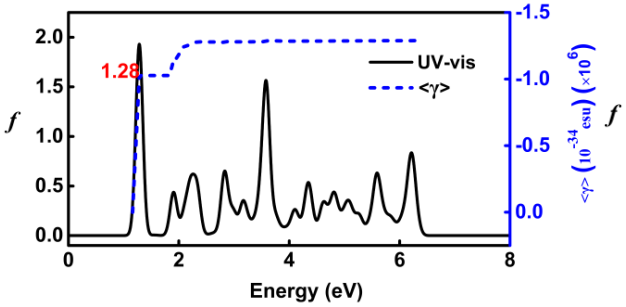
b) TPA –1.35 eV



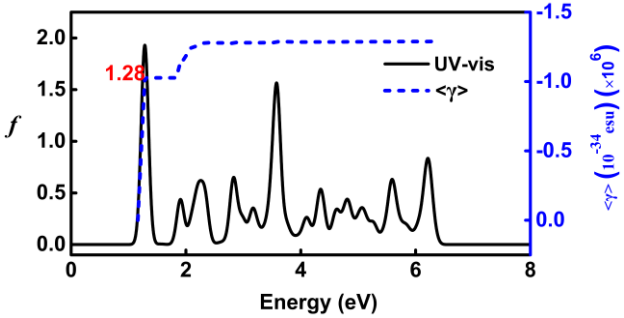
c) TPA –1.90 eV



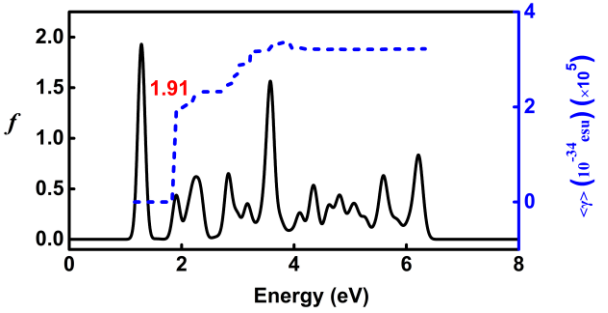
DFWM: a) DFWM –1.25 eV



b) DFWM –1.30 eV



c)DFWM –1.90 eV



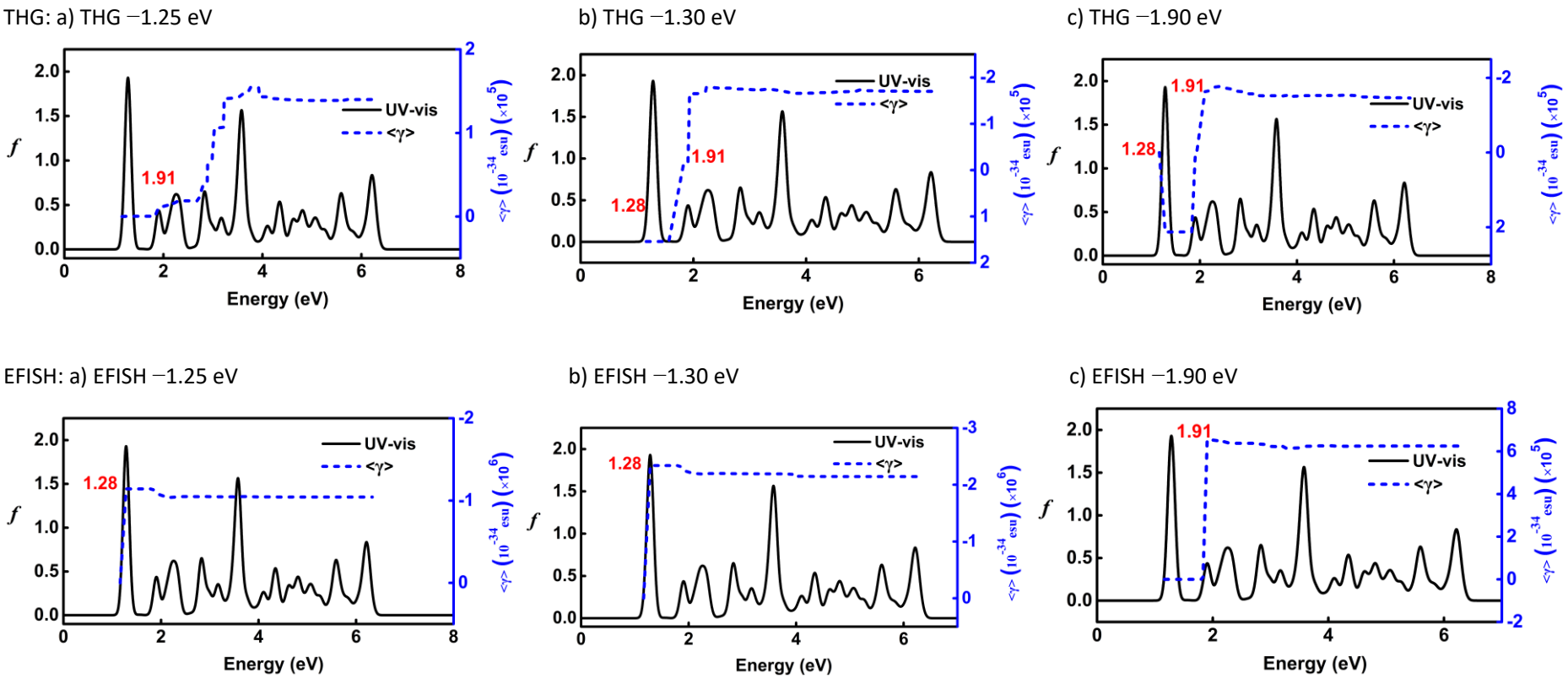
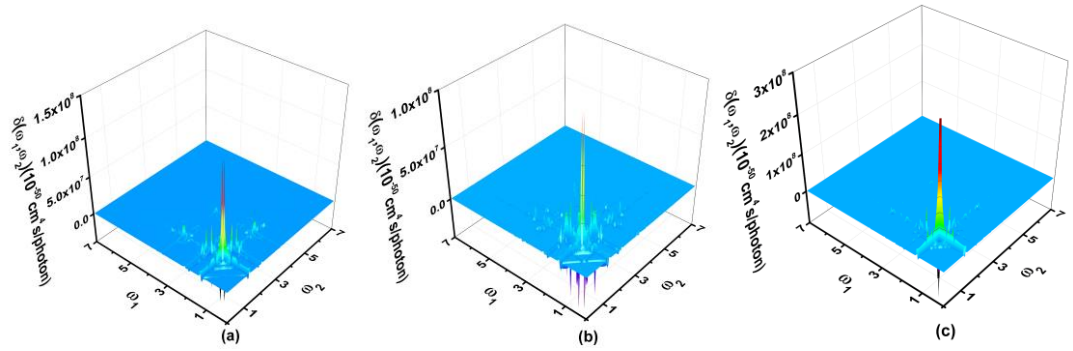


Figure S9 The evolution of third order nonlinear optic properties with electron excitations for Ni-P_N-3A-A at specific external fields.



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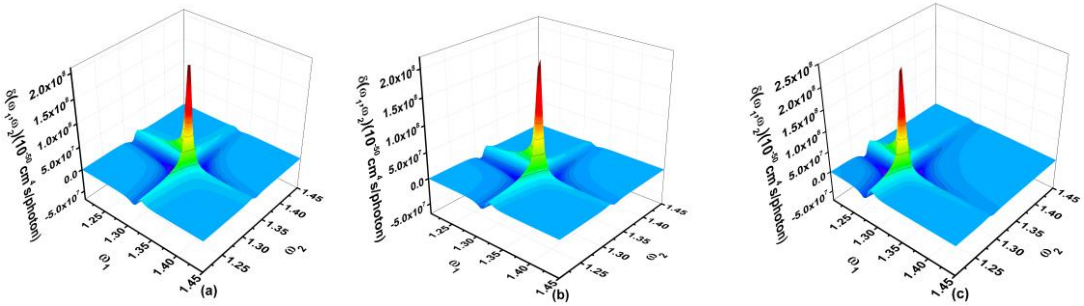

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Compounds	LVF (cm^{-1})	ΔE_{OS-CS} (Kcal/mol)	ΔE_{T-CS} (Kcal/mol)	<S^2>$_{OS}$	E_H (eV)	E_L (eV)	E_{gap} (eV)	D_g/Debye	<β_0>/(<β_0>/N) (10^{-30} esu)	<γ_0>/(<γ_0>/N) (10^{-30} esu)	<γ_0>$_{3L}$/<γ_0>$_{4L}$ (10^{-34} esu)
P_N-2A-2A (C_1)	5.27	0.00	5.31	0.00	−3.46	−4.45	0.99	16.00	22935.10/409.56	−621.19/−11.09	−268.33/−352.86
Mg-P_N-2A-2A (C_s)	6.05	0.00	21.32	0.00	−3.43	−4.41	0.98	15.68	22361.30/392.30	−573.93/−10.07	−275.94/−297.99
Ni-P_N-2A-2A(C_1)	3.30	0.00	5.89	0.00	−4.19	−3.39	0.80	26.25	17282.10/303.19	−385.27/−6.76	−277.50/−107.76
Zn-P_N-2A-2A (C_1)	4.39	0.00	3.12	0.00	−4.17	−3.43	0.74	27.71	/	/	/
P_N-3A-2A (C_1)	3.81	−0.33	3.57	0.02	−4.21	−3.48	0.73	28.71	59933.80/856.20	−2449.6/−34.99	−724.02/−1725.58
Ni-P_N-3A-2A (C_1)	3.30	0.00	3.93	0.00	−4.19	−3.39	0.80	26.25	54439.20/766.75	−1836.7/−25.87	−855.99/−980.71
Mg-P_N-3A-2A (C_s)	4.68	−0.04	3.99	0.00	−4.18	−3.44	0.74	28.13	59631.70/839.88	−2390.07/−33.66	−764.28/−1625.79
Zn-P_N-3A-2A (C_1)	4.39	−0.33	3.57	0.00	−3.43	−4.17	0.74	27.71	46932.40/661.02	−1461.25/−20.58	−729.87/−731.38
P_N-4A-A (C_s)	3.91	0.00	4.39	0.00	−4.23	−3.58	0.65	42.00	69183.40/910.31	−2222.7/−29.25	−845.54/−1377.16
Mg-P_N-4A-A (C_s)	3.37	0.00	4.53	0.00	−4.20	−3.56	0.64	41.18	70625.70/917.22	−2328.91/−30.25	−885.30/−1443.60
Ni-P_N-4A-A (C_1)	4.23	0.00	4.83	0.00	−4.18	−3.52	0.66	39.72	71367.60/926.85	−2401.82/−31.19	−936.91/−1464.91
Zn-P_N-4A-A (C_s)	3.84	0.00	1.30	0.00	−3.95	−3.54	0.41	39.95	/	/	/
P_N-2A-N-2A-N (C_s)	1.96	0.00	11.52	0.00	−4.54	−3.14	1.40	7.57	22935.10/364.05	−621.19/−9.86	−268.33/−352.86
P-A-A-N (C_s)	14.44	0.00	28.97	0.00	−2.87	−4.47	1.60	2.10	−242.95/−7.15	−1.46/−0.04	−6.26/4.80
P-2A-A-N (C_1)	9.01	0.00	10.00	0.00	−2.83	−4.20	1.37	4.27	−870.39/−18.13	6.43/0.13	−29.80/36.23

P-3A-N (C_{2V})	9.76	0.00	10.69	0.00	−2.65	−4.04	1.39	3.73	−2302.74/−40.40	23.46/0.41	−54.14/77.60
P-3A-A (C_s)	6.19	0.00	−4.74	0.00	−3.27	−3.70	0.43	21.03	/	/	/
P-3A-A-N(C_{2V})	6.24	0.00	9.87	0.00	−2.80	−4.07	1.27	4.20	−3439.85/−55.48	−1.46/−0.02	−83.84/82.38
P_N-A-2A (C_1)	8.73	0.00	5.84	0.00	−4.85	−3.64	1.21	2.11	4680.12/111.43	−77.75/−1.85	−86.90/9.16
Pc_N-3A-N (C_s)	8.21	0.00	9.56	0.00	−4.16	−2.91	2.01	6.91	−3338.99/−48.39	−36.51/-0.53	−116.61/80.10
Ni-Pc_N-3A-N (C_s)	8.57	0.00	16.58	0.00	−4.09	−2.77	1.32	5.40	−2877.10/−41.10	−37.44/−0.53	−110.79/73.35
Mg-Pc_N-3A-N(C_s)	8.50	0.00	9.48	0.00	−4.10	−2.80	1.30	5.78	−2497.61/−35.68	−48.68/−0.70	−118.10/69.42
Zn-Pc_N-3A-N (C_s)	8.53	0.00	1.30	0.00	−4.10	−2.79	1.31	5.72	/	/	/

Table S2 Major electronic spectra absorption peaks with transition nature in P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A (*f* is the oscillator strength in arbitrary unit, E is the transition energy in eV, λ is the wavelength in nm, TNMC to $<\beta_0>$ is the transition nature of electron excitation with a major contribution to $<\beta_0>$, $<\beta_0>_{Con}$ is contribution to $<\beta_0>$ in 10^{-30} esu).

Compounds	*f*	E	λ	Transition	TNMC to $<\beta_0>$	$<\beta_0>_{Con}$
P_N-3A-A	1.86	1.32	936.86	$S_0 \rightarrow S_2$	H−2→L (5.5 %) H→L (88.5 %)	22264.13
Mg-P_N-3A-A	1.83	1.32	940.20	$S_0 \rightarrow S_2$	H−2→L (5.3%) H→L (88.2%)	21620.92
Ni-P_N-3A-A	1.93	1.28	965.91	$S_0 \rightarrow S_2$	H−2→L (5.3%) H→L (87.6%)	20877.60

Table S3 Calculated important parameters of $(\beta_{ijk})_m$ [i, j, k∈(x, y, z)] (×10^{-30} esu) of P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. 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
P_N-3A-A (27899.8)				S_0		−0.24	39.16	0.00	39.16				
	0.00	22264.7	0.00	S_2 [$S_0 \rightarrow S_2$]	1.32	−0.64	−5.54	0.00	5.58	0.06	19.32	0.00	19.32
Mg-P_N-3A-A (28606.4)				S_0		0.00	−38.21	0.00	38.21				
	0.00	−21620.9	0.00	S_2 [$S_0 \rightarrow S_2$]	1.32	0.00	5.62	0.00	5.62	0.00	19.16	0.00	19.16
Ni-P_N-3A-A (26161.6)				S_0		35.85	0.00	0.00	35.85				
	208776	0.00	0.00	S_2 [$S_0 \rightarrow S_2$]	1.28	1.02	0.00	0.00	1.02	19.98	0.00	0.00	19.98

(1) P_N-3A-A:

$$\beta_{YYY}[S_0 \rightarrow S_2] = 6 \times \frac{19.32 \times [(-5.54) - 39.16] \times (-19.32)}{1.32^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu$$
$$= 22387.21 \times 10^{-30} esu$$

(2) Mg-P_N-3A-A:

$$\beta_{YYY}[S_0 \rightarrow S_2] = 6 \times \frac{19.16 \times [5.62 - (-38.21)] \times (-19.16)}{1.32^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu$$
$$= -21589.41 \times 10^{-30} esu$$

(3) Ni-P_N-3A-A:

$$\beta_{YYY}[S_0 \rightarrow S_2] = 6 \times \frac{19.98 \times [1.02 - 35.85] \times (-19.98)}{1.28^2} \times \frac{(10^{-18})^3}{(1.602 \times 10^{-12})^2} esu$$
$$= 19840.41 \times 10^{-30} esu$$

Table S4 Major electron excitations with transition nature in P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. *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 $< \gamma_0 >_{3L}$.

Compounds	*f*	E	λ	Transition	TNMC to $<\gamma_0>_{3L}$	$[<\gamma_0>_{3L}]_{Con}$	$[<\gamma_0>_{4L}]_{Con}$
P_N-3A-A	1.86	1.32	936.86	$S_0 \rightarrow S_2$	H−2→L (5.5 %) H→L (88.5 %)	−117.23	−625.65
Mg-P_N-3A-A	1.83	1.32	940.20	$S_0 \rightarrow S_2$	H−2→L (5.3%) H→L (88.2%)	−114.66	−597.68
Ni-P_N-3A-A	1.93	1.28	965.91	$S_0 \rightarrow S_2$	H−2→L (5.3%) H→L (87.6%)	−146.93	−498.68

Table S5 Calculated important parameters of $(\gamma_{ijk})_m$ (× 10^{-34} esu) of P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. 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 ($<\gamma_0>$), m = 0 is the ground state, and m > 0 is the mth excited state. (γxxxx represents γ along the X direction, γ_{YYYY} represents γ along the Y direction)

Structures ($<\gamma_0>_{3L}$)	$(\gamma_{zzzz})_{3Lm}$ (Contribution)	S_m	E_m	State dipole moment				Transition dipole moment			
				X	Y	Z	tot	X	Y	Z	tot
P_N-3A-A (−269.44)		S_0		−0.24	39.29	0.00	39.29				
		S_1 [$S_0 \rightarrow S_1$]	1.21	−0.05	8.91	0.00	8.91	0.00	0.00	−1.25	1.25
	−584.30	S_2 [$S_0 \rightarrow S_2$]	1.32	−0.64	−5.54	0.00	5.57	0.06	19.32	0.00	19.32
Mg-P_N-3A-A (−284.46)		S_0		0.00	−38.21	0.00	38.21				
		S_1 [$S_0 \rightarrow S_1$]	1.21	0.00	−8.32	0.00	8.32	0.00	0.00	−1.29	1.29
	−571.32	S_2 [$S_0 \rightarrow S_2$]	1.32	0.00	5.62	0.00	5.62	0.00	19.16	0.00	19.16
Ni-P_N-3A-A (−323.30)		S_0		35.85	0.00	0.00	35.85				
		S_1 [$S_0 \rightarrow S_1$]	1.16	6.21	0.00	0.00	6.21	0.00	1.13	0.17	1.14
	−732.80	S_2 [$S_0 \rightarrow S_2$]	1.28	−1.02	0.00	0.00	1.02	19.98	0.00	0.00	19.98

1. P_N-3A-A:

（1）$S_0 \rightarrow S_2$：

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

$$\gamma_{3L(YYYY)(\text{Contribution})}[S_0 \rightarrow S_2] \approx -\frac{24}{6}\frac{r_{01}^{Y}r_{10}^{Y}r_{02}^{Y}r_{20}^{Y}}{E_1E_2^2} - \frac{24}{6}\frac{r_{02}^{Y}r_{20}^{Y}r_{01}^{Y}r_{10}^{Y}}{E_2E_1^2} - \frac{24}{6}\frac{r_{02}^{Y}r_{20}^{Y}r_{02}^{Y}r_{20}^{Y}}{E_2^3}$$

$$= \left[-4 \times \frac{0 \times 0 \times (19.32) \times (-19.32)}{1.21 \times 1.32^2} - 4 \times \frac{(19.32) \times (-19.32) \times 0 \times 0}{1.32 \times 1.21^2} - 4 \times \frac{(19.32) \times (-19.32) \times (19.32) \times (-19.32)}{1.32^3}\right] \times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3}$$

$$= -589.35 \times 10^{-34}$$

2. Mg-P_N-3A-A:

（2）$S_0 \rightarrow S_2$：

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

$$\gamma_{3L(xxxx)(\text{Contribution})}[S_0 \rightarrow S_2] \approx -\frac{24}{6}\frac{r_{01}^{x}r_{10}^{x}r_{02}^{x}r_{20}^{x}}{E_1E_2^2} - \frac{24}{6}\frac{r_{02}^{x}r_{20}^{x}r_{01}^{x}r_{10}^{x}}{E_2E_1^2} - \frac{24}{6}\frac{r_{02}^{x}r_{20}^{x}r_{02}^{x}r_{20}^{x}}{E_2^3}$$

$$= \left[-4 \times \frac{0 \times 0 \times (19.16) \times (-19.16)}{1.21 \times 1.32^2} - 4 \times \frac{(19.16) \times (-19.16) \times 0 \times 0}{1.32 \times 1.21^2} - 4 \times \frac{(19.16) \times (-19.16) \times (19.16) \times (-19.16)}{1.32^3}\right] \times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3}$$

$$= -570.07 \times 10^{-34}$$

3. Ni-P_N-3A-A:

（3）$S_0 \rightarrow S_2$：

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

$$\gamma_{3L(YYYY)(\text{Contribution})}[S_0 \rightarrow S_2] \approx -\frac{24}{6}\frac{r_{01}^{Y}r_{10}^{Y}r_{02}^{Y}r_{20}^{Y}}{E_1E_2^2} - \frac{24}{6}\frac{r_{02}^{Y}r_{20}^{Y}r_{01}^{Y}r_{10}^{Y}}{E_2E_1^2} - \frac{24}{6}\frac{r_{02}^{Y}r_{20}^{Y}r_{02}^{Y}r_{20}^{Y}}{E_2^3}$$

$$= \left[-4 \times \frac{0 \times 0 \times (19.98) \times (-19.98)}{1.16 \times 1.28^2} - 4 \times \frac{(19.98) \times (-19.98) \times 0 \times 0}{1.28 \times 1.16^2} - 4 \times \frac{(19.98) \times (-19.98) \times (19.98) \times (-19.98)}{1.28^3}\right] \times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3}$$

$$= -739.30 \times 10^{-34}$$

Table S6 Important parameters of $(\gamma_{ijk})_m$ ($\times 10^{-34}$ esu) of P_N-3A-A, Mg-P_N-3A-A and Ni-P_N-3A-A. 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 ($<\gamma_0>$), m = 0 is the ground state, and m > 0 is the mth excited state. (γ_{xxxx} represents γ along the X direction, γ_{YYYY} represents γ along the Y direction)

Structures ($<\gamma_0>_{4L}$)	$(\gamma_{YYYY/xxxx})_{4Lm}$ (Contribution)	S_m	E_m	State dipole moment				Transition dipole moment			
				X	Y	Z	tot	X	Y	Z	tot
P_N-3A-A (−699.65)		S_0		−0.24	39.29	0.00	39.29				
		S_1 [$S_0 \rightarrow S_1$]	1.21	−0.05	8.91	0.00	8.91	0.00	0.00	−1.25	1.25
		$S_1 \rightarrow S_2$		0.00	0.00	1.33	1.33				
	−3129.03	S_2 [$S_0 \rightarrow S_2$]	1.32	−0.64	−5.54	0.00	5.57	0.06	19.32	0.00	19.32
Mg-P_N-3A-A (−716.40)		S_0		0.00	−38.21	0.00	38.21				
		S_1 [$S_0 \rightarrow S_1$]	1.21	0.00	−8.32	0.00	8.32	0.00	0.00	−1.29	1.29
		$S_1 \rightarrow S_2$		0.00	0.00	−1.29	1.29				
	−2989.35	S_2 [$S_0 \rightarrow S_2$]	1.32	0.00	5.62	0.00	5.62	0.00	19.16	0.00	19.16
Ni-P_N-3A-A (−592.60)		S_0		35.85	0.00	0.00	35.85				
		S_1 [$S_0 \rightarrow S_1$]	1.16	6.21	0.00	0.00	6.21	0.00	1.13	0.17	1.14
		$S_1 \rightarrow S_2$		0.00	−1.26	0.19					
	−2494.51	S_2 [$S_0 \rightarrow S_2$]	1.28	−1.02	0.00	0.00	1.02	19.98	0.00	0.00	19.98

1. P_N-3A-A:

(1) $S_0 \rightarrow S_2$:

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

$$\gamma_{4L(YYYY)(\text{Contribution})}[S_0 \rightarrow S_2] \approx \frac{24}{6}\frac{r_{02}^{Y}(r_{22}^{Y}-r_{00}^{Y})(r_{22}^{Y}-r_{00}^{Y})r_{20}^{Y}}{E_2^3} + \frac{24}{6}\frac{r_{01}^{Y}r_{12}^{Y}(r_{22}^{Y}-r_{00}^{Y})r_{20}^{Y}}{E_1E_2^2} + \frac{24}{6}\frac{r_{02}^{Y}r_{21}^{Y}r_{12}^{Y}r_{20}^{Y}}{E_2E_1E_2} + \frac{24}{6}\frac{r_{02}^{Y}(r_{22}^{Y}-r_{00}^{Y})r_{21}^{Y}r_{10}^{Y}}{E_2^2E_1} + \frac{24}{6}\frac{r_{01}^{Y}(r_{11}^{Y}-r_{00}^{Y})r_{12}^{Y}r_{20}^{Y}}{E_1^2E_2} + \frac{24}{6}\frac{r_{01}^{Y}r_{12}^{Y}r_{21}^{Y}r_{10}^{Y}}{E_1E_2E_1} + \frac{24}{6}\frac{r_{02}^{Y}r_{21}^{Y}(r_{11}^{Y}-r_{00}^{Y})r_{10}^{Y}}{E_2E_1^2}$$

$$= \left[4 \times \frac{(19.32) \times (-5.54 - 39.29) \times (-5.54 - 39.29) \times (-19.32)}{1.32^3} + 4 \right.$$
$$\times \frac{0 \times 0 \times (-5.54 - 39.29) \times (-19.32)}{1.21 \times 1.32^2} + 4 \times \frac{(19.32) \times 0 \times 0 \times (-19.32)}{1.32 \times 1.21 \times 1.32} + 4$$
$$\times \frac{(19.32) \times (-5.54 - 39.29) \times 0 \times 0}{1.32^2 \times 1.21} + 4 \times \frac{0 \times (8.91 - 39.29) \times 0 \times (-19.32)}{1.21^2 \times 1.32}$$
$$\left. + 4 \times \frac{0 \times 0 \times 0 \times 0}{1.21 \times 1.32 \times 1.21} + 4 \times \frac{(19.32) \times 0 \times (8.91 - 39.29) \times 0}{1.21 \times 1.32^2} \right]$$
$$\times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3} = -3461.71 \times 10^{-34}$$

2. Mg-P_N-3A-A:

(1) $S_0 \rightarrow S_2$:

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

$$\gamma_{4L(YYYY)(\text{Contribution})}[S_0 \rightarrow S_2] \approx \frac{24}{6}\frac{r_{02}^Y(r_{22}^Y - r_{00}^Y)(r_{22}^Y - r_{00}^Y)r_{20}^Y}{E_2^3} + \frac{24}{6}\frac{r_{01}^Y r_{12}^Y (r_{22}^Y - r_{00}^Y) r_{20}^Y}{E_1 E_2^2} +$$
$$\frac{24}{6}\frac{r_{02}^Y r_{21}^Y r_{12}^Y r_{20}^Y}{E_2 E_1 E_2} + \frac{24}{6}\frac{r_{02}^Y (r_{22}^Y - r_{00}^Y) r_{21}^Y r_{10}^Y}{E_2^2 E_1} + \frac{24}{6}\frac{r_{01}^Y (r_{11}^Y - r_{00}^Y) r_{12}^Y r_{20}^Y}{E_1^2 E_2} + \frac{24}{6}\frac{r_{01}^Y r_{12}^Y r_{21}^Y r_{10}^Y}{E_1 E_2 E_1} +$$
$$\frac{24}{6}\frac{r_{02}^Y r_{21}^Y (r_{11}^Y - r_{00}^Y) r_{10}^Y}{E_2 E_1^2}$$

$$= \left[4 \times \frac{(19.16) \times (5.62 + 38.21) \times (5.62 + 38.21) \times (-19.16)}{1.32^3} + 4 \right.$$
$$\times \frac{0 \times 0 \times (5.62 + 38.21) \times (-19.16)}{1.21 \times 1.32^2} + 4 \times \frac{(19.16) \times 0 \times 0 \times (-19.16)}{1.32 \times 1.21 \times 1.32} + 4$$
$$\times \frac{(19.32) \times (5.62 + 38.21) \times 0 \times 0}{1.32^2 \times 1.21} + 4 \times \frac{0 \times (-8.32 + 38.21) \times 0 \times (-19.16)}{1.21^2 \times 1.32}$$
$$\left. + 4 \times \frac{0 \times 0 \times 0 \times 0}{1.21 \times 1.32 \times 1.21} + 4 \times \frac{(19.16) \times 0 \times (-8.32 + 38.21) \times 0}{1.21 \times 1.32^2} \right]$$
$$\times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3} = -2983.21 \times 10^{-34}$$

3. Ni-P_N-3A-A:

(1) $S_0 \rightarrow S_2$:

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

$$\gamma_{4L(xxxx)(\text{Contribution})}[S_0 \to S_2] \approx \frac{24}{6}\frac{r^x_{02}(r^x_{22}-r^x_{00})(r^x_{22}-r^x_{00})r^x_{20}}{E_2^3} + \frac{24}{6}\frac{r^x_{01}r^x_{12}(r^x_{22}-r^x_{00})r^x_{20}}{E_1E_2^2} +$$

$$\frac{24}{6}\frac{r^x_{02}r^x_{21}r^x_{12}r^x_{20}}{E_2E_1E_2} + \frac{24}{6}\frac{r^x_{02}(r^x_{22}-r^x_{00})r^x_{21}r^x_{10}}{E_2^2E_1} + \frac{24}{6}\frac{r^x_{01}(r^x_{11}-r^x_{00})r^x_{12}r^x_{20}}{E_1^2E_2} + \frac{24}{6}\frac{r^x_{01}r^x_{12}r^x_{21}r^x_{10}}{E_1E_2E_1} +$$

$$\frac{24}{6}\frac{r^x_{02}r^x_{21}(r^x_{11}-r^x_{00})r^x_{10}}{E_2E_1^2}$$

$$= \left[4 \times \frac{(19.98) \times (-1.02 - 35.85) \times (-1.02 - 35.85) \times (-19.98)}{1.28^3} + 4 \right.$$

$$\times \frac{0 \times 0 \times (-1.02 - 35.85) \times (-19.98)}{1.16 \times 1.28^2} + 4 \times \frac{(19.98) \times 0 \times 0 \times (-19.98)}{1.28 \times 1.16 \times 1.28} + 4$$

$$\times \frac{(19.98) \times (-1.02 - 35.85) \times 0 \times 0}{1.28^2 \times 1.16} + 4 \times \frac{0 \times (6.21 - 35.85) \times 0 \times (-19.98)}{1.16^2 \times 1.28}$$

$$\left. + 4 \times \frac{0 \times 0 \times 0 \times 0}{1.16 \times 1.28 \times 1.16} + 4 \times \frac{(19.98) \times 0 \times (6.21 - 19.98) \times 0}{1.16 \times 1.28^2} \right]$$

$$\times \frac{(10^{-18})^4}{(1.602 \times 10^{-12})^3} = -2517.55 \times 10^{-34}$$

Table S7 The strong response and corresponding major electronic excitation contribution of the dynamic third order nonlinear optic process for P_N-3A-A. TPA is in 10^{-50} cm^4·s/photon. DFWM, THG and EFISH are in 10^{-34} esu.

processes	External Field/eV (λ/nm)	Responses	Major Electronic Excitation Contribution
TPA	1.30 (953.85)	−15037900	1.32 eV(939.39nm)(−13810599.41)
δ(−ω;ω,−ω,ω)	1.35 (918.52)	−9163540	1.32 eV(939.39nm)(−10119000.16)
	1.90 (652.63)	−2145170	1.91 eV(649.21nm)(−1060896.50)
DFWM	1.30 (953.85)	−1349860	1.32 eV(939.39nm)(−1014568.54)
γ(−ω;ω,−ω,ω)	1.35 (10888.43)	860869	1.32 eV(939.39nm)(1075601.32)
	1.90 (652.63)	292359	1.91 eV(649.21nm)(305851.60)
THG	0.45 (2755.56)	51364	1.91 eV(423.21nm)(−52446.08)
γ(−3ω;ω,ω,ω)	0.65 (1907.69)	118959	1.91 eV(423.21nm)(137033.04)
	1.30 (953.85)	97985	1.32 eV(939.39nm)(324431.96)
EFISH	1.30 (953.85)	−1603710	1.32 eV(939.39nm)(−1763147.71)
γ(−2ω;ω,ω,0)	1.35 (918.52)	2156870	1.32 eV(939.39nm)(1990442.93)
	2.10 (590.48)	−1888000	2.08 eV(596.15nm)(−1869219.45)

Table S8 The strong response and corresponding major electronic excitation contribution of the dynamic third order nonlinear optic process of Mg-P_N-3A-A. TPA is in 10^{-50} cm^4·s/photon. DFWM, THG and EFISH are in 10^{-34} esu.

processes	External Field/eV (λ/nm)	Responses	Major Electronic Excitation Contribution
	1.30 (953.85)	−25322800	1.32 eV(939.39nm)(−23495799.11)
TPA	1.35 (918.52)	−5289810	1.32 eV(939.39nm)(−5856190.13)
δ(−ω;ω,−ω,ω)	2.05 (604.88)	−2498190	2.07 eV(599.03nm)(−2098402.67)
	2.10 (590.48)	−2331620	2.07 eV(599.03nm)(−2656904.34)
DFWM	1.25 (992)	−251232	1.16 eV(1068.96nm)(627263.91); 2.37 eV(523.21nm)(−60384)
γ(−ω;ω,−ω,ω)	1.30 (953.85)	−362301	1.32 eV(939.39nm)(−159569)
	1.35 (918.52)	776070	1.32 eV(939.39nm)(938665.35)
	1.90 (652.63)	509618	1.91 eV(649.21nm)(425608.94)
THG	0.65 (1907.69)	97555	1.91 eV(649.21nm)(127610.73)
γ(−3ω;ω,ω,ω)	1.30 (953.85)	−192831	1.32 eV(939.39nm)(335485.88);1.91 eV(649.21nm)(−248625.70)
	1.90 (652.63)	73248	1.91 eV(649.21nm)(11934.64);3.11 eV(398.71nm)(69333.80)
EFISH	0.65 (1907.69)	−416333	1.32 eV(939.39nm)(−362659.71)
γ(−2ω;ω,ω,0)	1.35 (918.52)	1835940	1.32 eV(939.39nm)(1692150.85)
	1.90 (652.63)	821549	1.91 eV(649.21nm)(866985.02)

Table S9 The strong response and corresponding major electronic excitation contribution of the dynamic third order nonlinear optic process of Ni-P_N-3A-A. TPA is in 10^{-50} cm^4·s/photon. DFWM, THG and EFISH are in 10^{-34} esu.

processes	External Field/eV (λ/nm)	Responses	Major Electronic Excitation Contribution
	1.25 (992.00)	−5370200	1.28 eV(968.75nm)(602881.30)
TPA	1.30 (953.85)	−32617600	1.28 eV(968.75nm)(−35208200.18)
δ(−ω;ω,−ω,ω)	1.90 (652.63)	−1254690	1.91 eV(649.21nm)(2095888.10)
DFWM	1.25 (992.00)	−1287140	1.28 eV(968.75nm)(−1026638.51)
γ(−ω;ω,−ω,ω)	1.30 (953.85)	−2389890	1.28 eV(968.75nm)(−2099328.77)
	1.90 (652.63)	322944	1.91 eV(649.21nm)(192594.05)
THG	1.25 (992.00)	−169773	1.28 eV(968.75nm)(154323.64);1.91 eV(649.21nm)(−171166.6)
γ(−3ω;ω,ω,ω)	1.30 (953.85)	−145642	1.28 eV(968.75nm)(212962.42);1.91 eV(649.21nm)(−210234.57)
	1.90 (652.63)	139193	1.91 eV(649.21nm)(10855.48)
EFISH	1.25 (992.00)	−1041750	1.28 eV(968.75nm)(−1142327.49)
γ(−2ω;ω,ω,0)	1.30 (953.85)	−2185260	1.28 eV(968.75nm)(−2338033.40)
	1.90 (652.63)	627103	1.91 eV(649.21nm)(654806.96)

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

P

C	0	4.148037	0.675857
C	0	4.148037	-0.675857
C	0	2.737322	1.083406
C	0	-0.683169	4.151174
C	0	0.683169	4.151174
C	0	1.130312	2.775405
C	0	-4.148037	-0.675857
C	0	-4.148037	0.675857
C	0	-2.737322	-1.083406
C	0	-2.737322	1.083406
C	0	-0.683169	-4.151174
C	0	0.683169	-4.151174
C	0	-1.130312	-2.775405
C	0	1.130312	-2.775405
C	0	2.737322	-1.083406
C	0	-1.130312	2.775405
N	0	0	1.995603
N	0	1.909874	0
N	0	-1.909874	0
H	0	0	0.983696
H	0	0	-0.983696
N	0	2.39197	2.375544
N	0	2.39197	-2.375544
N	0	-2.39197	-2.375544
N	0	-2.39197	2.375544
H	0	-4.978805	1.367351
H	0	-4.978805	-1.367351
H	0	-1.359832	4.993234
H	0	1.359832	4.993234
H	0	4.978805	1.367351
H	0	4.978805	-1.367351
H	0	1.359832	-4.993234
H	0	-1.359832	-4.993234
N	0	0	-1.995603

Pc

N	0	0	2.026254
N	0	1.948458	0
N	0	0	-2.026254
N	0	-1.948458	0
C	0	-1.145443	2.791776
C	0	-0.706787	4.176474
C	0	0.706787	4.176474
C	0	1.145443	2.791776
C	0	2.760998	1.097306
C	0	4.173748	0.70203
C	0	4.173748	-0.70203
C	0	2.760998	-1.097306
C	0	1.145443	-2.791776
C	0	0.706787	-4.176474
C	0	-0.706787	-4.176474
C	0	-1.145443	-2.791776
C	0	-2.760998	-1.097306
C	0	-4.173748	-0.70203
C	0	-4.173748	0.70203
C	0	-2.760998	1.097306
H	0	0	1.013059
N	0	2.39828	2.383138
N	0	2.39828	-2.383138
N	0	-2.39828	2.383138
N	0	-2.39828	-2.383138
H	0	0	-1.013059
C	0	5.364184	-1.424898
C	0	6.55958	-0.702557
C	0	6.55958	0.702557
C	0	5.364184	1.424898
H	0	5.355402	-2.509906
H	0	7.507338	-1.232952
H	0	7.507338	1.232952
H	0	5.355402	2.509906
C	0	-1.426356	5.374402
C	0	1.426356	5.374402
C	0	0.705101	6.563894

C	0	-0.705101	6.563894
H	0	-2.511006	5.363998
H	0	2.511006	5.363998
H	0	1.234187	7.512101
H	0	-1.234187	7.512101
C	0	-1.426356	-5.374402
C	0	-0.705101	-6.563894
C	0	0.705101	-6.563894
C	0	1.426356	-5.374402
H	0	-2.511006	-5.363998
H	0	2.511006	-5.363998
C	0	-6.55958	0.702557
C	0	-6.55958	-0.702557
C	0	-5.364184	-1.424898
C	0	-5.364184	1.424898
H	0	-7.507338	1.232952
H	0	-7.507338	-1.232952
H	0	-5.355402	-2.509906
H	0	-5.355402	2.509906
H	0	-1.234187	-7.512101
H	0	1.234187	-7.512101

P_N-2A-2A

C	6.544567	1.35441	-0.096214
C	6.635818	-0.106836	-0.080845
C	7.854135	1.858423	-0.089806
C	0.645041	-3.929197	0.043059
C	1.98334	-3.856884	-0.070123
C	2.324554	-2.40901	-0.039494
C	-1.689312	1.316078	0.298639
C	-1.555641	-0.989596	0.300374
C	0.158268	4.488459	0.035901
C	1.495328	4.573772	-0.081506
C	-0.151695	3.043477	0.134756
C	2.004229	3.176446	-0.052292
C	8.050544	-0.452659	-0.063027
C	0.168008	-2.530476	0.141312
N	1.194055	-1.65245	0.09145
N	3.581007	-2.046602	-0.118877
N	3.29259	2.965017	-0.136778
N	-1.426643	2.625026	0.225399
N	-1.144817	-2.261801	0.230055

Mg-P_N-2A-2A

C	-2.831058	-6.0374	0
C	-1.437321	-6.467216	0
C	-3.630973	-7.192378	0
C	3.696286	-1.521624	0
C	3.326976	-2.823528	0
C	1.852481	-2.852487	0
C	-0.848201	1.983603	0
C	1.332	1.324622	0
C	-4.393961	0.925021	0
C	-4.811333	-0.361206	0
C	-2.922146	0.905528	0
C	-3.601559	-1.206657	0
C	-1.43196	-7.924241	0
C	2.463034	-0.720609	0
N	1.387551	-1.558704	0
N	1.17567	-3.971573	0
N	-3.664509	-2.510729	0
N	-2.196018	2.031898	0
N	2.481412	0.619249	0

C	5.394922	2.129301	-0.124035	C	-3.31731	-4.737366	0
C	5.591971	-0.986358	-0.096274	C	-0.336742	-5.655889	0
H	5.829782	-2.045319	-0.098068	H	0.634506	-6.141742	0
H	5.544012	3.20521	-0.144129	H	-4.400077	-4.639293	0
C	-2.983014	-0.640357	0.229129	C	1.345512	2.800981	0
C	-3.06759	0.803924	0.229074	C	-0.041282	3.220533	0
C	-3.992516	-1.564117	0.157072	C	2.479257	3.572242	0
C	-5.400777	-1.367466	0.093087	C	2.616982	4.989246	0
C	-6.097082	-0.098823	0.067326	C	1.546531	5.963579	0
C	-5.554371	1.242513	0.096011	C	0.115433	5.746523	0
C	-4.178143	1.603158	0.158746	C	-0.556513	4.491181	0
H	-3.958521	2.668653	0.154613	H	-1.643848	4.530032	0
H	-3.649357	-2.596441	0.152121	H	3.40539	3.001199	0
C	-12.737174	-0.49154	-0.247412	C	3.477794	12.33708	0
C	-12.067779	-1.71809	-0.220506	C	4.514121	11.399571	0
C	-10.691168	-1.960985	-0.156832	C	4.429354	10.002739	0
C	-12.217764	0.805256	-0.21832	C	2.095401	12.132662	0
C	-9.640744	-1.05195	-0.104241	C	3.300251	9.191517	0
C	-10.879172	1.209657	-0.154131	C	1.389897	10.924041	0
C	-9.7287	0.431419	-0.102775	C	1.87829	9.622356	0
H	-10.403836	-3.010659	-0.147236	H	5.383118	9.478548	0
H	-10.71829	2.285962	-0.14275	H	0.305643	11.017951	0
C	-8.254097	-1.39042	-0.040488	C	3.305666	7.762744	0
C	-7.509262	-0.181828	-0.000134	C	1.956676	7.318691	0
C	-8.391021	0.930846	-0.037918	C	1.080793	8.436667	0
C	-6.17823	-2.573485	0.049049	C	3.971317	5.466003	0
C	-7.552878	-2.611068	-0.014652	C	4.328813	6.79554	0
C	-7.837895	2.225188	-0.008649	C	-0.306985	8.199242	0
H	-5.627634	-3.508429	0.068806	H	4.752263	4.712467	0
H	-8.067365	-3.567048	-0.044232	H	5.378718	7.073849	0
H	-8.461171	3.114246	-0.035797	H	-1.026343	9.013025	0
C	-6.468103	2.348875	0.055253	C	-0.746794	6.894595	0
H	-6.031331	3.341989	0.077463	H	-1.814576	6.700931	0
H	0.235585	0.270009	0.493717	C	-0.202361	-4.212411	0
C	4.158331	-0.789887	-0.108022	N	-2.493699	-0.387961	0
N	0.967745	2.291326	0.081676	C	-2.816676	-8.34678	0
C	8.783702	0.793685	-0.068554	C	-2.648534	-3.477879	0
C	4.014634	1.782757	-0.123222	C	-1.228135	-3.217771	0
C	3.481364	0.452923	-0.120234	H	-4.714819	-7.198139	0
H	2.39955	0.391363	-0.13932	C	0	0.854735	0
H	8.116064	2.909937	-0.099747	C	-3.342958	-9.665168	0
C	-0.828261	0.20861	0.402104	C	-0.276877	-8.723002	0

C	10.189865	0.995982	-0.056479	C	-2.665477	-10.85926	0
C	8.555027	-1.764049	-0.043307	C	-0.176595	-10.106214	0
C	11.190993	0.05788	-0.037281	C	-1.192006	-11.078137	0
C	9.874799	-2.186822	-0.026546	C	-3.270222	-12.155943	0
C	11.058498	-1.427622	-0.023294	C	-0.99759	-12.460966	0
C	12.593677	0.342	-0.026713	C	-2.263749	-13.108098	0
C	12.355919	-1.939679	-0.0055	H	-4.4309	-9.729049	0
C	13.282174	-0.859097	-0.007781	H	0.669173	-8.189103	0
H	10.506896	2.03856	-0.064081	H	0.837258	-10.503663	0
H	7.813806	-2.558123	-0.040532	H	-0.033289	-12.95457	0
H	10.022948	-3.265512	-0.013397	H	-4.337357	-12.339264	0
H	12.610544	-2.992498	0.007893	H	-2.411894	-14.181769	0
H	13.021981	1.336348	-0.032821	H	-5.819105	-0.753375	0
H	14.360603	-0.967091	0.003635	H	-4.981451	1.833113	0
H	2.129499	5.44395	-0.18246	H	3.946716	-3.709751	0
H	-0.586655	5.272506	0.057837	H	4.689814	-1.09432	0
H	2.715203	-4.646927	-0.169393	H	1.485374	13.031896	0
H	-0.002924	-4.795121	0.063124	H	3.79327	13.378114	0
H	-12.949491	1.607885	-0.24972	H	5.520816	11.80858	0
H	-13.82187	-0.555938	-0.298431	Mg	-0.605543	-1.149584	0
H	-12.699473	-2.601551	-0.253308				

Zn-P$_N$-2A-2A

C	6.416755	1.324246	0.0214	C	-6.369151	1.170823	-0.471473
C	6.507367	-0.125831	-0.037945	C	-6.342202	-0.170995	0.082104
C	7.724885	1.832517	0.068289	C	-7.688681	1.642809	-0.384952
C	0.545603	-3.978691	-0.085508	C	-0.522732	-3.766698	-1.583809
C	1.894569	-3.92	-0.150028	C	-1.863665	-3.757158	-1.447038
C	2.255202	-2.489396	-0.162527	C	-2.237216	-2.394453	-1.076097
C	-1.732652	1.272852	0.146478	C	1.602711	1.252823	-0.202447
C	-1.602601	-0.991322	0.163154	C	1.565553	-0.928666	-0.750125
C	0.054249	4.486671	-0.145766	C	-0.227999	4.353195	-0.476496
C	1.400656	4.589132	-0.189394	C	-1.50815	4.422915	-0.888759
C	-0.259723	3.049905	-0.087187	C	0.095817	2.937579	-0.336687
C	1.930716	3.211522	-0.160986	C	-2.013282	3.050745	-0.923147
C	7.920547	-0.477181	-0.029097	C	-7.685686	-0.483739	0.546039
C	0.063121	-2.589628	-0.059843	C	-0.05675	-2.420996	-1.271695
N	1.113919	-1.735569	-0.149881	N	-1.123144	-1.578931	-1.030749
N	3.493813	-2.084414	-0.128429	N	-3.457764	-2.100863	-0.745328
N	3.206269	2.960374	-0.101154	N	-3.266717	2.817453	-1.139987
N	-1.508422	2.591006	0.018291	N	1.335649	2.552581	-0.070374
N	-1.228872	-2.27686	0.050827	N	1.233038	-2.161432	-1.144218

Ni-P$_N$-2A-2A

C	5.257096	2.082217	0.012868	C	-5.274021	1.877647	-0.942749
C	5.451381	-0.988749	-0.083335	C	-5.270838	-1.012452	0.011926
H	5.687153	-2.047474	-0.123946	H	-5.428647	-2.041654	0.323028
H	5.402404	3.158565	0.041925	H	-5.478032	2.88492	-1.295741
C	-3.037946	-0.659079	0.103775	C	2.959507	-0.610777	-0.455358
C	-3.120416	0.77713	0.091456	C	2.984006	0.779667	-0.084108
C	-4.048676	-1.585457	0.063033	C	3.999607	-1.504531	-0.535502
C	-5.457687	-1.388428	0.047011	C	5.379288	-1.311735	-0.258519
C	-6.15467	-0.119637	0.033974	C	6.013823	-0.085114	0.180394
C	-5.608541	1.221462	0.030885	C	5.420899	1.211081	0.427225
C	-4.231822	1.580276	0.042429	C	4.047823	1.561072	0.284666
H	-4.011072	2.644971	0.014016	H	3.791824	2.596512	0.497238
H	-3.706551	-2.617839	0.048463	H	3.708307	-2.501698	-0.857289
C	-12.802248	-0.507255	-0.057773	C	12.587176	-0.462088	1.17806
C	-12.132859	-1.73377	-0.04261	C	11.978448	-1.648647	0.755678
C	-10.755215	-1.978054	-0.022035	C	10.63088	-1.884206	0.466729
C	-12.280158	0.789279	-0.056796	C	12.018766	0.789572	1.421203
C	-9.702451	-1.069643	-0.011275	C	9.552916	-1.006189	0.523523
C	-10.940552	1.1928	-0.040357	C	10.678536	1.179976	1.302462
C	-9.788728	0.413379	-0.020085	C	9.576891	0.427877	0.915234
H	-10.468729	-3.027944	-0.0133	H	10.392445	-2.898714	0.152933
H	-10.778407	2.268953	-0.043833	H	10.473453	2.219962	1.549164
C	-8.314894	-1.409176	0.009485	C	8.200297	-1.332759	0.208284
C	-7.567502	-0.201468	0.014203	C	7.411408	-0.165293	0.392746
C	-8.449874	0.91153	-0.004542	C	8.234351	0.91003	0.820708
C	-6.237895	-2.593861	0.038949	C	6.20233	-2.476323	-0.43995
C	-7.613946	-2.630213	0.022169	C	7.559735	-2.512385	-0.221464
C	-7.89433	2.205548	-0.007282	C	7.633172	2.161241	1.055621
H	-5.687776	-3.529299	0.047762	H	5.699637	-3.379475	-0.770721
H	-8.130056	-3.58585	0.01812	H	8.109484	-3.435351	-0.381118
H	-8.517518	3.095054	-0.022007	H	8.210603	3.02062	1.383776
C	-6.523327	2.328383	0.008302	C	6.276058	2.281045	0.857981
H	-6.085241	3.321201	0.005088	H	5.802672	3.241362	1.035254
C	4.010846	-0.793262	-0.065728	C	-3.924799	-0.836305	-0.499028
N	0.885123	2.32602	-0.139858	N	-1.001949	2.154066	-0.600643
C	8.655463	0.768288	0.039608	C	-8.506768	0.668119	0.234017
C	3.871409	1.73496	-0.028187	C	-3.875029	1.594536	-0.925872
C	3.255505	0.422782	0.015024	C	-3.165321	0.354843	-0.735449
H	7.985411	2.883492	0.115842	H	-8.030259	2.613683	-0.724719
C	-0.825795	0.189934	0.308401	C	0.721518	0.198466	-0.563118
C	10.060778	0.96752	0.07442	C	-9.890789	0.859725	0.478467
C	8.423023	-1.787456	-0.078703	C	-8.059484	-1.683895	1.16928

C	11.061174	0.027558	0.051501	C	-10.784187	-0.000244	1.069729
C	9.743158	-2.211893	-0.073478	C	-9.309508	-2.06735	1.63381
C	10.92672	-1.455368	-0.017526	C	-10.525756	-1.364446	1.61148
C	12.463624	0.308085	0.089943	C	-12.172684	0.265661	1.282284
C	12.224369	-1.970333	-0.017153	C	-11.745842	-1.830399	2.107775
C	13.151403	-0.893786	0.048562	C	-12.739971	-0.835918	1.904198
H	10.379459	2.008415	0.126678	H	-10.29143	1.818551	0.15009
H	7.680088	-2.578642	-0.128349	H	-7.264272	-2.410594	1.31244
H	9.890699	-3.289838	-0.119697	H	-9.360272	-3.057054	2.085264
H	12.476991	-3.022884	-0.060078	H	-11.901155	-2.796724	2.572101
H	12.893318	1.300584	0.142336	H	-12.676476	1.180861	0.997618
H	14.229638	-1.003594	0.063446	H	-13.78038	-0.929912	2.193028
H	2.021582	5.4738	-0.222979	H	-2.123686	5.282025	-1.114041
H	-0.692908	5.268481	-0.134006	H	0.490199	5.140727	-0.296943
H	2.61643	-4.724894	-0.168855	H	-2.581439	-4.558235	-1.551314
H	-0.101868	-4.843762	-0.041989	H	0.146789	-4.580248	-1.824807
H	-13.011845	1.592547	-0.070922	H	12.706316	1.565845	1.745893
H	-13.888066	-0.570708	-0.072668	H	13.660973	-0.524166	1.340855
H	-12.765928	-2.616947	-0.047446	H	12.640632	-2.50182	0.636007
Zn	1.191311	0.30485	0.16456	Ni	-1.156325	0.281584	-0.740199

	P_N-A-2A				P_N-2A-N-2A-N		
C	3.412637	1.424721	-0.115911	C	-1.787572	-8.104185	0
C	3.576791	-0.029069	-0.123865	C	-3.180245	-7.628453	0
C	4.696949	1.993923	-0.135117	C	-1.823512	-9.502044	0
C	-2.215355	-4.145788	0.118101	C	-4.352903	-0.617027	0
C	-0.881296	-4.003352	0.130615	C	-4.799815	-1.885148	0
C	-0.614406	-2.541768	0.028672	C	-3.600392	-2.754712	0
C	-4.797466	0.979723	-0.037837	C	1.333593	-0.35655	0
C	-4.552133	-1.314294	-0.053938	C	-0.833711	0.390915	0
C	-3.115785	4.247251	-0.015029	C	3.48223	-3.319314	0
C	-1.783096	4.396843	0.056733	C	3.055334	-4.594452	0
C	-3.356097	2.790025	0.061814	C	2.263667	-2.491381	0
C	-1.20827	3.026137	0.014928	C	1.575462	-4.543634	0
C	5.007745	-0.303216	0.415089	C	-4.037594	-8.80362	0
C	-2.76243	-2.776385	-0.155744	C	-2.882254	-0.713376	0
N	-1.777492	-1.845322	0.026641	N	-2.444429	-1.976875	0
N	0.625833	-2.112909	-0.001791	N	-3.770531	-4.042821	0
N	0.092831	2.875509	-0.150348	N	0.919735	-5.664688	0
N	-4.603423	2.305129	-0.167622	N	2.378182	-1.137168	0
N	-4.082664	-2.56909	-0.206795	N	-2.138716	0.422314	0
C	2.230931	2.143901	-0.035255	C	-0.631102	-7.334724	0

C	2.580161	-0.959007	0.313168	C	-3.596937	-6.328736	0
H	2.869156	-2.005086	0.044185	H	-4.666517	-6.143792	0
H	2.327443	3.22589	0.003897	H	0.308239	-7.880958	0
C	-5.985748	-1.033612	0.081691	C	0.021243	1.582874	0
C	-6.139942	0.403328	0.049365	C	1.394788	1.109826	0
C	-6.966156	-2.012463	0.084543	C	-0.458051	2.850778	0
C	-8.352109	-1.830102	0.127178	C	0.265516	4.101348	0
C	-9.081894	-0.636755	0.130477	C	1.708611	4.256387	0
C	-8.621595	0.683282	0.156053	C	2.751014	3.246468	0
C	-7.305123	1.153741	0.049858	C	2.552423	1.814887	0
H	-7.150933	2.230231	-0.014377	H	3.457197	1.211243	0
H	-6.587601	-3.031831	0.060365	H	-1.542729	2.930986	0
H	-2.824155	0.028423	0.144239	C	3.914469	10.678134	0
C	1.136656	-0.833012	0.136594	C	2.476136	10.478747	0
N	-2.196601	2.092035	0.192555	C	1.760496	9.21225	0
C	5.677843	0.979545	-0.222412	C	4.926966	9.637235	0
C	0.865303	1.73053	-0.004975	C	2.19208	7.929051	0
C	0.399469	0.376769	-0.307723	C	4.713941	8.198067	0
H	-0.6773	0.262183	-0.099353	C	3.585239	7.450435	0
H	4.904565	3.057596	-0.048635	H	0.679822	9.339426	0
C	-3.882629	-0.083886	-0.111161	H	5.645033	7.634975	0
C	7.071358	1.254828	-0.08706	C	1.330474	6.742881	0
C	5.57638	-1.586151	-0.115911	C	2.168116	5.593206	0
C	8.116685	0.36774	-0.123865	C	3.535563	5.98499	0
C	6.916985	-1.940388	-0.135117	C	-0.538426	5.257525	0
C	8.058139	-1.122014	0.118101	C	-0.041085	6.56663	0
C	9.502849	0.7208	0.130615	C	4.508646	5.002371	0
C	9.3796	-1.568887	0.028672	H	-1.614823	5.114638	0
C	10.250615	-0.444431	-0.037837	H	-0.730975	7.40501	0
H	7.334723	2.312076	-0.053938	H	5.568257	5.239342	0
H	4.877256	-2.417101	-0.015029	C	4.095857	3.664045	0
H	7.12003	-3.010022	0.056733	H	4.856861	2.889543	0
H	9.686084	-2.607745	0.061814	C	3.468295	13.131089	0
H	9.881365	1.735095	0.014928	C	4.383217	12.043484	0
H	11.332298	-0.498497	0.415089	C	5.773224	12.339665	0
H	-1.19138	5.297057	-0.155744	C	1.635491	11.597475	0
H	-3.897366	4.99472	0.026641	C	2.114048	12.913601	0
H	-0.110308	-4.753738	-0.001791	C	6.277498	10.003665	0
H	-2.818252	-5.043758	-0.150348	C	6.708309	11.336174	0
H	-9.392838	1.449153	-0.167622	H	0.562644	11.431032	0
H	-10.161783	-0.751999	-0.206795	H	1.415787	13.744791	0
H	-8.943816	-2.741136	-0.035255	H	7.021734	9.213194	0

H	7.769874	11.563159	0
H	-0.334631	-1.672881	0
C	-2.859419	-5.086781	0
N	1.141565	-3.217141	0
C	-3.166079	-9.954448	0
C	-0.439926	-5.930956	0
C	-1.463488	-4.937185	0
H	-1.107189	-3.914641	0

P_N-2A-A

C	0.099521	-8.454	0.735944
C	0.099521	-8.454	-0.735944
C	0.088622	-9.81226	1.144197
C	-0.02775	-2.256578	-4.216543
C	0.085179	-3.596949	-4.223449
C	0.056054	-4.023712	-2.799065
C	-0.283843	-0.230242	1.155223
C	-0.283843	-0.230242	-1.155223
C	-0.02775	-2.256578	4.216543
C	0.085179	-3.596949	4.223449
C	-0.124533	-1.862942	2.792284
C	0.056054	-4.023712	2.799065
C	0.088622	-9.81226	-1.144197
C	-0.124533	-1.862942	-2.792284
N	-0.074577	-2.934038	-1.976279
N	0.137412	-5.295343	-2.510474
N	0.137412	-5.295343	2.510474
N	-0.212437	-0.563789	2.446623
N	-0.212437	-0.563789	-2.446623
C	0.12114	-7.358246	1.567347
C	0.12114	-7.358246	-1.567347
H	0.132309	-7.558851	-2.635196
H	0.132309	-7.558851	2.635196
C	-0.218424	1.176393	-0.722164
C	-0.218424	1.176393	0.722164
C	-0.151303	2.238487	-1.58629
C	-0.092919	3.63255	-1.307293
C	-0.067885	4.253649	0
C	-0.092919	3.63255	1.307293
C	-0.151303	2.238487	1.58629
H	-0.14589	1.955176	2.636654

P_N-3A-A

C	0.17951	-11.635535	0.736204
C	0.17951	-11.635535	-0.736204
C	0.184639	-12.993339	1.144652
C	-0.022948	-5.437707	-4.214374
C	0.106189	-6.776422	-4.222411
C	0.083441	-7.20469	-2.797926
C	-0.300818	-3.410684	1.155424
C	-0.300818	-3.410684	-1.155424
C	-0.022948	-5.437707	4.214374
C	0.106189	-6.776422	4.222411
C	-0.122815	-5.045485	2.789168
C	0.083441	-7.20469	2.797926
C	0.184639	-12.993339	-1.144652
C	-0.122815	-5.045485	-2.789168
N	-0.059113	-6.115856	-1.974523
N	0.179902	-8.474862	-2.511353
N	0.179902	-8.474862	2.511353
N	-0.226828	-3.746271	2.445936
N	-0.226828	-3.746271	-2.445936
C	0.187813	-10.538371	1.567096
C	0.187813	-10.538371	-1.567096
H	0.201121	-10.738866	-2.634998
H	0.201121	-10.738866	2.634998
C	-0.259811	-2.000484	-0.723683
C	-0.259811	-2.000484	0.723683
C	-0.212538	-0.940899	-1.586344
C	-0.178003	0.459333	-1.308072
C	-0.163543	1.080726	0
C	-0.178003	0.459333	1.308072
C	-0.212538	-0.940899	1.586344
H	-0.202991	-1.222675	2.637128

H	-0.14589	1.955176	-2.636654	H	-0.202991	-1.222675	-2.637128
C	0.228105	10.906035	0	C	0.023095	7.79091	0
C	0.201249	10.310126	-1.263752	C	0.004866	7.168985	-1.305055
C	0.140448	8.95045	-1.588082	C	-0.034988	5.776458	-1.579663
C	0.201249	10.310126	1.263752	C	0.004866	7.168985	1.305055
C	0.091324	7.847567	-0.742606	C	-0.065372	4.687347	-0.737953
C	0.140448	8.95045	1.588082	C	-0.034988	5.776458	1.579663
C	0.091324	7.847567	0.742606	C	-0.065372	4.687347	0.737953
H	0.130483	8.725986	-2.652916	H	-0.04186	5.535416	-2.640787
H	0.130483	8.725986	2.652916	H	-0.04186	5.535416	2.640787
C	0.031045	6.48305	-1.162503	C	-0.102966	3.310666	-1.162213
C	-0.005432	5.668247	0	C	-0.125509	2.49584	0
C	0.031045	6.48305	1.162503	C	-0.102966	3.310666	1.162213
C	-0.053474	4.480035	-2.465779	C	-0.153453	1.304494	-2.460477
C	0.005605	5.854581	-2.422208	C	-0.117685	2.686017	-2.415422
C	0.005605	5.854581	2.422208	C	-0.117685	2.686017	2.415422
H	-0.072855	3.985419	-3.431415	H	-0.164327	0.812534	-3.427706
H	0.032026	6.424349	-3.346415	H	-0.101105	3.255316	-3.340362
H	0.032026	6.424349	3.346415	H	-0.101105	3.255316	3.340362
C	-0.053474	4.480035	2.465779	C	-0.153453	1.304494	2.460477
H	-0.072855	3.985419	3.431415	H	-0.164327	0.812534	3.427706
H	-0.47047	-2.092061	0	C	0.201636	13.849623	-1.264928
C	0.125729	-5.951874	-1.288046	C	0.161059	12.488145	-1.588798
N	-0.074577	-2.934038	1.976279	C	0.201636	13.849623	1.264928
C	0.080474	-10.622983	0	C	0.128531	11.384891	-0.744797
H	0.070458	-11.706509	0	C	0.161059	12.488145	1.588798
C	0.125729	-5.951874	1.288046	C	0.128531	11.384891	0.744797
C	0.128893	-5.347314	0	H	0.221912	14.53353	-2.108833
H	0.146157	-4.263896	0	H	0.154301	12.264029	-2.653963
H	0.087277	-10.151382	2.172741	H	0.221912	14.53353	2.108833
H	0.087277	-10.151382	-2.172741	H	0.154301	12.264029	2.653963
C	-0.382963	-1.026081	0	C	0.088321	10.021502	-1.164214
H	0.183332	-4.280986	-5.055347	C	0.064508	9.206626	0
H	-0.048243	-1.55899	-5.043041	C	0.088321	10.021502	1.164214
H	0.183332	-4.280986	5.055347	C	0.029129	8.017409	-2.46676
H	-0.048243	-1.55899	5.043041	C	0.069438	9.390379	-2.425571
H	0.231751	10.993088	2.10831	C	0.029129	8.017409	2.46676
H	0.276701	11.992693	0	C	0.069438	9.390379	2.425571
H	0.231751	10.993088	-2.10831	H	0.014327	7.52377	-3.433588
				H	0.085851	9.960036	-3.34984
				H	0.014327	7.52377	3.433588
				H	0.085851	9.960036	3.34984

H	0.251933	15.531034	0
H	-0.452222	-5.274825	0
C	0.175794	-9.133203	-1.288048
N	-0.059113	-6.115856	1.974523
C	0.186117	-13.803681	0
H	0.188875	-14.887417	0
C	0.175794	-9.133203	1.288048
C	0.171724	-8.528496	0
H	0.175836	-7.444885	0
H	0.187194	-13.332466	2.173202
H	0.187194	-13.332466	-2.173202
C	-0.384893	-4.207392	0
C	0.219523	14.443553	0
H	0.211527	-7.458934	-5.05477
H	-0.052763	-4.739563	-5.040222
H	0.211527	-7.458934	5.05477
H	-0.052763	-4.739563	5.040222

Mg-P_N-3A-A

C	0	0.732964	11.511593
C	0	-0.732964	11.511593
C	0	1.142874	12.870967
C	0	-4.226008	5.296218
C	0	-4.252491	6.648679
C	0	-2.850286	7.107313
C	0	1.138841	3.257947
C	0	-1.138841	3.257947
C	0	4.226008	5.296218
C	0	4.252491	6.648679
C	0	2.811719	4.889347
C	0	2.850286	7.107313
C	0	-1.142874	12.870967
C	0	-2.811719	4.889347
N	0	-2.027718	5.999783
N	0	-2.529476	8.371143
N	0	2.529476	8.371143
N	0	2.441685	3.598322
N	0	-2.441685	3.598322
C	0	1.564753	10.4139
C	0	-1.564753	10.4139
H	0	-2.63193	10.622677
H	0	2.63193	10.622677

Zn-P_N-3A-A

C	0.01143	-11.177664	0.730895
C	0.01143	-11.177664	-0.730895
C	-0.010032	-12.534757	1.144486
C	0.118827	-5.004638	-4.236686
C	0.169562	-6.354712	-4.260237
C	0.165817	-6.803122	-2.854425
C	-0.151265	-3.034283	1.133296
C	-0.151265	-3.034283	-1.133296
C	0.118827	-5.004638	4.236686
C	0.169562	-6.354712	4.260237
C	0.08313	-4.60762	2.820391
C	0.165817	-6.803122	2.854425
C	-0.010032	-12.534757	-1.144486
C	0.08313	-4.60762	-2.820391
N	0.158229	-5.704066	-2.031344
N	0.109687	-8.059474	-2.527521
N	0.109687	-8.059474	2.527521
N	-0.02346	-3.331978	2.434491
N	-0.02346	-3.331978	-2.434491
C	0.032846	-10.069533	1.544263
C	0.032846	-10.069533	-1.544263
H	0.040513	-10.266637	-2.612905
H	0.040513	-10.266637	2.612905

C	0	-0.724581	1.836772	C	-0.098611	-1.61629	-0.719186
C	0	0.724581	1.836772	C	-0.098611	-1.61629	0.719186
C	0	-1.585968	0.773852	C	-0.06082	-0.557324	-1.585626
C	0	-1.307718	-0.626808	C	-0.055801	0.84255	-1.308221
C	0	0	-1.249477	C	-0.054513	1.46565	0
C	0	1.307718	-0.626808	C	-0.055801	0.84255	1.308221
C	0	1.585968	0.773852	C	-0.06082	-0.557324	1.585626
H	0	2.637871	1.05218	H	-0.0369	-0.839228	2.635931
H	0	-2.637871	1.05218	H	-0.0369	-0.839228	-2.635931
C	0	0	-7.962491	C	0.00082	8.178164	0
C	0	-1.304918	-7.340011	C	-0.004693	7.555167	-1.305106
C	0	-1.579638	-5.947151	C	-0.016595	6.163065	-1.579804
C	0	1.304918	-7.340011	C	-0.004693	7.555167	1.305106
C	0	-0.737954	-4.857249	C	-0.025935	5.072591	-0.737469
C	0	1.579638	-5.947151	C	-0.016595	6.163065	1.579804
C	0	0.737954	-4.857249	C	-0.025935	5.072591	0.737469
H	0	-2.64077	-5.706033	H	-0.018294	5.921737	-2.640864
H	0	2.64077	-5.706033	H	-0.018294	5.921737	2.640864
C	0	-1.161926	-3.480315	C	-0.036254	3.696067	-1.161857
C	0	0	-2.664707	C	-0.04316	2.879922	0
C	0	1.161926	-3.480315	C	-0.036254	3.696067	1.161857
C	0	-2.459925	-1.47315	C	-0.045422	1.688913	-2.460323
C	0	-2.415073	-2.855083	C	-0.037485	3.070888	-2.414988
C	0	2.415073	-2.855083	C	-0.037485	3.070888	2.414988
H	0	-3.427251	-0.981149	H	-0.045108	1.197037	-3.42771
H	0	-3.340129	-3.424554	H	-0.031553	3.640502	-3.339951
H	0	3.340129	-3.424554	H	-0.031553	3.640502	3.339951
C	0	2.459925	-1.47315	C	-0.045422	1.688913	2.460323
H	0	3.427251	-0.981149	H	-0.045108	1.197037	3.42771
C	0	-1.264878	-14.023868	C	0.056598	14.238975	-1.264807
C	0	-1.588804	-12.661816	C	0.043815	12.877334	-1.58889
C	0	1.264878	-14.023868	C	0.056598	14.238975	1.264807
C	0	-0.74486	-11.557976	C	0.033565	11.773112	-0.744595
C	0	1.588804	-12.661816	C	0.043815	12.877334	1.58889
C	0	0.74486	-11.557976	C	0.033565	11.773112	0.744595
H	0	-2.108816	-14.708067	H	0.063001	14.923145	-2.108803
H	0	-2.653982	-12.437627	H	0.041708	12.653115	-2.654035
H	0	2.108816	-14.708067	H	0.063001	14.923145	2.108803
H	0	2.653982	-12.437627	H	0.041708	12.653115	2.654035
C	0	-1.164141	-10.194094	C	0.021008	10.409575	-1.163968
C	0	0	-9.378783	C	0.013599	9.59385	0
C	0	1.164141	-10.194094	C	0.021008	10.409575	1.163968

C	0	-2.46669	-8.18903	C	0.002766	8.404608	-2.466855
C	0	-2.425528	-9.562485	C	0.015173	9.777915	-2.425399
C	0	2.46669	-8.18903	C	0.002766	8.404608	2.466855
C	0	2.425528	-9.562485	C	0.015173	9.777915	2.425399
H	0	-3.433511	-7.695135	H	-0.001743	7.910869	-3.433752
H	0	-3.349822	-10.13237	H	0.020265	10.347876	-3.349663
H	0	3.433511	-7.695135	H	-0.001743	7.910869	3.433752
H	0	3.349822	-10.13237	H	0.020265	10.347876	3.349663
H	0	0	-15.706137	H	0.072472	15.921587	0
C	0	-1.276144	9.006035	C	0.040326	-8.656879	-1.265156
N	0	2.027718	5.999783	N	0.158229	-5.704066	2.031344
C	0	0	13.683672	C	-0.024147	-13.34622	0
H	0	0	14.767294	H	-0.041386	-14.429793	0
C	0	1.276144	9.006035	C	0.040326	-8.656879	1.265156
C	0	0	8.349944	C	-0.019284	-7.97119	0
H	0	2.172192	13.208592	H	-0.013766	-12.873005	2.173467
H	0	-2.172192	13.208592	H	-0.013766	-12.873005	-2.173467
C	0	0	4.093698	C	-0.314169	-3.878353	0
C	0	0	-14.618171	C	0.062244	14.833698	0
H	0	-5.103508	7.316043	H	0.189325	-7.027021	-5.107014
H	0	-5.051324	4.597147	H	0.088855	-4.304277	-5.060265
H	0	5.103508	7.316043	H	0.189325	-7.027021	5.107014
H	0	5.051324	4.597147	H	0.088855	-4.304277	5.060265
Mg	0	0	6.191737	Zn	-0.159928	-5.903438	0

Ni-P_N-3A-A				**P_N-A-A**			
C	-11.107357	-0.601155	-0.412814	C	0.002813	5.415304	0.735184
C	-11.107321	0.601085	0.413184	C	0.002813	5.415304	-0.735184
C	-12.464705	-0.936887	-0.65808	C	0.04602	6.774205	1.143119
C	-5.081422	4.117675	0.049767	C	-0.024491	-0.778097	-4.222112
C	-6.386799	4.111779	0.382749	C	-0.104534	0.564914	-4.226452
C	-6.815712	2.714992	0.37744	C	-0.060577	0.988183	-2.802072
C	-3.083849	-1.115698	0.139406	C	0.19155	-2.800953	1.153629
C	-3.083848	1.115733	-0.139589	C	0.19155	-2.800953	-1.153629
C	-5.081398	-4.117645	-0.050018	C	-0.024491	-0.778097	4.222112
C	-6.386774	-4.111748	-0.383011	C	-0.104534	0.564914	4.226452
C	-4.676777	-2.724093	0.094016	C	0.068428	-1.175109	2.799817
C	-6.815706	-2.714968	-0.377623	C	-0.060577	0.988183	2.802072
C	-12.46465	0.936776	0.658626	C	0.04602	6.774205	-1.143119
C	-4.676784	2.724119	-0.094199	C	0.068428	-1.175109	-2.799817
N	-5.752069	1.881304	0.06034	N	0.047044	-0.100686	-1.98083
N	-8.041418	2.398631	0.64418	N	-0.110662	2.263456	-2.509165

N	-8.041429	-2.398606	-0.644273	N	-0.110662	2.263456	2.509165
N	-3.396812	-2.407856	0.234103	N	0.125647	-2.471099	2.449463
N	-3.396819	2.407893	-0.234274	N	0.125647	-2.471099	-2.449463
C	-9.990169	-1.320897	-0.762006	C	-0.045455	4.323114	1.567747
C	-9.990114	1.320872	0.762219	C	-0.045455	4.323114	-1.567747
H	-10.166437	2.249724	1.29896	H	-0.052356	4.5238	-2.635506
H	-10.16653	-2.249744	-1.298744	H	-0.052356	4.5238	2.635506
C	-1.675295	0.712628	-0.101591	C	0.080341	-4.196866	-0.720642
C	-1.675295	-0.712588	0.101433	C	0.080341	-4.196866	0.720642
C	-0.615639	1.571205	-0.223362	C	-0.024643	-5.273213	-1.592257
C	0.783192	1.294767	-0.186996	C	-0.123896	-6.629443	-1.263856
C	1.40545	0.000015	-0.000044	C	-0.165277	-7.227739	0
C	0.783187	-1.294736	0.1869	C	-0.123896	-6.629443	1.263856
C	-0.615645	-1.571167	0.223242	C	-0.024643	-5.273213	1.592257
H	-0.894995	-2.612543	0.365714	H	-0.022998	-5.003715	2.645804
H	-0.894977	2.612585	-0.365826	H	-0.022998	-5.003715	-2.645804
C	8.117839	-0.000004	0.000018	H	0.438438	-0.944355	0
C	7.495717	1.29207	-0.18344	C	-0.083454	2.914194	-1.288385
C	6.102869	1.563877	-0.223997	N	0.047044	-0.100686	1.98083
C	7.495706	-1.292074	0.183461	C	0.073597	7.58551	0
C	5.012817	0.730814	-0.105398	H	0.109356	8.66817	0
C	6.102857	-1.563873	0.223988	C	-0.083454	2.914194	1.288385
C	5.012811	-0.730801	0.105371	C	-0.100869	2.31028	0
H	5.861966	2.614315	-0.374676	H	-0.144202	1.227756	0
H	5.861941	-2.614309	0.374657	H	0.055144	7.113015	2.171739
C	3.636658	1.15013	-0.166337	H	0.055144	7.113015	-2.171739
C	2.820739	0.000012	-0.000033	C	0.315547	-2.006574	0
C	3.636651	-1.15011	0.166285	H	-0.189438	1.251775	-5.057337
C	1.630351	2.435856	-0.35235	H	-0.024193	-1.474318	-5.049811
C	3.011436	2.391167	-0.345854	H	-0.189438	1.251775	5.057337
C	3.011423	-2.391144	0.345798	H	-0.024193	-1.474318	5.049811
H	1.138213	3.39319	-0.490888	H	-0.180406	-7.313844	2.107029
H	3.581516	3.30633	-0.478224	H	-0.180406	-7.313844	-2.107029
H	3.581498	-3.306309	0.47818	H	-0.246736	-8.312048	0
C	1.630338	-2.435828	0.352273				
H	1.138194	-3.39316	0.490806				
C	14.179438	1.252624	-0.176363				
C	12.817171	1.573291	-0.221578				
C	14.179425	-1.252671	0.176541				
C	11.713466	0.737805	-0.104023				
C	12.817159	-1.57333	0.221723				
C	11.713458	-0.737835	0.104143				

H	14.863675	2.088314	-0.29384
H	12.59284	2.628074	-0.369973
H	14.863656	-2.088363	0.294034
H	12.592815	-2.628111	0.370112
C	10.349769	1.152781	-0.16269
C	9.534317	-0.000008	0.000035
C	10.349761	-1.152802	0.162778
C	8.344956	2.442588	-0.345542
C	9.718274	2.402042	-0.339078
C	8.344935	-2.442599	0.34558
C	9.718253	-2.402061	0.339149
H	7.850851	3.39977	-0.481289
H	10.28847	3.317145	-0.468031
H	7.850822	-3.399778	0.481313
H	10.288441	-3.317168	0.468114
H	15.861513	-0.000028	0.000109
C	-8.59539	1.151283	0.445256
N	-5.752066	-1.881284	-0.0605
C	-13.276165	-0.000068	0.000329
H	-14.359773	-0.000084	0.000397
C	-8.595412	-1.151277	-0.445212
C	-7.864663	0	0.000008
H	-12.803935	-1.785874	-1.238948
H	-12.803834	1.785753	1.239538
C	-3.952052	0.000016	-0.000124
C	14.773503	-0.000023	0.000096
H	-7.055767	4.931428	0.602902
H	-4.392803	4.943755	-0.058168
H	-7.055724	-4.931401	-0.603203
H	-4.39278	-4.94373	0.057882
Ni	-5.841231	0.000006	-0.000025

	P_N-N-3A-N				**Mg-P_N-N-3A-N**		
C	0	4.147011	7.999241	C	-0.001926	-7.824381	4.179124
C	0	4.144812	6.647741	C	-0.000812	-6.46209	4.179803
C	0	2.739169	8.412368	C	-0.001115	-8.257876	2.785808
C	0	-0.688436	11.468001	C	-0.004377	-11.311933	-0.684495
C	0	0.688436	11.468001	C	-0.004377	-11.311933	0.684495
C	0	1.128138	10.104275	C	-0.001912	-9.925791	1.109909
C	0	-4.144812	6.647741	C	-0.000812	-6.46209	-4.179803
C	0	-4.147011	7.999241	C	-0.001926	-7.824381	-4.179124

C	0	-2.732629	6.244107	C	0.000683	-6.032823	-2.784226
C	0	-2.739169	8.412368	C	-0.001115	-8.257876	-2.785808
C	0	-0.724691	3.121824	C	0.002033	-2.926134	-0.725703
C	0	0.724691	3.121824	C	0.002033	-2.926134	0.725703
C	0	-1.147142	4.526089	C	0.002404	-4.342232	-1.127071
C	0	1.147142	4.526089	C	0.002404	-4.342232	1.127071
C	0	2.732629	6.244107	C	0.000683	-6.032823	2.784226
C	0	-1.128138	10.104275	C	-0.001912	-9.925791	-1.109909
N	0	0	9.322696	N	-0.000144	-9.124102	0
N	0	1.906632	7.308668	N	0.000491	-7.132741	1.984714
N	0	-1.906632	7.308668	N	0.000491	-7.132741	-1.984714
H	0	0	8.311017	N	-0.002096	-9.526957	2.396141
H	0	0	6.300609	N	0.001691	-4.745791	2.395404
N	0	2.398622	9.6902	N	0.001691	-4.745791	-2.395404
N	0	2.391756	4.936697	N	-0.002096	-9.526957	-2.396141
N	0	-2.391756	4.936697	C	0.0016	-1.878871	-1.593265
N	0	-2.398622	9.6902	C	0.00128	-0.466351	-1.31665
C	0	-1.59345	2.074017	C	0.001168	0.152747	0
C	0	-1.317146	0.663007	C	0.00128	-0.466351	1.31665
C	0	0	0.043649	C	0.0016	-1.878871	1.593265
C	0	1.317146	0.663007	H	0.001523	-2.154703	2.645437
C	0	1.59345	2.074017	H	0.001523	-2.154703	-2.645437
H	0	2.645141	2.351517	H	-0.003305	-8.500427	-5.022784
H	0	-2.645141	2.351517	H	-0.001082	-5.785962	-5.023217
H	0	-4.979359	8.688904	H	-0.006141	-12.156674	-1.359002
H	0	-4.974837	5.955106	H	-0.006141	-12.156674	1.359002
H	0	-1.361458	12.312875	H	-0.003305	-8.500427	5.022784
H	0	1.361458	12.312875	H	-0.001082	-5.785962	5.023217
H	0	4.979359	8.688904	N	0.003166	-5.118826	0
H	0	4.974837	5.955106	C	-0.000236	6.884186	0
N	0	0	5.283712	C	-0.000128	6.249754	-1.317829
C	0	0	-6.686192	C	0.000124	4.859081	-1.583799
C	0	-1.31798	-6.051629	C	-0.000128	6.249754	1.317829
C	0	-1.584058	-4.661598	C	0.000344	3.777053	-0.724433
C	0	1.31798	-6.051629	C	0.000124	4.859081	1.583799
C	0	-0.724313	-3.579112	C	0.000344	3.777053	0.724433
C	0	1.584058	-4.661598	H	0.000161	4.609445	-2.643127
C	0	0.724313	-3.579112	H	0.000161	4.609445	2.643127
H	0	-2.643306	-4.411837	C	0.000631	2.382471	-1.160593
H	0	2.643306	-4.411837	C	0.000831	1.55919	0
C	0	-1.160812	-2.185381	C	0.000631	2.382471	1.160593
C	0	0	-1.361579	C	0.001049	0.370892	-2.451768

C	0	1.160812	-2.185381	C	0.000742	1.7694	-2.402577
C	0	-2.452509	-0.174098	C	0.000742	1.7694	2.402577
C	0	-2.402961	-1.572455	H	0.001126	-0.111689	-3.424533
C	0	2.402961	-1.572455	H	0.000595	2.338809	-3.327301
H	0	-3.425245	0.308433	H	0.000595	2.338809	3.327301
H	0	-3.327583	-2.141926	C	0.001049	0.370892	2.451768
H	0	3.327583	-2.141926	H	0.001126	-0.111689	3.424533
C	0	2.452509	-0.174098	C	-0.001231	12.933542	-1.258297
H	0	3.425245	0.308433	C	-0.001025	11.625897	-1.589392
C	0	-1.258135	-12.734707	C	-0.001231	12.933542	1.258297
C	0	-1.589343	-11.426814	C	-0.000839	10.468417	-0.708073
C	0	1.258135	-12.734707	C	-0.001025	11.625897	1.589392
C	0	-0.708657	-10.269611	C	-0.000839	10.468417	0.708073
C	0	1.589343	-11.426814	H	-0.001506	14.536563	0
C	0	0.708657	-10.269611	H	-0.001347	13.670341	-2.055652
H	0	0	-14.337447	H	-0.000992	11.42058	-2.655208
H	0	-2.055471	-13.471466	H	-0.001347	13.670341	2.055652
H	0	-2.655193	-11.22178	H	-0.000992	11.42058	2.655208
H	0	2.055471	-13.471466	C	-0.000614	9.112526	-1.15627
H	0	2.655193	-11.22178	C	-0.000472	8.269928	0
C	0	-1.156436	-8.914315	C	-0.000614	9.112526	1.15627
C	0	0	-8.071643	C	-0.00028	7.100525	-2.460855
C	0	1.156436	-8.914315	C	-0.000514	8.488298	-2.408112
C	0	-2.461334	-6.902635	C	-0.00028	7.100525	2.460855
C	0	-2.408609	-8.290021	C	-0.000514	8.488298	2.408112
C	0	2.461334	-6.902635	H	-0.000201	6.618433	-3.434313
C	0	2.408609	-8.290021	H	-0.000613	9.05912	-3.332712
H	0	-3.434706	-6.420433	H	-0.000201	6.618433	3.434313
H	0	-3.333105	-8.860958	H	-0.000613	9.05912	3.332712
H	0	3.434706	-6.420433	N	-0.001318	13.530451	0
H	0	3.333105	-8.860958	Mg	0.003983	-7.132976	0

Zn-P_N-N-3A-N				**Ni-P_N-N-3A-N**			
C	0.017311	-7.498767	4.161451	C	0	4.110907	7.493695
C	0.010793	-6.138241	4.162361	C	0	4.109472	6.138793
C	0.009403	-7.930409	2.769397	C	0	2.724899	7.914498
C	0.036068	-10.981329	-0.683723	C	0	-0.679988	10.908945
C	0.036068	-10.981329	0.683723	C	0	0.679988	10.908945
C	0.017837	-9.595819	1.107332	C	0	1.094938	9.529389
C	0.010793	-6.138241	-4.162361	C	0	-4.109472	6.138793
C	0.017311	-7.498767	-4.161451	C	0	-4.110907	7.493695
C	-0.001304	-5.710321	-2.76824	C	0	-2.720465	5.724039

C	0.009403	-7.930409	-2.769397	C	0	-2.724899	7.914498
C	-0.0072	-2.610767	-0.724367	C	0	-0.718308	2.673487
C	-0.0072	-2.610767	0.724367	C	0	0.718308	2.673487
C	-0.008922	-4.026726	-1.122445	C	0	-1.108911	4.083888
C	-0.008922	-4.026726	1.122445	C	0	1.108911	4.083888
C	-0.001304	-5.710321	2.76824	C	0	2.720465	5.724039
C	0.017837	-9.595819	-1.107332	C	0	-1.094938	9.529389
N	0.006869	-8.790657	0	N	0	0	8.690421
N	-0.002156	-6.80763	1.962654	N	0	1.887346	6.808887
N	-0.002156	-6.80763	-1.962654	N	0	-1.887346	6.808887
N	0.017777	-9.199714	2.390132	N	0	2.377136	9.181547
N	-0.005742	-4.424862	2.389366	N	0	2.374805	4.442483
N	-0.005742	-4.424862	-2.389366	N	0	-2.374805	4.442483
N	0.017777	-9.199714	-2.390132	N	0	-2.377136	9.181547
C	-0.005379	-1.564854	-1.59336	C	0	-1.593615	1.631618
C	-0.00401	-0.152321	-1.31678	C	0	-1.31722	0.220072
C	-0.003511	0.466716	0	C	0	0	-0.399297
C	-0.00401	-0.152321	1.31678	C	0	1.31722	0.220072
C	-0.005379	-1.564854	1.59336	C	0	1.593615	1.631618
H	-0.005112	-1.841069	2.645385	H	0	2.644466	1.910166
H	-0.005112	-1.841069	-2.645385	H	0	-2.644466	1.910166
H	0.028372	-8.178239	-5.002117	H	0	-4.939992	8.186552
H	0.015303	-5.458911	-5.00303	H	0	-4.936551	5.443693
H	0.04894	-11.823789	-1.360802	H	0	-1.373176	11.737584
H	0.04894	-11.823789	1.360802	H	0	1.373176	11.737584
H	0.028372	-8.178239	5.002117	H	0	4.939992	8.186552
H	0.015303	-5.458911	5.00303	H	0	4.936551	5.443693
N	-0.01041	-4.80909	0	N	0	0	4.901834
C	0.001667	7.198163	0	C	0	0	-7.130185
C	0.001246	6.563717	-1.317834	C	0	-1.317874	-6.495573
C	0.00028	5.173068	-1.583798	C	0	-1.583838	-5.105418
C	0.001246	6.563717	1.317834	C	0	1.317874	-6.495573
C	-0.00049	4.091016	-0.724422	C	0	-0.724428	-4.022799
C	0.00028	5.173068	1.583798	C	0	1.583838	-5.105418
C	-0.00049	4.091016	0.724422	C	0	0.724428	-4.022799
H	0.000091	4.923428	-2.643125	H	0	-2.643163	-4.855759
H	0.000091	4.923428	2.643125	H	0	2.643163	-4.855759
C	-0.001568	2.696451	-1.1606	C	0	-1.160697	-2.628873
C	-0.00227	1.873138	0	C	0	0	-1.805301
C	-0.001568	2.696451	1.1606	C	0	1.160697	-2.628873
C	-0.003147	0.684911	-2.451846	C	0	-2.452519	-0.617503
C	-0.001971	2.083426	-2.402584	C	0	-2.402833	-2.015705

C	-0.001971	2.083426	2.402584	C	0	2.402833	-2.015705
H	-0.003468	0.202372	-3.424633	H	0	-3.425288	-0.134962
H	-0.001404	2.652879	-3.327282	H	0	-3.327434	-2.585346
H	-0.001404	2.652879	3.327282	H	0	3.327434	-2.585346
C	-0.003147	0.684911	2.451846	C	0	2.452519	-0.617503
H	-0.003468	0.202372	3.424633	H	0	3.425288	-0.134962
C	0.005222	13.2475	-1.258297	C	0	-1.258254	-13.179114
C	0.004585	11.939855	-1.589394	C	0	-1.589379	-11.871358
C	0.005222	13.2475	1.258297	C	0	1.258254	-13.179114
C	0.003898	10.782369	-0.708084	C	0	-0.708424	-10.713907
C	0.004585	11.939855	1.589394	C	0	1.589379	-11.871358
C	0.003898	10.782369	0.708084	C	0	0.708424	-10.713907
H	0.005814	14.85052	0	H	0	0	-14.781976
H	0.005656	13.984301	-2.055652	H	0	-2.055565	-13.915954
H	0.004573	11.734542	-2.655211	H	0	-2.655234	-11.666174
H	0.005656	13.984301	2.055652	H	0	2.055565	-13.915954
H	0.004573	11.734542	2.655211	H	0	2.655234	-11.666174
C	0.00307	9.426502	-1.156274	C	0	-1.15638	-9.358525
C	0.002545	8.583896	0	C	0	0	-8.515844
C	0.00307	9.426502	1.156274	C	0	1.15638	-9.358525
C	0.001801	7.414502	-2.46087	C	0	-2.461231	-7.34665
C	0.002691	8.802261	-2.408124	C	0	-2.408493	-8.734028
C	0.001801	7.414502	2.46087	C	0	2.461231	-7.34665
C	0.002691	8.802261	2.408124	C	0	2.408493	-8.734028
H	0.001484	6.932406	-3.434327	H	0	-3.43462	-6.864411
H	0.003052	9.373086	-3.332722	H	0	-3.333064	-9.304913
H	0.001484	6.932406	3.434327	H	0	3.43462	-6.864411
H	0.003052	9.373086	3.332722	H	0	3.333064	-9.304913
N	0.005448	13.844409	0	N	0	0	-13.775852
Zn	-0.043519	-6.819935	0	Ni	0	0	6.802196

P_N-N-3A				**Mg-P_N-N-3A**			
C	-0.111339	-7.900512	4.206268	C	-7.781377	-4.193992	0.157523
C	0.147133	-6.572455	4.217924	C	-6.427715	-4.200761	0.005753
C	-0.20371	-8.281294	2.787256	C	-8.207018	-2.795755	0.125478
C	-0.795249	-11.251329	-0.681164	C	-11.241385	0.68068	0.5726
C	-0.795249	-11.251329	0.681164	C	-11.241377	-0.680703	0.572593
C	-0.559955	-9.894898	1.135578	C	-9.867773	-1.115672	0.314005
C	0.147133	-6.572455	-4.217924	C	-6.427767	4.200774	0.005581
C	-0.111339	-7.900512	-4.206268	C	-7.781408	4.19399	0.157458
C	0.224619	-6.155065	-2.807867	C	-5.992377	2.809675	-0.128829
C	-0.20371	-8.281294	-2.787256	C	-8.20703	2.795732	0.125528

C	0.448886	-3.144135	-0.727437	C	-2.91166	0.731099	-0.283608
C	0.448886	-3.144135	0.727437	C	-2.911658	-0.731072	-0.283615
C	0.520862	-4.54305	-1.155784	C	-4.324646	1.146504	-0.333037
C	0.520862	-4.54305	1.155784	C	-4.324639	-1.146479	-0.333067
C	0.224619	-6.155065	2.807867	C	-5.992367	-2.809684	-0.128905
C	-0.559955	-9.894898	-1.135578	C	-9.867776	1.115663	0.314038
N	-0.435349	-9.117535	0	N	-9.090562	0.000011	0.146018
N	0.006379	-7.224702	1.979217	N	-7.113442	-2.007161	-0.062518
N	0.006379	-7.224702	-1.979217	N	-7.113438	2.007136	-0.062281
H	-0.298281	-8.111474	0	N	-9.481469	-2.395285	0.289837
H	0.789681	-6.393322	0	N	-4.712429	-2.444069	-0.241779
N	-0.47123	-9.54387	2.406143	N	-4.712449	2.444082	-0.241742
N	0.433623	-4.891292	2.454365	N	-9.481489	2.395282	0.289869
N	0.433623	-4.891292	-2.454365	C	-1.842372	1.585264	-0.229407
N	-0.47123	-9.54387	-2.406143	C	-0.443972	1.30707	-0.189504
C	0.371092	-2.079919	-1.585546	C	0.17804	0.000007	-0.173389
C	0.308874	-0.68299	-1.307536	C	-0.443973	-1.307057	-0.189511
C	0.281423	-0.06237	0	C	-1.842376	-1.585244	-0.229422
C	0.308874	-0.68299	1.307536	H	-2.115131	-2.638722	-0.220283
C	0.371092	-2.079919	1.585546	H	-2.115122	2.638743	-0.220253
H	0.363237	-2.356971	2.637587	H	-8.450721	5.031971	0.295473
H	0.363237	-2.356971	-2.637587	H	-5.756259	5.048532	-0.008926
H	-0.247367	-8.582362	-5.034597	H	-12.068385	1.356195	0.742653
H	0.284379	-5.907384	-5.059709	H	-12.068374	-1.356224	0.742639
H	-0.928848	-12.081691	-1.359377	H	-8.450694	-5.031953	0.295628
H	-0.928848	-12.081691	1.359377	H	-5.75616	-5.048484	-0.00858
H	-0.247367	-8.582362	5.034597	C	6.88767	0	0.023471
H	0.284379	-5.907384	5.059709	C	6.265853	1.304969	0.005016
C	-0.034046	6.642317	0	C	4.8735	1.579701	-0.035814
C	-0.004069	6.021216	-1.305128	C	6.265851	-1.304966	0.005009
C	0.062104	4.629628	-1.579767	C	3.783663	0.739017	-0.067423
C	-0.004069	6.021216	1.305128	C	4.873496	-1.579696	-0.035821
C	0.11295	3.540705	-0.739223	C	3.783662	-0.73901	-0.067425
C	0.062104	4.629628	1.579767	H	4.63289	2.641055	-0.042931
C	0.11295	3.540705	0.739223	H	4.632885	-2.641049	-0.042943
H	0.073686	4.389258	-2.641161	C	2.408675	1.162409	-0.107209
H	0.073686	4.389258	2.641161	C	1.593746	0.000006	-0.131521
C	0.176947	2.166772	-1.162814	C	2.408671	-1.1624	-0.107213
C	0.215184	1.352647	0	C	0.402846	2.461202	-0.16212
C	0.176947	2.166772	1.162814	C	1.782484	2.416948	-0.123034
C	0.267772	0.162776	-2.462194	C	1.78248	-2.416937	-0.123042
C	0.204511	1.541234	-2.417793	H	-0.089675	3.42832	-0.174163

C	0.204511	1.541234	2.417793	H	2.352039	3.341748	-0.104857
H	0.288828	-0.329686	-3.429177	H	2.352033	-3.341737	-0.104867
H	0.176762	2.110659	-3.34236	C	0.40284	-2.46119	-0.162129
H	0.176762	2.110659	3.34236	H	-0.089681	-3.428308	-0.174176
C	0.267772	0.162776	2.462194	C	12.946883	1.265091	0.202016
H	0.288828	-0.329686	3.429177	C	11.584945	1.588922	0.161664
C	-0.325312	12.697255	-1.265187	C	12.946881	-1.2651	0.202008
C	-0.259354	11.33617	-1.588952	C	10.481746	0.745633	0.129312
C	-0.325312	12.697255	1.265187	C	11.584942	-1.588929	0.161654
C	-0.206468	10.233878	-0.745762	C	10.481745	-0.745639	0.129307
C	-0.259354	11.33617	1.588952	H	14.627964	-0.000006	0.251968
C	-0.206468	10.233878	0.745762	H	13.630869	2.108963	0.222149
H	-0.406965	14.376936	0	H	11.360905	2.654195	0.154903
H	-0.358246	13.380765	-2.109028	H	13.630867	-2.108972	0.222135
H	-0.248335	11.112273	-2.654235	H	11.360902	-2.654202	0.154886
H	-0.358246	13.380765	2.109028	C	9.118822	1.164475	0.089154
H	-0.248335	11.112273	2.654235	C	8.303846	-0.000001	0.06525
C	-0.140947	8.871944	-1.164609	C	9.11882	-1.164478	0.089147
C	-0.101992	8.057555	0	C	7.114721	2.467017	0.029681
C	-0.140947	8.871944	1.164609	C	8.487188	2.426386	0.070255
C	-0.044146	6.86936	-2.467124	C	7.114716	-2.467016	0.029667
C	-0.110167	8.240872	-2.426599	C	8.487184	-2.426388	0.07024
C	-0.044146	6.86936	2.467124	H	6.620602	3.433716	0.014768
C	-0.110167	8.240872	2.426599	H	9.057043	3.350553	0.086833
H	-0.01991	6.375547	-3.433816	H	6.620596	-3.433714	0.014747
H	-0.137156	8.810386	-3.35072	H	9.057037	-3.350556	0.086812
H	-0.01991	6.375547	3.433816	C	-5.134133	0.000016	-0.429386
H	-0.137156	8.810386	3.35072	C	13.540369	-0.000005	0.219776
C	0.641378	-5.334736	0	Mg	-7.149034	-0.000041	-0.239831
C	-0.354325	13.290117	0				

Zn-P_N-N-3A

C	0.17403	-7.432989	4.208776
C	0.013927	-6.081846	4.217443
C	0.198019	-7.845019	2.805463
C	0.601657	-10.844328	-0.678979
C	0.601657	-10.844328	0.678979
C	0.353847	-9.471482	1.112884
C	0.013927	-6.081846	-4.217443
C	0.17403	-7.432989	-4.208776
C	-0.074781	-5.648433	-2.82173
C	0.198019	-7.845019	-2.805463

Ni-P_N-N-3A

C	0.006381	-7.468792	4.10798
C	0.006701	-6.114397	4.13035
C	0.002948	-7.866259	2.712917
C	-0.003059	-10.898878	-0.676902
C	-0.003059	-10.898878	0.676902
C	-0.002449	-9.504938	1.09454
C	0.006701	-6.114397	-4.13035
C	0.006381	-7.468792	-4.10798
C	0.003442	-5.669745	-2.750873
C	0.002948	-7.866259	-2.712917

C	-0.288609	-2.618722	-0.727684	C	-0.001515	-2.659884	-0.722435
C	-0.288609	-2.618722	0.727684	C	-0.001515	-2.659884	0.722435
C	-0.345416	-4.027763	-1.144582	C	-0.001605	-4.062289	-1.131267
C	-0.345416	-4.027763	1.144582	C	-0.001605	-4.062289	1.131267
C	-0.074781	-5.648433	2.82173	C	0.003442	-5.669745	2.750873
C	0.353847	-9.471482	-1.112884	C	-0.002449	-9.504938	-1.09454
N	0.186513	-8.679458	0	N	-0.003274	-8.675345	0
N	0.057467	-6.75301	2.013975	N	0.002463	-6.760301	1.89321
N	0.057467	-6.75301	-2.013975	N	0.002463	-6.760301	-1.89321
N	0.344741	-9.114352	2.396793	N	0.000382	-9.14873	2.366861
N	-0.234147	-4.381363	2.445344	N	0.001411	-4.389782	2.427601
N	-0.234147	-4.381363	-2.445344	N	0.001411	-4.389782	-2.427601
N	0.344741	-9.114352	-2.396793	N	0.000382	-9.14873	-2.366861
C	-0.229852	-1.552054	-1.584853	C	-0.000874	-1.59517	-1.585834
C	-0.192308	-0.153958	-1.307257	C	-0.000814	-0.198065	-1.307607
C	-0.176488	0.46786	0	C	-0.000846	0.424377	0
C	-0.192308	-0.153958	1.307257	C	-0.000814	-0.198065	1.307607
C	-0.229852	-1.552054	1.584853	C	-0.000874	-1.59517	1.585834
H	-0.215936	-1.827508	2.637415	H	-0.000383	-1.871977	2.637746
H	-0.215936	-1.827508	-2.637415	H	-0.000383	-1.871977	-2.637746
H	0.278484	-8.109456	-5.045884	H	0.007986	-8.176777	-4.924301
H	-0.049948	-5.413803	-5.065603	H	0.008649	-5.436112	-4.97174
H	0.767515	-11.666917	-1.360548	H	-0.002818	-11.728373	-1.369617
H	0.767515	-11.666917	1.360548	H	-0.002818	-11.728373	1.369617
H	0.278484	-8.109456	5.045884	H	0.007986	-8.176777	4.924301
H	-0.049948	-5.413803	5.065603	H	0.008649	-5.436112	4.97174
C	0.023516	7.177113	0	C	-0.000168	7.13628	0
C	0.00434	6.555368	-1.305023	C	-0.00024	6.514102	-1.304983
C	-0.037806	5.16305	-1.579729	C	-0.000388	5.121493	-1.579757
C	0.00434	6.555368	1.305023	C	-0.00024	6.514102	1.304983
C	-0.070195	4.073213	-0.739075	C	-0.000482	4.030744	-0.739106
C	-0.037806	5.16305	1.579729	C	-0.000388	5.121493	1.579757
C	-0.070195	4.073213	0.739075	C	-0.000482	4.030744	0.739106
H	-0.045078	4.922463	-2.641096	H	-0.000421	4.880826	-2.641131
H	-0.045078	4.922463	2.641096	H	-0.000421	4.880826	2.641131
C	-0.110443	2.698368	-1.162565	C	-0.000594	2.655873	-1.162492
C	-0.134716	1.883516	0	C	-0.000698	1.840305	0
C	-0.110443	2.698368	1.162565	C	-0.000594	2.655873	1.162492
C	-0.16534	0.692696	-2.461639	C	-0.000632	0.649826	-2.462364
C	-0.126497	2.072207	-2.417277	C	-0.000557	2.029369	-2.41756
C	-0.126497	2.072207	2.417277	C	-0.000557	2.029369	2.41756
H	-0.177235	0.200006	-3.428664	H	-0.000577	0.157113	-3.429434

H	-0.108448	2.64189	-3.34198	H	-0.000447	2.599547	-3.342143
H	-0.108448	2.64189	3.34198	H	-0.000447	2.599547	3.342143
C	-0.16534	0.692696	2.461639	C	-0.000632	0.649826	2.462364
H	-0.177235	0.200006	3.428664	H	-0.000577	0.157113	3.429434
C	0.210398	13.236083	-1.26512	C	0.00055	13.198027	-1.265103
C	0.168014	11.874176	-1.588939	C	0.000381	11.835531	-1.588962
C	0.210398	13.236083	1.26512	C	0.00055	13.198027	1.265103
C	0.134054	10.77104	-0.745675	C	0.000253	10.731778	-0.745709
C	0.168014	11.874176	1.588939	C	0.000381	11.835531	1.588962
C	0.134054	10.77104	0.745675	C	0.000253	10.731778	0.745709
H	0.2629	14.917048	0	H	0.00077	14.879855	0
H	0.231557	13.920048	-2.108981	H	0.000633	13.882329	-2.108967
H	0.160929	11.650144	-2.654216	H	0.000349	11.611421	-2.654248
H	0.231557	13.920048	2.108981	H	0.000633	13.882329	2.108967
H	0.160929	11.650144	2.654216	H	0.000349	11.611421	2.654248
C	0.092001	9.408196	-1.164515	C	0.000094	9.368422	-1.16449
C	0.067037	8.593239	0	C	-0.000002	8.553043	0
C	0.092001	9.408196	1.164515	C	0.000094	9.368422	1.16449
C	0.029932	7.404201	-2.467073	C	-0.000149	7.363539	-2.467198
C	0.072226	8.776604	-2.426464	C	0.000012	8.736419	-2.426546
C	0.029932	7.404201	2.467073	C	-0.000149	7.363539	2.467198
C	0.072226	8.776604	2.426464	C	0.000012	8.736419	2.426546
H	0.014384	6.910084	-3.433772	H	-0.000212	6.86915	-3.433882
H	0.08949	9.346461	-3.350613	H	0.000073	9.30658	-3.350674
H	0.014384	6.910084	3.433772	H	-0.000212	6.86915	3.433882
H	0.08949	9.346461	3.350613	H	0.000073	9.30658	3.350674
Zn	-0.263917	-6.768319	0	C	-0.003477	-4.9202	0
C	-0.480017	-4.844432	0	C	0.000629	13.791783	0
C	0.229063	13.829499	0	Ni	-0.004448	-6.766805	0

Pc_N-3A-N

C	0.000022	-6.413568	4.171597	C	0.000456	-6.301862	4.196778
C	0.000061	-5.009486	4.168689	C	-0.00042	-4.889401	4.194711
C	0.00015	-6.813745	2.760726	C	-0.000315	-6.723612	2.797098
C	0.000121	-9.888105	-0.708301	C	0.002189	-9.790765	-0.707308
C	0.000121	-9.888105	0.708301	C	0.002189	-9.790765	0.707308
C	0.000097	-8.508166	1.144173	C	-0.000129	-8.393501	1.122992
C	0.000061	-5.009486	-4.168689	C	-0.00042	-4.889401	-4.194711
C	0.000022	-6.413568	-4.171597	C	0.000456	-6.301862	-4.196778
C	0.000213	-4.618277	-2.754658	C	-0.001751	-4.473981	-2.792335
C	0.00015	-6.813745	-2.760726	C	-0.000315	-6.723612	-2.797098

Mg-Pc_N-3A-N

C	0.000165	-1.513683	-0.724754	C	-0.002888	-1.381541	-0.725376
C	0.000165	-1.513683	0.724754	C	-0.002888	-1.381541	0.725376
C	0.000189	-2.914427	-1.146485	C	-0.003504	-2.794228	-1.124772
C	0.000189	-2.914427	1.146485	C	-0.003504	-2.794228	1.124772
C	0.000213	-4.618277	2.754658	C	-0.001751	-4.473981	2.792335
C	0.000097	-8.508166	-1.144173	C	-0.000129	-8.393501	-1.122992
N	0.000046	-7.742844	0	N	-0.001933	-7.604721	0
N	0.000151	-5.706621	1.944267	N	-0.001546	-5.593395	2.006086
N	0.000151	-5.706621	-1.944267	N	-0.001546	-5.593395	-2.006086
H	0.000066	-6.729733	0	N	0.00024	-7.989918	2.398491
N	0.000115	-8.09224	2.401064	N	-0.002715	-3.198742	2.394074
N	0.000208	-3.325355	2.393874	N	-0.002715	-3.198742	-2.394074
N	0.000208	-3.325355	-2.393874	N	0.00024	-7.989918	-2.398491
N	0.000115	-8.09224	-2.401064	C	-0.002316	-0.331773	-1.592673
C	0.000137	-0.462733	-1.592885	C	-0.001811	1.078944	-1.316701
C	0.000102	0.94626	-1.317276	C	-0.001617	1.698669	0
C	0.000092	1.56638	0	C	-0.001811	1.078944	1.316701
C	0.000102	0.94626	1.317276	C	-0.002316	-0.331773	1.592673
C	0.000137	-0.462733	1.592885	H	-0.002283	-0.606869	2.644926
H	0.000128	-0.739265	2.644559	H	-0.002283	-0.606869	-2.644926
H	0.000128	-0.739265	-2.644559	C	0.000468	8.429561	0
C	-0.000218	8.295447	0	C	0.00029	7.794735	-1.317842
C	-0.000205	7.660425	-1.317992	C	-0.000107	6.405063	-1.583749
C	-0.000133	6.271605	-1.584056	C	0.00029	7.794735	1.317842
C	-0.000205	7.660425	1.317992	C	-0.00042	5.321754	-0.724482
C	-0.000063	5.187635	-0.7244	C	-0.000107	6.405063	1.583749
C	-0.000133	6.271605	1.584056	C	-0.00042	5.321754	0.724482
C	-0.000063	5.187635	0.7244	H	-0.000183	6.155389	-2.643107
H	-0.000136	6.021795	-2.643336	H	-0.000183	6.155389	2.643107
H	-0.000136	6.021795	2.643336	C	-0.000849	3.928519	-1.160628
C	0.000015	3.795457	-1.160915	C	-0.001126	3.105028	0
C	0.00006	2.971406	0	C	-0.000849	3.928519	1.160628
C	0.000015	3.795457	1.160915	C	-0.001489	1.917301	-2.452762
C	0.000074	1.784567	-2.453662	C	-0.001028	3.314694	-2.403173
C	0.000025	3.181714	-2.40369	C	-0.001028	3.314694	2.403173
C	0.000025	3.181714	2.40369	H	-0.001626	1.434509	-3.425432
H	0.000081	1.301852	-3.426318	H	-0.000817	3.884477	-3.327747
H	0.000001	3.751565	-3.328153	H	-0.000817	3.884477	3.327747
H	0.000001	3.751565	3.328153	C	-0.001489	1.917301	2.452762
C	0.000074	1.784567	2.453662	H	-0.001626	1.434509	3.425432
H	0.000081	1.301852	3.426318	C	0.002133	14.478338	-1.258363
C	0.000563	14.34324	-1.258093	C	0.001724	13.170527	-1.589411

C	-0.000549	13.035131	-1.589297	C	0.002133	14.478338	1.258363
C	0.000563	14.34324	1.258093	C	0.001438	12.012972	-0.708707
C	-0.0004	11.877856	-0.709431	C	0.001724	13.170527	1.589411
C	-0.000549	13.035131	1.589297	C	0.001438	12.012972	0.708707
C	-0.0004	11.877856	0.709431	H	0.00231	15.215234	-2.055642
H	0.000416	15.080117	-2.055329	H	0.001607	12.965412	-2.655314
H	-0.001593	12.830408	-2.655262	H	0.00231	15.215234	2.055642
H	0.000416	15.080117	2.055329	H	0.001607	12.965412	2.655314
H	-0.001593	12.830408	2.655262	C	0.00108	10.658044	-1.156452
C	-0.000324	10.523719	-1.15666	C	0.000853	9.815249	0
C	-0.000265	9.680814	0	C	0.00108	10.658044	1.156452
C	-0.000324	10.523719	1.15666	C	0.000528	8.64619	-2.461569
C	-0.000271	8.512255	-2.462165	C	0.000909	10.033141	-2.408848
C	-0.000333	9.89864	-2.4095	C	0.000528	8.64619	2.461569
C	-0.000271	8.512255	2.462165	C	0.000909	10.033141	2.408848
C	-0.000333	9.89864	2.4095	H	0.000394	8.163723	-3.434872
H	-0.000263	8.029606	-3.435349	H	0.001066	10.604124	-3.333391
H	-0.000362	10.469732	-3.333937	H	0.000394	8.163723	3.434872
H	-0.000263	8.029606	3.435349	H	0.001066	10.604124	3.333391
H	-0.000362	10.469732	3.333937	C	0.00182	-7.01756	5.39434
C	-0.000135	-7.13256	5.364254	C	0.00006	-4.168099	5.388788
C	-0.000055	-4.283548	5.357074	C	0.002265	-6.293693	6.585834
C	-0.000497	-6.407224	6.558089	C	0.001393	-4.8863	6.583658
C	-0.000457	-5.001999	6.555041	C	0.004395	-10.988688	1.425405
C	0.000109	-11.089076	1.426797	C	0.004395	-10.988688	-1.425405
C	0.000109	-11.089076	-1.426797	C	0.006446	-12.180306	0.704499
C	-0.000047	-12.276894	0.70612	C	0.006446	-12.180306	-0.704499
C	-0.000047	-12.276894	-0.70612	C	0.00182	-7.01756	-5.39434
C	-0.000135	-7.13256	-5.364254	C	0.00006	-4.168099	-5.388788
C	-0.000055	-4.283548	-5.357074	C	0.002265	-6.293693	-6.585834
C	-0.000497	-6.407224	-6.558089	C	0.001393	-4.8863	-6.583658
C	-0.000457	-5.001999	-6.555041	H	0.00331	-6.822239	7.534622
H	-0.000742	-6.935793	7.506943	H	0.001774	-4.354207	7.530394
H	-0.000672	-4.46879	7.501245	H	-0.000612	-3.083125	5.378139
H	-0.000016	-3.198514	5.345819	H	0.002504	-8.102521	5.38793
H	-0.000165	-8.217595	5.358246	H	0.004456	-10.980518	2.510423
H	0.000114	-11.079532	2.511535	H	0.004456	-10.980518	-2.510423
H	0.000114	-11.079532	-2.511535	H	0.008112	-13.128442	1.234257
H	-0.00013	-13.225481	1.23473	H	0.008112	-13.128442	-1.234257
H	-0.00013	-13.225481	-1.23473	H	0.002504	-8.102521	-5.38793
H	-0.000165	-8.217595	-5.358246	H	-0.000612	-3.083125	-5.378139
H	-0.000016	-3.198514	-5.345819	H	0.00331	-6.822239	-7.534622

H	-0.000742	-6.935793	-7.506943	H	0.001774	-4.354207	-7.530394
H	-0.000672	-4.46879	-7.501245	N	-0.004434	-3.574253	0
N	0.000158	-3.672855	0	N	0.002434	15.075091	0
H	0.000199	-4.688542	0	H	0.0025	16.081188	0
N	0.002166	14.939543	0	Mg	-0.005945	-5.593761	0
H	0.002286	15.945719	0				

	Zn-Pc$_N$-3A-N				**Ni-Pc$_N$-3A-N**		
C	-0.001856	-6.085371	4.180607	C	-0.00043	-6.077791	4.126442
C	-0.00069	-4.675518	4.178947	C	-0.000095	-4.677726	4.123381
C	0.000286	-6.505095	2.782042	C	-0.000639	-6.488533	2.733814
C	-0.004476	-9.567045	-0.706286	C	-0.000144	-9.498892	-0.700868
C	-0.004476	-9.567045	0.706286	C	-0.000144	-9.498892	0.700868
C	-0.000433	-8.170704	1.120147	C	-0.000291	-8.108578	1.106675
C	-0.00069	-4.675518	-4.178947	C	-0.000095	-4.677726	-4.123381
C	-0.001856	-6.085371	-4.180607	C	-0.00043	-6.077791	-4.126442
C	0.002121	-4.261353	-2.77791	C	-0.000133	-4.274111	-2.727538
C	0.000286	-6.505095	-2.782042	C	-0.000639	-6.488533	-2.733814
C	0.003188	-1.178018	-0.723886	C	0.000825	-1.236634	-0.717904
C	0.003188	-1.178018	0.723886	C	0.000825	-1.236634	0.717904
C	0.004065	-2.590472	-1.120433	C	0.000467	-2.644131	-1.106352
C	0.004065	-2.590472	1.120433	C	0.000467	-2.644131	1.106352
C	0.002121	-4.261353	2.77791	C	-0.000133	-4.274111	2.727538
C	-0.000433	-8.170704	-1.120147	C	-0.000291	-8.108578	-1.106675
N	0.002053	-7.377696	0	N	-0.000163	-7.28178	0
N	0.00231	-5.377175	1.985301	N	-0.000583	-5.376704	1.905041
N	0.00231	-5.377175	-1.985301	N	-0.000583	-5.376704	-1.905041
N	-0.000867	-7.771089	2.392976	N	-0.000525	-7.752884	2.37925
N	0.003089	-2.987491	2.388546	N	0.000343	-3.002718	2.373394
N	0.003089	-2.987491	-2.388546	N	0.000343	-3.002718	-2.373394
N	-0.000867	-7.771089	-2.392976	N	-0.000525	-7.752884	-2.37925
C	0.002378	-0.12968	-1.592737	C	0.00097	-0.192384	-1.593154
C	0.001709	1.281054	-1.316827	C	0.000983	1.217337	-1.317353
C	0.001462	1.900733	0	C	0.000942	1.837306	0
C	0.001709	1.281054	1.316827	C	0.000983	1.217337	1.317353
C	0.002378	-0.12968	1.592737	C	0.00097	-0.192384	1.593154
H	0.002328	-0.405287	2.644789	H	0.00095	-0.470213	2.644141
H	0.002328	-0.405287	-2.644789	H	0.00095	-0.470213	-2.644141
C	-0.000978	8.631602	0	C	0.000028	8.567593	0
C	-0.000795	7.996762	-1.317846	C	0.000159	7.932542	-1.317896
C	-0.000363	6.607128	-1.583754	C	0.000419	6.543484	-1.583805
C	-0.000795	7.996762	1.317846	C	0.000159	7.932542	1.317896

C	0.00001	5.523788	-0.724465	C	0.000573	5.459524	-0.724431
C	-0.000363	6.607128	1.583754	C	0.000419	6.543484	1.583805
C	0.00001	5.523788	0.724465	C	0.000573	5.459524	0.724431
H	-0.000292	6.357447	-2.643109	H	0.00048	6.293748	-2.643146
H	-0.000292	6.357447	2.643109	H	0.00048	6.293748	2.643146
C	0.000527	4.130574	-1.160636	C	0.000759	4.067015	-1.160726
C	0.000865	3.307047	0	C	0.000837	3.243162	0
C	0.000527	4.130574	1.160636	C	0.000759	4.067015	1.160726
C	0.001299	2.11938	-2.452831	C	0.000968	2.056074	-2.453569
C	0.00073	3.516797	-2.403176	C	0.000847	3.453159	-2.403446
C	0.00073	3.516797	2.403176	C	0.000847	3.453159	2.403446
H	0.001466	1.636625	-3.42552	H	0.001007	1.573385	-3.426269
H	0.000466	4.086619	-3.327724	H	0.000803	4.023192	-3.32788
H	0.000466	4.086619	3.327724	H	0.000803	4.023192	3.32788
C	0.001299	2.11938	2.452831	C	0.000968	2.056074	2.453569
H	0.001466	1.636625	3.42552	H	0.001007	1.573385	3.426269
C	-0.002369	14.680341	-1.258357	C	-0.000676	14.61585	-1.25831
C	-0.002292	13.372524	-1.589408	C	-0.001157	13.307904	-1.589392
C	-0.002369	14.680341	1.258357	C	-0.000676	14.61585	1.25831
C	-0.001967	12.214975	-0.708734	C	-0.000794	12.150391	-0.709156
C	-0.002292	13.372524	1.589408	C	-0.001157	13.307904	1.589392
C	-0.001967	12.214975	0.708734	C	-0.000794	12.150391	0.709156
H	-0.002583	15.417234	-2.055637	H	-0.000953	15.352782	-2.055545
H	-0.002464	13.167432	-2.655317	H	-0.001833	13.102958	-2.655341
H	-0.002583	15.417234	2.055637	H	-0.000953	15.352782	2.055545
H	-0.002464	13.167432	2.655317	H	-0.001833	13.102958	2.655341
C	-0.001606	10.860081	-1.15645	C	-0.000474	10.796057	-1.156585
C	-0.001372	10.017277	0	C	-0.00027	9.953152	0
C	-0.001606	10.860081	1.15645	C	-0.000474	10.796057	1.156585
C	-0.001051	8.848238	-2.461594	C	-0.000026	8.784353	-2.46201
C	-0.001442	10.235163	-2.408871	C	-0.000339	10.170845	-2.409299
C	-0.001051	8.848238	2.461594	C	-0.000026	8.784353	2.46201
C	-0.001442	10.235163	2.408871	C	-0.000339	10.170845	2.409299
H	-0.000915	8.36576	-3.434892	H	0.000076	8.301711	-3.435227
H	-0.001602	10.806161	-3.333405	H	-0.00046	10.741914	-3.333798
H	-0.000915	8.36576	3.434892	H	0.000076	8.301711	3.435227
H	-0.001602	10.806161	3.333405	H	-0.00046	10.741914	3.333798
C	-0.004755	-6.802885	5.377225	C	-0.00038	-6.80094	5.320822
C	-0.002398	-3.95307	5.372475	C	0.000282	-3.947915	5.313592
C	-0.006289	-6.079338	6.568644	C	-0.000069	-6.075718	6.509864
C	-0.005122	-4.67163	6.566863	C	0.00027	-4.66624	6.506806
C	-0.008287	-10.764316	1.425563	C	-0.000063	-10.693193	1.427142

C	-0.008287	-10.764316	-1.425563	C	-0.000063	-10.693193	-1.427142
C	-0.011831	-11.955721	0.704601	C	0.000048	-11.882834	0.705513
C	-0.011831	-11.955721	-0.704601	C	0.000048	-11.882834	-0.705513
C	-0.004755	-6.802885	-5.377225	C	-0.00038	-6.80094	-5.320822
C	-0.002398	-3.95307	-5.372475	C	0.000282	-3.947915	-5.313592
C	-0.006289	-6.079338	-6.568644	C	-0.000069	-6.075718	-6.509864
C	-0.005122	-4.67163	-6.566863	C	0.00027	-4.66624	-6.506806
H	-0.008454	-6.608011	7.517346	H	-0.00008	-6.60258	7.459532
H	-0.006403	-4.139936	7.513808	H	0.000535	-4.134717	7.453778
H	-0.001548	-2.868147	5.36166	H	0.000575	-2.863266	5.300335
H	-0.005713	-7.887792	5.369972	H	-0.000632	-7.885613	5.312609
H	-0.008396	-10.755909	2.510544	H	-0.000058	-10.682531	2.51184
H	-0.008396	-10.755909	-2.510544	H	-0.000058	-10.682531	-2.51184
H	-0.014706	-12.903887	1.234271	H	0.000153	-12.831501	1.23419
H	-0.014706	-12.903887	-1.234271	H	0.000153	-12.831501	-1.23419
H	-0.005713	-7.887792	-5.369972	H	-0.000632	-7.885613	-5.312609
H	-0.001548	-2.868147	-5.36166	H	0.000575	-2.863266	-5.300335
H	-0.008454	-6.608011	-7.517346	H	-0.00008	-6.60258	-7.459532
H	-0.006403	-4.139936	-7.513808	H	0.000535	-4.134717	-7.453778
N	0.004799	-3.376885	0	N	0.000377	-3.464577	0
N	-0.002112	15.277084	0	N	0.000434	15.21241	0
H	-0.002576	16.283182	0	H	-0.000223	16.218527	0
Zn	0.016809	-5.389191	0	Ni	-0.000939	-5.376479	0

Pc-3A-N				**Mg-Pc-3A-N**			
C	0.04259	-6.334035	4.228978	C	0.000197	-6.283165	4.217368
C	0.299529	-4.951634	4.242688	C	0.009976	-4.870383	4.225643
C	-0.051974	-6.698417	2.806518	C	0.002081	-6.688705	2.80885
C	-0.630591	-9.689953	-0.703883	C	-0.025081	-9.770975	-0.705945
C	-0.630591	-9.689953	0.703883	C	-0.025081	-9.770975	0.705945
C	-0.395674	-8.320618	1.15121	C	-0.008922	-8.364728	1.129596
C	0.299529	-4.951634	-4.242688	C	0.009976	-4.870383	-4.225643
C	0.04259	-6.334035	-4.228978	C	0.000197	-6.283165	-4.217368
C	0.359262	-4.539688	-2.828361	C	0.018035	-4.431573	-2.822666
C	-0.051974	-6.698417	-2.806518	C	0.002081	-6.688705	-2.80885
C	0.528599	-1.541551	-0.729364	C	0.025172	-1.352835	-0.733712
C	0.528599	-1.541551	0.729364	C	0.025172	-1.352835	0.733712
C	0.616965	-2.935085	-1.154961	C	0.031352	-2.76136	-1.145918
C	0.616965	-2.935085	1.154961	C	0.031352	-2.76136	1.145918
C	0.359262	-4.539688	2.828361	C	0.018035	-4.431573	2.822666
C	-0.395674	-8.320618	-1.15121	C	-0.008922	-8.364728	-1.129596
N	-0.276677	-7.556497	0	N	0.001903	-7.583496	0

N	0.143178	-5.635157	2.014178	N	0.013448	-5.576372	2.032023
N	0.143178	-5.635157	-2.014178	N	0.013448	-5.576372	-2.032023
H	-0.141707	-6.548893	0	N	-0.007733	-7.971203	2.400333
N	-0.308482	-7.963398	2.410084	N	0.025003	-3.159556	2.448652
N	0.548863	-3.287817	2.458349	N	0.025003	-3.159556	-2.448652
N	0.548863	-3.287817	-2.458349	N	-0.007733	-7.971203	-2.400333
N	-0.308482	-7.963398	-2.410084	C	0.019339	-0.280492	-1.585339
C	0.440289	-0.476346	-1.585273	C	0.01465	1.118656	-1.306985
C	0.359141	0.919565	-1.307405	C	0.012844	1.740485	0
C	0.322842	1.539431	0	C	0.01465	1.118656	1.306985
C	0.359141	0.919565	1.307405	C	0.019339	-0.280492	1.585339
C	0.440289	-0.476346	1.585273	H	0.018978	-0.550108	2.639674
H	0.438785	-0.750832	2.637977	H	0.018978	-0.550108	-2.639674
H	0.438785	-0.750832	-2.637977	C	-0.004901	8.453815	0
C	-0.084106	8.239724	0	C	-0.003449	7.831899	-1.304984
C	-0.045446	7.6193	-1.305159	C	-0.000101	6.438169	-1.579649
C	0.04002	6.228119	-1.57976	C	-0.003449	7.831899	1.304984
C	-0.045446	7.6193	1.305159	C	0.002612	5.348214	-0.739717
C	0.105684	5.140175	-0.739972	C	-0.000101	6.438169	1.579649
C	0.04002	6.228119	1.57976	C	0.002612	5.348214	0.739717
C	0.105684	5.140175	0.739972	H	0.000517	6.197783	-2.641188
H	0.054947	5.988265	-2.641337	H	0.000517	6.197783	2.641188
H	0.054947	5.988265	2.641337	C	0.00628	3.972713	-1.162726
C	0.188399	3.767556	-1.163156	C	0.008605	3.157285	0
C	0.237522	2.953866	0	C	0.00628	3.972713	1.162726
C	0.188399	3.767556	1.163156	C	0.011802	1.966083	-2.461052
C	0.307147	1.765015	-2.462268	C	0.007832	3.346075	-2.417612
C	0.224956	3.142091	-2.418655	C	0.007832	3.346075	2.417612
C	0.224956	3.142091	2.418655	H	0.013093	1.473346	-3.428295
H	0.335325	1.272669	-3.429295	H	0.006023	3.916009	-3.342325
H	0.189752	3.711285	-3.343095	H	0.006023	3.916009	3.342325
H	0.189752	3.711285	3.343095	C	0.011802	1.966083	2.461052
C	0.307147	1.765015	2.462268	H	0.013093	1.473346	3.428295
H	0.335325	1.272669	3.429295	C	-0.018177	14.516413	-1.26525
C	-0.460609	14.290707	-1.265363	C	-0.01524	13.153266	-1.58898
C	-0.37527	12.930091	-1.589023	C	-0.018177	14.516413	1.26525
C	-0.460609	14.290707	1.265363	C	-0.012883	12.049853	-0.746294
C	-0.30686	11.828905	-0.746445	C	-0.01524	13.153266	1.58898
C	-0.37527	12.930091	1.589023	C	-0.012883	12.049853	0.746294
C	-0.30686	11.828905	0.746445	H	-0.019632	15.200706	-2.109127
H	-0.503224	14.973703	-2.109205	H	-0.014733	12.929154	-2.654345
H	-0.361042	12.706379	-2.654392	H	-0.019632	15.200706	2.109127

H	-0.503224	14.973703	2.109205	H	-0.014733	12.929154	2.654345
H	-0.361042	12.706379	2.654392	C	-0.009898	10.686323	-1.164761
C	-0.222175	10.468088	-1.164881	C	-0.008107	9.870918	0
C	-0.171826	9.654221	0	C	-0.009898	10.686323	1.164761
C	-0.222175	10.468088	1.164881	C	-0.005378	8.680947	-2.466718
C	-0.097238	8.466746	-2.466929	C	-0.00848	10.054137	-2.426729
C	-0.182463	9.837247	-2.427023	C	-0.005378	8.680947	2.466718
C	-0.097238	8.466746	2.466929	C	-0.00848	10.054137	2.426729
C	-0.182463	9.837247	2.427023	H	-0.004227	8.186366	-3.433411
H	-0.065975	7.973023	-3.433586	H	-0.009752	10.624201	-3.350922
H	-0.217348	10.406371	-3.351139	H	-0.004227	8.186366	3.433411
H	-0.065975	7.973023	3.433586	H	-0.009752	10.624201	3.350922
H	-0.217348	10.406371	3.351139	C	-0.009465	-7.011827	5.406071
C	-0.079595	-7.059437	5.410398	C	0.01028	-4.16559	5.428196
C	0.445112	-4.26168	5.442184	C	-0.008851	-6.302437	6.607223
C	0.066232	-6.367379	6.616155	C	0.000899	-4.896333	6.617043
C	0.324615	-4.987409	6.631167	C	-0.039235	-10.964854	1.423739
C	-0.825156	-10.868634	1.424437	C	-0.039235	-10.964854	-1.423739
C	-0.825156	-10.868634	-1.424437	C	-0.052922	-12.160331	0.702685
C	-1.022915	-12.044791	0.703929	C	-0.052922	-12.160331	-0.702685
C	-1.022915	-12.044791	-0.703929	C	-0.009465	-7.011827	-5.406071
C	-0.079595	-7.059437	-5.410398	C	0.01028	-4.16559	-5.428196
C	0.445112	-4.26168	-5.442184	C	-0.008851	-6.302437	-6.607223
C	0.066232	-6.367379	-6.616155	C	0.000899	-4.896333	-6.617043
C	0.324615	-4.987409	-6.631167	H	-0.016035	-6.84103	7.550481
H	-0.020812	-6.902723	7.557371	H	0.001044	-4.372557	7.568872
H	0.432217	-4.477556	7.58449	H	0.017682	-3.080426	5.428414
H	0.644803	-3.194883	5.446787	H	-0.017065	-8.096826	5.386342
H	-0.279999	-8.125828	5.388608	H	-0.039362	-10.954747	2.508776
H	-0.820613	-10.855592	2.509081	H	-0.039362	-10.954747	-2.508776
H	-0.820613	-10.855592	-2.509081	H	-0.063881	-13.107621	1.234011
H	-1.179333	-12.979403	1.234458	H	-0.063881	-13.107621	-1.234011
H	-1.179333	-12.979403	-1.234458	H	-0.017065	-8.096826	-5.386342
H	-0.279999	-8.125828	-5.388608	H	0.017682	-3.080426	-5.428414
H	0.644803	-3.194883	-5.446787	H	-0.016035	-6.84103	-7.550481
H	-0.020812	-6.902723	-7.557371	H	0.001044	-4.372557	-7.568872
H	0.432217	-4.477556	-7.58449	H	-0.0218	16.197894	0
H	0.889846	-4.785295	0	C	0.040517	-3.573583	0
H	-0.566173	15.968723	0	C	-0.019467	15.109724	0
C	0.736834	-3.727059	0	Mg	0.028925	-5.591658	0
C	-0.498081	14.882647	0				

Zn-Pc-3A-N				Ni-Pc-3A-N			
C	-6.037076	4.234289	0.021473	C	-0.000558	-6.046302	4.122421
C	-4.632309	4.244355	-0.113919	C	-0.000623	-4.647605	4.148112
C	-6.432723	2.822803	0.052875	C	-0.000125	-6.430824	2.718171
C	-9.45012	-0.7031	0.382967	C	0.000764	-9.479907	-0.700258
C	-9.450089	0.703069	0.382907	C	0.000764	-9.479907	0.700258
C	-8.060628	1.126435	0.185217	C	0.000276	-8.077327	1.105451
C	-4.632285	-4.244328	-0.11404	C	-0.000623	-4.647605	-4.148112
C	-6.037051	-4.234309	0.021409	C	-0.000558	-6.046302	-4.122421
C	-4.205085	-2.838952	-0.171383	C	-0.000217	-4.210535	-2.75926
C	-6.432717	-2.822855	0.052982	C	-0.000125	-6.430824	-2.718171
C	-1.187379	-0.729684	-0.321564	C	0.00015	-1.215782	-0.723735
C	-1.18738	0.729723	-0.321601	C	0.00015	-1.215782	0.723735
C	-2.590977	-1.143848	-0.381814	C	0.000129	-2.614274	-1.128149
C	-2.590994	1.143889	-0.381814	C	0.000129	-2.614274	1.128149
C	-4.205079	2.838998	-0.171395	C	-0.000217	-4.210535	2.75926
C	-8.060664	-1.126534	0.185311	C	0.000276	-8.077327	-1.105451
N	-7.273479	-0.000062	0.053456	N	-0.000127	-7.259252	0
N	-5.33269	2.045246	-0.050439	N	0.00005	-5.320247	1.909699
N	-5.332741	-2.045241	-0.050316	N	0.00005	-5.320247	-1.909699
N	-7.700853	2.402637	0.173353	N	0.000071	-7.710893	2.369113
N	-2.948832	2.450385	-0.300087	N	-0.000123	-2.943263	2.428126
N	-2.948858	-2.45033	-0.300095	N	-0.000123	-2.943263	-2.428126
N	-7.70089	-2.402724	0.173543	N	0.000071	-7.710893	-2.369113
C	-0.119395	-1.584701	-0.261059	C	0.000086	-0.150532	-1.585705
C	1.278561	-1.307153	-0.212713	C	0.000124	1.246967	-1.307599
C	1.899778	0.000012	-0.191847	C	0.000148	1.868822	0
C	1.278568	1.307178	-0.212879	C	0.000124	1.246967	1.307599
C	-0.119387	1.584734	-0.261213	C	0.000086	-0.150532	1.585705
H	-0.392483	2.637951	-0.254114	H	0.000019	-0.425328	2.63807
H	-0.392493	-2.637918	-0.253899	H	0.000019	-0.425328	-2.63807
C	8.608197	0.000002	0.054821	C	0.000147	8.581488	0
C	7.986828	-1.305059	0.031401	C	0.000162	7.95955	-1.305027
C	6.594042	-1.579689	-0.020439	C	0.000187	6.566138	-1.579718
C	7.986842	1.305065	0.031166	C	0.000162	7.95955	1.305027
C	5.504798	-0.739817	-0.060278	C	0.000191	5.475769	-0.73982
C	6.594056	1.579699	-0.020707	C	0.000187	6.566138	1.579718
C	5.504804	0.739831	-0.060393	C	0.000191	5.475769	0.73982
H	6.353846	-2.641244	-0.029403	H	0.000198	6.325793	-2.641274
H	6.353871	2.641254	-0.029845	H	0.000198	6.325793	2.641274
C	4.13038	-1.162929	-0.110161	C	0.000187	4.10094	-1.162872
C	3.315631	0.000011	-0.140095	C	0.000183	3.285322	0

C	4.130389	1.162948	-0.110336	C	0.000187	4.10094	1.162872
C	2.12515	-2.461581	-0.180373	C	0.000127	2.094888	-2.462326
C	3.504091	-2.418055	-0.131268	C	0.00016	3.474246	-2.418326
C	3.504108	2.418075	-0.131618	C	0.00016	3.474246	2.418326
H	1.632401	-3.428679	-0.19646	H	0.000109	1.602029	-3.429481
H	4.073776	-3.342648	-0.109493	H	0.000168	4.044564	-3.342789
H	4.073799	3.342668	-0.109988	H	0.000168	4.044564	3.342789
C	2.125167	2.461604	-0.18071	C	0.000127	2.094888	2.462326
H	1.632423	3.428703	-0.196924	H	0.000109	1.602029	3.429481
C	14.666507	-1.265305	0.283834	C	-0.000015	14.644	-1.265268
C	13.30429	-1.589003	0.231986	C	0.000027	13.28089	-1.589013
C	14.666522	1.265289	0.283588	C	-0.000015	14.644	1.265268
C	12.201698	-0.74636	0.19035	C	0.000062	12.177409	-0.746354
C	13.304303	1.58899	0.23168	C	0.000027	13.28089	1.589013
C	12.201707	0.746351	0.190208	C	0.000062	12.177409	0.746354
H	15.35032	-2.109168	0.309803	H	-0.000037	15.328319	-2.109128
H	13.080316	-2.654369	0.223418	H	0.000034	13.056794	-2.654385
H	15.350341	2.109152	0.309391	H	-0.000037	15.328319	2.109128
H	13.080341	2.654356	0.22291	H	0.000034	13.056794	2.654385
C	10.839175	-1.164817	0.138893	C	0.000101	10.814033	-1.164782
C	10.024335	0	0.108189	C	0.00012	9.998585	0
C	10.839184	1.164813	0.138674	C	0.000101	10.814033	1.164782
C	8.835287	-2.466809	0.062914	C	0.00015	8.808789	-2.466937
C	10.207481	-2.426852	0.114772	C	0.000119	10.181802	-2.42691
C	8.83531	2.466812	0.06246	C	0.00015	8.808789	2.466937
C	10.207506	2.426849	0.11432	C	0.000119	10.181802	2.42691
H	8.341019	-3.433489	0.043917	H	0.000167	8.314153	-3.433607
H	10.777201	-3.351014	0.136016	H	0.000109	10.751953	-3.351051
H	8.341053	3.433493	0.043285	H	0.000167	8.314153	3.433607
H	10.777235	3.35101	0.135387	H	0.000109	10.751953	3.351051
C	-6.763336	5.421062	0.102402	C	-0.000874	-6.797033	5.298907
C	-3.929957	5.446172	-0.173881	C	-0.001016	-3.947622	5.355253
C	-6.056947	6.623194	0.043921	C	-0.001248	-6.101126	6.506179
C	-4.657833	6.63463	-0.092569	C	-0.001321	-4.692889	6.533094
C	-10.62931	1.423927	0.560757	C	0.001147	-10.670021	1.425383
C	-10.629354	-1.423913	0.56089	C	0.001147	-10.670021	-1.425383
C	-11.811833	0.703087	0.733441	C	0.001556	-11.864255	0.703375
C	-11.811857	-0.703022	0.73351	C	0.001556	-11.864255	-0.703375
C	-6.763285	-5.421113	0.102211	C	-0.000874	-6.797033	-5.298907
C	-3.929899	-5.446118	-0.174179	C	-0.001016	-3.947622	-5.355253
C	-6.056861	-6.623209	0.043567	C	-0.001248	-6.101126	-6.506179
C	-4.657746	-6.634597	-0.092977	C	-0.001321	-4.692889	-6.533094

H	-6.593264	7.56588	0.103654	H	-0.001488	-6.649834	7.443551
H	-4.136725	7.586944	-0.135108	H	-0.001621	-4.181633	7.491613
H	-2.849943	5.448337	-0.280093	H	-0.001057	-2.862785	5.366228
H	-7.843369	5.400973	0.206391	H	-0.000802	-7.881275	5.263155
H	-10.616798	2.508817	0.562726	H	0.001141	-10.658635	2.510221
H	-10.616868	-2.508803	0.562963	H	0.001141	-10.658635	-2.510221
H	-12.74921	1.234134	0.871676	H	0.001877	-12.812091	1.233773
H	-12.74925	-1.234025	0.871803	H	0.001877	-12.812091	-1.233773
H	-7.843315	-5.401067	0.206233	H	-0.000802	-7.881275	-5.263155
H	-2.84989	-5.448231	-0.280443	H	-0.001057	-2.862785	-5.366228
H	-6.593149	-7.565918	0.103208	H	-0.001488	-6.649834	-7.443551
H	-4.136619	-7.586895	-0.135643	H	-0.001621	-4.181633	-7.491613
H	16.34671	-0.00001	0.347906	H	-0.000062	16.325471	0
C	-3.410445	0.000013	-0.495275	C	0.000278	-3.473943	0
C	15.259313	-0.000007	0.306517	C	-0.000032	15.237295	0
Zn	-5.335897	-0.000023	-0.327995	Ni	0.000064	-5.332543	0

	P_N-N-A				**P_N-N-2A**		
C	0	4.148312	-1.775592	C	0	4.146561	-4.804659
C	0	4.148217	-0.423355	C	0	4.144021	-3.452973
C	0	2.737921	-2.183147	C	0	2.7384	-5.217157
C	0	-0.68253	-5.25293	C	0	-0.686997	-8.27581
C	0	0.68253	-5.25293	C	0	0.686997	-8.27581
C	0	1.131634	-3.875936	C	0	1.128881	-6.909135
C	0	-4.148217	-0.423355	C	0	-4.144021	-3.452973
C	0	-4.148312	-1.775592	C	0	-4.146561	-4.804659
C	0	-2.738172	-0.015577	C	0	-2.732052	-3.049562
C	0	-2.737921	-2.183147	C	0	-2.7384	-5.217157
C	0	-0.693972	3.051096	C	0	-0.715028	0.062478
C	0	0.693972	3.051096	C	0	0.715028	0.062478
C	0	-1.126832	1.674534	C	0	-1.141201	-1.33748
C	0	1.126832	1.674534	C	0	1.141201	-1.33748
C	0	2.738172	-0.015577	C	0	2.732052	-3.049562
C	0	-1.131634	-3.875936	C	0	-1.128881	-6.909135
N	0	0	-3.096388	N	0	0	-6.128033
N	0	1.911496	-1.103203	N	0	1.906653	-4.119128
N	0	-1.911496	-1.103203	N	0	-1.906653	-4.119128
H	0	0	-2.084628	H	0	0	-5.116255
H	0	0	-0.123756	H	0	0	-3.118063
N	0	2.392227	-3.478695	N	0	2.39708	-6.498706
N	0	2.390171	1.273862	N	0	2.389306	-1.745801
N	0	-2.390171	1.273862	N	0	-2.389306	-1.745801

N	0	-2.392227	-3.478695
C	0	-1.604541	4.188383
C	0	-1.263532	5.490316
C	0	1.263532	5.490316
C	0	1.604541	4.188383
H	0	2.661275	3.949499
H	0	-2.661275	3.949499
H	0	-4.979949	-2.466168
H	0	-4.980077	0.266976
H	0	-1.358593	-6.095553
H	0	1.358593	-6.095553
H	0	4.979949	-2.466168
H	0	4.980077	0.266976
N	0	0	0.886101
H	0	2.057053	6.231333
H	0	0	7.091239
H	0	-2.057053	6.231333
N	0	0	6.08514

N	0	-2.39708	-6.498706
C	0	-1.598233	1.121907
C	0	-1.324827	2.510047
C	0	0	3.140712
C	0	1.324827	2.510047
C	0	1.598233	1.121907
H	0	2.647569	0.837534
H	0	-2.647569	0.837534
H	0	-4.979044	-5.494221
H	0	-4.97395	-2.76034
H	0	-1.360614	-9.120248
H	0	1.360614	-9.120248
H	0	4.979044	-5.494221
H	0	4.97395	-2.76034
N	0	0	-2.102775
C	0	-1.257758	9.18977
C	0	-1.589931	7.882386
C	0	1.257758	9.18977
C	0	-0.70763	6.725231
C	0	1.589931	7.882386
C	0	0.70763	6.725231
H	0	-2.655347	7.676543
H	0	2.655347	7.676543
C	0	-1.156463	5.369226
C	0	0	4.524732
C	0	1.156463	5.369226
C	0	-2.464897	3.361711
C	0	-2.40929	4.750256
C	0	2.40929	4.750256
H	0	-3.438061	2.879961
H	0	-3.332262	5.323325
H	0	3.332262	5.323325
C	0	2.464897	3.361711
H	0	3.438061	2.879961
H	0	2.055088	9.926491
H	0	0	10.792493
H	0	-2.055088	9.926491
N	0	0	9.786107

P_N-A-N

C	0	4.211288	1.744035
C	0	4.225175	0.392123

P_N-2A-N

C	-0.026401	-4.727154	4.206833
C	0.197482	-3.393189	4.220106

C	0	2.789481	2.133288	C	-0.10642	-5.108849	2.786835
C	0	-0.678805	5.174891	C	-0.620987	-8.09515	-0.680342
C	0	0.678805	5.174891	C	-0.620987	-8.09515	0.680342
C	0	1.137757	3.791213	C	-0.420263	-6.731138	1.135534
C	0	-4.225175	0.392123	C	0.197482	-3.393189	-4.220106
C	0	-4.211288	1.744035	C	-0.026401	-4.727154	-4.206833
C	0	-2.815129	-0.038893	C	0.266566	-2.972825	-2.810397
C	0	-2.789481	2.133288	C	-0.10642	-5.108849	-2.786835
C	0	-0.730444	-3.068457	C	0.400628	0.035195	-0.726824
C	0	0.730444	-3.068457	C	0.400628	0.035195	0.726824
C	0	-1.157456	-1.68081	C	0.519236	-1.356919	-1.155433
C	0	1.157456	-1.68081	C	0.519236	-1.356919	1.155433
C	0	2.815129	-0.038893	C	0.266566	-2.972825	2.810397
C	0	-1.137757	3.791213	C	-0.420263	-6.731138	-1.135534
N	0	0	3.00835	N	-0.315758	-5.950716	0
N	0	1.98483	1.06415	N	0.077461	-4.049465	1.979813
N	0	-1.98483	1.06415	N	0.077461	-4.049465	-1.979813
H	0	0	1.996738	H	-0.204649	-4.941446	0
H	0	0	0.17159	H	0.850407	-3.198114	0
N	0	2.402838	3.43129	N	-0.341311	-6.379739	2.404569
N	0	2.463623	-1.313602	N	0.44181	-1.706532	2.456058
N	0	-2.463623	-1.313602	N	0.44181	-1.706532	-2.456058
N	0	-2.402838	3.43129	N	-0.341311	-6.379739	-2.404569
C	0	-1.593144	-4.156014	C	0.285564	1.099566	-1.585578
C	0	-1.264609	-5.516095	C	0.175464	2.488749	-1.306783
C	0	0	-6.113127	C	0.126269	3.107868	0
C	0	1.264609	-5.516095	C	0.175464	2.488749	1.306783
C	0	1.593144	-4.156014	C	0.285564	1.099566	1.585578
H	0	2.649153	-3.895361	H	0.287267	0.821853	2.637438
H	0	-2.649153	-3.895361	H	0.287267	0.821853	-2.637438
H	0	-5.038571	2.440245	H	-0.146272	-5.413118	-5.03417
H	0	-5.068816	-0.28438	H	0.315896	-2.725558	-5.062629
H	0	-1.357529	6.015509	H	-0.733341	-8.928181	-1.359102
H	0	1.357529	6.015509	H	-0.733341	-8.928181	1.359102
H	0	5.038571	2.440245	H	-0.146272	-5.413118	5.03417
H	0	5.068816	-0.28438	H	0.315896	-2.725558	5.062629
C	0	0	-0.890356	C	-0.420001	9.743328	0
H	0	2.107321	-6.203097	C	-0.370579	9.150176	-1.264343
H	0	0	-7.200801	C	-0.258299	7.792989	-1.58847
H	0	-2.107321	-6.203097	C	-0.370579	9.150176	1.264343
C	0	4.211288	1.744035	C	-0.167855	6.692894	-0.744361
C	0	4.225175	0.392123	C	-0.258299	7.792989	1.58847

C	0	2.789481	2.133288	C	-0.167855	6.692894	0.744361
C	0	-0.678805	5.174891	H	-0.239746	7.569262	-2.653523
C	0	0.678805	5.174891	H	-0.239746	7.569262	2.653523
C	0	1.137757	3.791213	C	-0.056387	5.332978	-1.16329
C	0	-4.225175	0.392123	C	0.010447	4.520264	0
C	0	-4.211288	1.744035	C	-0.056387	5.332978	1.16329
C	0	-2.815129	-0.038893	C	0.104811	3.335233	-2.46721
C	0	-2.789481	2.133288	C	-0.006327	4.704783	-2.424615
C	0	-0.730444	-3.068457	C	-0.006327	4.704783	2.424615
C	0	0.730444	-3.068457	H	0.143642	2.840897	-3.432628
C	0	-1.157456	-1.68081	H	-0.053903	5.2737	-3.348486
C	0	1.157456	-1.68081	H	-0.053903	5.2737	3.348486
C	0	2.815129	-0.038893	C	0.104811	3.335233	2.46721
C	0	-1.137757	3.791213	H	0.143642	2.840897	3.432628
N	0	0	3.00835	C	0.665712	-2.145142	0
N	0	1.98483	1.06415	H	-0.426823	9.831805	2.108624
N	0	-1.98483	1.06415	H	-0.509698	10.827568	0
H	0	0	1.996738	H	-0.426823	9.831805	-2.108624
H	0	0	0.17159				
N	0	2.402838	3.43129				
N	0	2.463623	-1.313602				
N	0	-2.463623	-1.313602				
N	0	-2.402838	3.43129				
C	0	-1.593144	-4.156014				
C	0	-1.264609	-5.516095				
C	0	0	-6.113127				
C	0	1.264609	-5.516095				
C	0	1.593144	-4.156014				
H	0	2.649153	-3.895361				
H	0	-2.649153	-3.895361				
H	0	-5.038571	2.440245				
H	0	-5.068816	-0.28438				
H	0	-1.357529	6.015509				
H	0	1.357529	6.015509				
H	0	5.038571	2.440245				
H	0	5.068816	-0.28438				
C	0	0	-0.890356				
H	0	2.107321	-6.203097				

Pc_N-A-N

C	0.000036	-0.903053	4.172779

Pc_N-2A-N

C	0	4.171057	-3.504867

C	0.00001	0.501056	4.175102	C	0	4.168749	-2.100797
C	0.00007	-1.294415	2.758018	C	0	2.759359	-3.903274
C	0.000089	-4.383687	-0.705	C	0	-0.707407	-6.981392
C	0.000089	-4.383687	0.705	C	0	0.707407	-6.981392
C	0.000089	-2.992743	1.148091	C	0	1.145089	-5.598548
C	0.00001	0.501056	-4.175102	C	0	-4.168749	-2.100797
C	0.000036	-0.903053	-4.172779	C	0	-4.171057	-3.504867
C	0.000029	0.902225	-2.761706	C	0	-2.754604	-1.708114
C	0.00007	-1.294415	-2.758018	C	0	-2.759359	-3.903274
C	-0.000097	3.94592	-0.698053	C	0	-0.714983	1.382818
C	-0.000097	3.94592	0.698053	C	0	0.714983	1.382818
C	-0.000035	2.578879	-1.126696	C	0	-1.140015	-0.011025
C	-0.000035	2.578879	1.126696	C	0	1.140015	-0.011025
C	0.000029	0.902225	2.761706	C	0	2.754604	-1.708114
C	0.000089	-2.992743	-1.148091	C	0	-1.145089	-5.598548
N	0.000107	-2.227109	0	N	0	0	-4.833183
N	-0.000013	-0.214056	1.948605	N	0	1.944307	-2.803531
N	-0.000013	-0.214056	-1.948605	N	0	-1.944307	-2.803531
H	0.000129	-1.213914	0	H	0	0	-3.819965
N	0.000089	-2.593555	2.395883	N	0	2.399488	-5.186883
N	-0.000015	2.173223	2.396056	N	0	2.392391	-0.420805
N	-0.000015	2.173223	-2.396056	N	0	-2.392391	-0.420805
N	0.000089	-2.593555	-2.395883	N	0	-2.399488	-5.186883
C	-0.000151	5.085586	-1.60353	C	0	-1.59797	2.447834
C	-0.00021	6.388129	-1.263281	C	0	-1.324934	3.831798
C	-0.00021	6.388129	1.263281	C	0	0	4.464248
C	-0.000151	5.085586	1.60353	C	0	1.324934	3.831798
H	-0.000142	4.84976	2.661093	C	0	1.59797	2.447834
H	-0.000142	4.84976	-2.661093	H	0	2.647434	2.164399
C	0.000036	-1.629977	5.360422	H	0	-2.647434	2.164399
C	-0.000019	1.219222	5.367676	C	0	-1.257811	10.51046
C	0.000017	-0.911633	6.558512	C	0	-1.590167	9.20254
C	-0.000011	0.493275	6.561502	C	0	1.257811	10.51046
C	0.000089	-5.577946	1.42538	C	0	-0.710093	8.045256
C	0.000089	-5.577946	-1.42538	C	0	1.590167	9.20254
C	0.000089	-6.770188	0.703705	C	0	0.710093	8.045256
C	0.000089	-6.770188	-0.703705	H	0	-2.65582	8.99743
C	0.000036	-1.629977	-5.360422	H	0	2.65582	8.99743
C	-0.000019	1.219222	-5.367676	C	0	-1.157204	6.692944
C	0.000017	-0.911633	-6.558512	C	0	0	5.847528
C	-0.000011	0.493275	-6.561502	C	0	1.157204	6.692944
H	0.000024	-1.444957	7.504638	C	0	-2.467517	4.686101

H	-0.000025	1.021834	7.51039	C	0	-2.412041	6.071594
H	-0.000038	2.30427	5.362584	C	0	2.412041	6.071594
H	0.00006	-2.714958	5.347985	H	0	-3.44022	4.203255
H	0.000089	-5.566514	2.509982	H	0	-3.33479	6.645188
H	0.000089	-5.566514	-2.509982	H	0	3.33479	6.645188
H	0.000089	-7.717762	1.233888	C	0	2.467517	4.686101
H	0.000089	-7.717762	-1.233888	H	0	3.44022	4.203255
H	0.00006	-2.714958	-5.347985	C	0	5.362818	-4.225292
H	-0.000038	2.30427	-5.362584	C	0	5.357776	-1.376122
H	0.000024	-1.444957	-7.504638	C	0	6.557329	-3.501057
H	-0.000025	1.021834	-7.51039	C	0	6.555041	-2.095906
N	0.000016	1.787057	0	C	0	1.426398	-8.180566
H	0.000097	0.778866	0	C	0	-1.426398	-8.180566
H	-0.000249	7.129272	2.056734	C	0	0.70546	-9.369563
H	-0.000285	7.988601	0	C	0	-0.70546	-9.369563
H	-0.000249	7.129272	-2.056734	C	0	-5.362818	-4.225292
N	-0.000236	6.982648	0	C	0	-5.357776	-1.376122
				C	0	-6.557329	-3.501057
				C	0	-6.555041	-2.095906
				H	0	7.50578	-4.030334
				H	0	7.501632	-1.563345
				H	0	5.347458	-0.291106
				H	0	5.355819	-5.310319
				H	0	2.511095	-8.170505
				H	0	-2.511095	-8.170505
				H	0	1.234499	-10.317874
				H	0	-1.234499	-10.317874
				H	0	-5.355819	-5.310319
				H	0	-5.347458	-0.291106
				H	0	-7.50578	-4.030334
				H	0	-7.501632	-1.563345
				N	0	0	-0.778445
				H	0	0	-1.792257
				H	0	2.054811	11.24754
				H	0	0	12.112344
				H	0	-2.054811	11.24754
				N	0	0	11.10588

Pc-A-N

C	0.091564	-0.86513	4.230478
C	0.190878	0.536359	4.250808
C	0.044676	-1.231423	2.80502

Pc-2A-N

C	0.099661	-3.444754	4.229448
C	0.310878	-2.054894	4.245122
C	0.01886	-3.810286	2.80618

C	-0.185087	-4.276372	-0.702501	C	-0.45815	-6.821525	-0.703464
C	-0.185087	-4.276372	0.702501	C	-0.45815	-6.821525	0.703464
C	-0.109392	-2.884404	1.151593	C	-0.269648	-5.443601	1.15127
C	0.190878	0.536359	-4.250808	C	0.310878	-2.054894	-4.245122
C	0.091564	-0.86513	-4.230478	C	0.099661	-3.444754	-4.229448
C	0.208792	0.959473	-2.837238	C	0.358509	-1.63951	-2.831085
C	0.044676	-1.231423	-2.80502	C	0.01886	-3.810286	-2.80618
C	0.004227	3.929078	-0.73205	C	0.417872	1.354967	-0.729119
C	0.004227	3.929078	0.73205	C	0.417872	1.354967	0.729119
C	0.276659	2.574794	-1.154227	C	0.561013	-0.030033	-1.154831
C	0.276659	2.574794	1.154227	C	0.561013	-0.030033	1.154831
C	0.208792	0.959473	2.837238	C	0.358509	-1.63951	2.831085
C	-0.109392	-2.884404	-1.151593	C	-0.269648	-5.443601	-1.15127
N	-0.079779	-2.110543	0	N	-0.176558	-4.675537	0
N	0.120971	-0.161131	2.015699	N	0.179545	-2.743413	2.0148
N	0.120971	-0.161131	-2.015699	N	0.179545	-2.743413	-2.0148
H	-0.060333	-1.094001	0	H	-0.076018	-3.66391	0
N	-0.065306	-2.524837	2.40625	N	-0.195276	-5.085091	2.408837
N	0.255477	2.21537	2.467011	N	0.506077	-0.384554	2.460517
N	0.255477	2.21537	-2.467011	N	0.506077	-0.384554	-2.460517
N	-0.065306	-2.524837	-2.40625	N	-0.195276	-5.085091	-2.408837
C	-0.231189	4.991211	-1.592662	C	0.28628	2.419474	-1.585242
C	-0.494017	6.326788	-1.265203	C	0.149424	3.80628	-1.30659
C	-0.609584	6.911034	0	C	0.088014	4.424034	0
C	-0.494017	6.326788	1.265203	C	0.149424	3.80628	1.30659
C	-0.231189	4.991211	1.592662	C	0.28628	2.419474	1.585242
H	-0.196442	4.734177	2.648904	H	0.296042	2.1448	2.637838
H	-0.196442	4.734177	-2.648904	H	0.296042	2.1448	-2.637838
C	0.047217	-1.606877	5.406634	C	-0.584329	11.047984	0
C	0.253266	1.232602	5.453055	C	-0.523607	10.456604	-1.264727
C	0.109443	-0.908501	6.616344	C	-0.38531	9.101076	-1.588747
C	0.210883	0.491035	6.638214	C	-0.523607	10.456604	1.264727
C	-0.24121	-5.466474	1.424436	C	-0.273944	8.003154	-0.745555
C	-0.24121	-5.466474	-1.424436	C	-0.38531	9.101076	1.588747
C	-0.300859	-6.659119	0.702923	C	-0.273944	8.003154	0.745555
C	-0.300859	-6.659119	-0.702923	H	-0.362481	8.877748	-2.65392
C	0.047217	-1.606877	-5.406634	H	-0.362481	8.877748	2.65392
C	0.253266	1.232602	-5.453055	C	-0.136676	6.646133	-1.163726
C	0.109443	-0.908501	-6.616344	C	-0.054514	5.834618	0
C	0.210883	0.491035	-6.638214	C	-0.136676	6.646133	1.163726
H	0.079701	-1.454707	7.554639	C	0.063073	4.65176	-2.467371
H	0.256969	1.005174	7.593984	C	-0.074265	6.018371	-2.425775

H	0.331473	2.314933	5.464585	C	-0.074265	6.018371	2.425775
H	-0.031264	-2.68884	5.379118	H	0.111704	4.157776	-3.43272
H	-0.237995	-5.452888	2.508953	H	-0.132463	6.586559	-3.349507
H	-0.237995	-5.452888	-2.508953	H	-0.132463	6.586559	3.349507
H	-0.347458	-7.605176	1.233807	C	0.063073	4.65176	2.467371
H	-0.347458	-7.605176	-1.233807	H	0.111704	4.157776	3.43272
H	-0.031264	-2.68884	-5.379118	C	0.000045	-4.175879	5.409278
H	0.331473	2.314933	-5.464585	C	0.432406	-1.36222	5.445511
H	0.079701	-1.454707	-7.554639	C	0.12164	-3.481037	6.61621
H	0.256969	1.005174	-7.593984	C	0.334559	-2.093525	6.633302
H	0.793919	0.774668	0	C	-0.611894	-8.005215	1.424458
C	0.498256	1.802597	0	C	-0.611894	-8.005215	-1.424458
H	-0.63007	7.000012	-2.107954	C	-0.769098	-9.187902	0.703616
				C	-0.769098	-9.187902	-0.703616
				C	0.000045	-4.175879	-5.409278
				C	0.432406	-1.36222	-5.445511
				C	0.12164	-3.481037	-6.61621
				C	0.334559	-2.093525	-6.633302
				H	0.051219	-4.020224	7.556535
				H	0.424404	-1.581783	7.587381
				H	0.596972	-0.289493	5.452327
				H	-0.164972	-5.248233	5.385776
				H	-0.607683	-7.992034	2.509056
				H	-0.607683	-7.992034	-2.509056
				H	-0.893231	-10.12722	1.234231
				H	-0.893231	-10.12722	-1.234231
				H	-0.164972	-5.248233	-5.385776
				H	0.596972	-0.289493	-5.452327
				H	0.051219	-4.020224	-7.556535
				H	0.424404	-1.581783	-7.587381
				H	0.906751	-1.868881	0
				C	0.71122	-0.817552	0
				H	-0.592902	11.137198	2.108877
				H	-0.694771	12.130409	0
				H	-0.592902	11.137198	-2.108877

P_N-3A-2A

C	9.753109	1.273176	-0.15567
C	9.811367	-0.189958	-0.130345
C	11.072666	1.747419	-0.173025
C	3.737593	-3.874032	0.114226
C	5.075139	-3.833854	-0.018599

Mg-P_N-3A-2A

C	-9.766785	-0.004518	0
C	-9.63966	1.448687	0
C	-11.136947	-0.310871	0
C	-3.122418	4.338227	0
C	-4.467007	4.487803	0

C	5.45018	-2.393533	-0.006157	C	-5.051094	3.13287	0
C	1.520953	1.421768	0.357789	C	-1.58743	-1.191434	0
C	1.603186	-0.886305	0.374839	C	-1.375215	1.075902	0
C	3.438711	4.547869	0.050148	C	-3.905824	-4.075922	0
C	4.775147	4.603533	-0.087335	C	-5.254169	-3.978679	0
C	3.098434	3.10981	0.161699	C	-3.369426	-2.704331	0
C	5.254314	3.195198	-0.057068	C	-5.582544	-2.539121	0
C	11.217569	-0.567925	-0.131433	C	-10.986865	2.002577	0
C	3.293606	-2.463097	0.205877	C	-2.84557	2.893008	0
N	4.33784	-1.610068	0.133665	N	-4.027097	2.2141	0
N	6.712448	-2.062039	-0.106923	N	-6.341653	2.929095	0
N	6.535448	2.956411	-0.159063	N	-6.813551	-2.107745	0
N	1.814245	2.722879	0.272334	N	-2.052197	-2.457651	0
N	1.987118	-2.166755	0.309726	N	-1.596879	2.40632	0
C	8.619031	2.073078	-0.17163	C	-8.744396	-0.944813	0
C	8.746991	-1.045576	-0.122734	C	-8.471949	2.161406	0
H	8.96116	-2.109604	-0.119594	H	-8.555515	3.244187	0
H	8.791997	3.145197	-0.201902	H	-9.062246	-1.984545	0
C	0.180081	-0.507038	0.321129	C	0	0.53253	0
C	0.127712	0.941314	0.311673	C	-0.135333	-0.912665	0
C	-0.846919	-1.406958	0.270477	C	1.138552	1.289735	0
C	-2.256673	-1.179984	0.222797	C	2.508041	0.881453	0
C	-2.924701	0.104628	0.1971	C	3.005427	-0.478723	0
C	-2.351827	1.434447	0.210037	C	2.263705	-1.722568	0
C	-0.961572	1.763841	0.252168	C	0.842238	-1.868611	0
H	-0.719279	2.824374	0.237866	H	0.467704	-2.890234	0
H	-0.528205	-2.447156	0.268891	H	0.960985	2.363258	0
C	-9.629268	-0.143367	-0.044464	C	9.689771	-1.10729	0
C	-8.959703	-1.424471	-0.016507	C	9.192433	0.250212	0
C	-7.557861	-1.646676	0.03645	C	7.830626	0.654243	0
C	-9.056639	1.183919	-0.025425	C	8.947962	-2.348209	0
C	-6.501603	-0.765205	0.072908	C	6.667329	-0.081413	0
C	-7.674614	1.51044	0.024664	C	7.534762	-2.491002	0
C	-6.556045	0.710052	0.066929	C	6.529156	-1.551212	0
H	-7.277731	-2.698133	0.049271	H	7.690159	1.733353	0
H	-7.473449	2.579869	0.029512	H	7.195355	-3.524932	0
C	-5.110292	-1.138412	0.123772	C	5.335381	0.469573	0
C	-4.338686	0.053013	0.147847	C	4.414702	-0.611095	0
C	-5.195192	1.184668	0.11382	C	5.117948	-1.844374	0
C	-3.058583	-2.361947	0.196694	C	3.457951	1.948865	0
C	-4.440924	-2.367662	0.149167	C	4.830228	1.775318	0
C	-4.617026	2.459438	0.12818	C	4.378629	-3.033278	0

H	-2.531927	-3.310687	0.21616	H	3.058794	2.958113	0
H	-4.975911	-3.312792	0.132067	H	5.483562	2.643156	0
H	-5.219551	3.362942	0.103249	H	4.859011	-4.007555	0
C	-3.23766	2.554519	0.174269	C	2.998076	-2.948252	0
H	-2.781642	3.539239	0.184465	H	2.417866	-3.865457	0
C	-15.634744	-1.635178	-0.269477	C	15.843487	-0.416081	0
C	-14.26232	-1.907119	-0.216403	C	14.517422	0.034058	0
C	-15.730097	0.893019	-0.278557	C	15.606341	-2.934831	0
C	-13.192111	-1.022158	-0.177778	C	13.339617	-0.702506	0
C	-14.381646	1.268193	-0.227861	C	14.219622	-3.129522	0
C	-13.248053	0.466714	-0.183052	C	13.199957	-2.186037	0
H	-16.286242	-2.504271	-0.292366	H	16.603745	0.360032	0
H	-13.998186	-2.963049	-0.203916	H	14.394062	1.115586	0
H	-16.445026	1.710541	-0.30755	H	16.208402	-3.83919	0
H	-14.197881	2.341088	-0.223075	H	13.896528	-4.16901	0
C	-11.814406	-1.390051	-0.124655	C	12.020743	-0.157285	0
C	-11.043698	-0.196076	-0.09797	C	11.099955	-1.240019	0
C	-11.90118	0.936911	-0.132718	C	11.802571	-2.47557	0
C	-9.763738	-2.616651	-0.044145	C	10.146175	1.326939	0
C	-11.137141	-2.626848	-0.096246	C	11.510105	1.157516	0
C	-9.947146	2.312722	-0.06066	C	9.684042	-3.583998	0
C	-11.317671	2.22069	-0.112596	C	11.055607	-3.672036	0
H	-9.234603	-3.56443	-0.021973	H	9.745072	2.335833	0
H	-11.671851	-3.571707	-0.114427	H	12.163985	2.024421	0
H	-9.49014	3.297368	-0.044887	H	9.101709	-4.500319	0
H	-11.921228	3.123076	-0.136947	H	11.536273	-4.645711	0
H	-17.361974	-0.434446	-0.338213	H	17.399606	-1.833104	0
H	3.424217	0.334247	0.531762	C	-7.085342	1.741662	0
C	7.319038	-0.817089	-0.114605	N	-4.405888	-1.821095	0
N	4.199321	2.333689	0.097144	C	-11.899365	0.879153	0
C	11.978187	0.661004	-0.157714	C	-7.327608	-0.800589	0
C	7.23337	1.757721	-0.147507	C	-6.55016	0.41717	0
C	6.669888	0.439929	-0.126551	H	-11.551089	-1.312501	0
H	5.586716	0.402807	-0.129024	C	-2.312969	0.019827	0
H	11.358668	2.792437	-0.195063	C	16.316392	-1.731113	0
C	2.3579	0.29591	0.457402	C	-13.318651	0.887618	0
C	-16.27554	-0.393351	-0.296798	C	-11.293532	3.373951	0
C	13.388379	0.830586	-0.168547	C	-14.171479	1.963699	0
C	11.693324	-1.89075	-0.109423	C	-12.537058	3.986677	0
C	14.369114	-0.129366	-0.157331	C	-13.820475	3.411477	0
C	13.002667	-2.343503	-0.109458	C	-15.600435	1.890273	0
C	14.204006	-1.611494	-0.129973	C	-15.028548	4.111335	0

C	15.777703	0.123868	-0.170136	C	-16.104149	3.18085	0
C	15.489656	-2.15219	-0.127931	H	-13.786174	-0.096887	0
C	16.439371	-1.092201	-0.152433	H	-10.443142	4.049994	0
H	13.728664	1.865717	-0.188862	H	-12.524281	5.075652	0
H	10.934286	-2.667682	-0.089376	H	-15.123525	5.190493	0
H	13.126441	-3.425237	-0.090378	H	-16.171209	0.970136	0
H	15.721079	-3.210319	-0.110334	H	-17.154887	3.447182	0
H	16.227577	1.108486	-0.19031	H	-5.997049	-4.764577	0
H	17.515316	-1.224096	-0.156479	H	-3.285124	-4.961696	0
H	5.42675	5.458992	-0.202606	H	-5.053814	5.396225	0
H	2.710977	5.34778	0.078301	H	-2.351328	5.096657	0
H	5.787455	-4.641271	-0.120777	Mg	-4.398158	0.2142	0
H	3.069907	-4.724336	0.151463				

Zn-P_N-3A-2A

C	-9.454189	1.239184	0.015394
C	-9.511176	-0.212511	-0.054708
C	-10.772449	1.716687	0.070017
C	-3.460839	-3.924085	-0.103476
C	-4.809559	-3.897489	-0.183388
C	-5.204872	-2.475534	-0.189475
C	-1.303719	1.373406	0.162662
C	-1.381913	-0.891422	0.182671
C	-3.163855	4.541816	-0.163243
C	-4.511449	4.6143	-0.216821
C	-2.818154	3.112057	-0.096926
C	-5.011472	3.225099	-0.186941
C	-10.915256	-0.596723	-0.044483
C	-3.011582	-2.523554	-0.063997
N	-4.080563	-1.694487	-0.161704
N	-6.45206	-2.101984	-0.160553
N	-6.280431	2.947844	-0.126153
N	-1.559496	2.684496	0.022501
N	-1.727577	-2.183932	0.061368
C	-8.310746	2.02337	0.003113
C	-8.43488	-1.050244	-0.111108
H	-8.646724	-2.113577	-0.162272
H	-8.480786	3.096109	0.03346
C	0.048239	-0.52851	0.131287
C	0.097892	0.911514	0.116686
C	1.076204	-1.430166	0.09834
C	2.485855	-1.201659	0.087965

Ni-P_N-3A-2A

C	-9.404431	1.030207	-0.581449
C	-9.399373	-0.20111	0.188695
C	-10.739347	1.438968	-0.727092
C	-3.504343	-3.85193	-0.816061
C	-4.821582	-3.843821	-0.530144
C	-5.204225	-2.445151	-0.353781
C	-1.38577	1.301019	-0.136634
C	-1.423217	-0.904615	-0.577926
C	-3.297046	4.360652	-0.293702
C	-4.590195	4.402037	-0.66699
C	-2.935997	2.951525	-0.174225
C	-5.062104	3.018134	-0.701448
C	-10.777504	-0.504189	0.543692
C	-3.053158	-2.466502	-0.764225
N	-4.113442	-1.615668	-0.537321
N	-6.418171	-2.121563	-0.029029
N	-6.300059	2.750403	-0.963762
N	-1.672286	2.595834	0.006308
N	-1.763765	-2.173723	-0.815254
C	-8.280565	1.732861	-0.987579
C	-8.297288	-0.978217	0.396645
H	-8.453048	-1.937495	0.882455
H	-8.469433	2.688744	-1.469172
C	-0.011742	-0.545034	-0.442768
C	0.013688	0.862685	-0.133814
C	1.033165	-1.419294	-0.584231
C	2.434143	-1.184734	-0.461974

C	3.153425	0.083809	0.075021	C	3.077363	0.073598	-0.140451
C	2.576683	1.412805	0.067208	C	2.478709	1.365934	0.118752
C	1.186423	1.73908	0.071757	C	1.084922	1.678991	0.102755
H	0.942344	2.798612	0.039363	H	0.825561	2.71544	0.306238
H	0.759128	-2.470582	0.083784	H	0.737326	-2.43798	-0.824149
C	9.862191	-0.152599	0.001338	C	9.780048	-0.115244	0.180348
C	9.193974	-1.434621	0.016631	C	9.136885	-1.368921	-0.146987
C	7.792029	-1.659425	0.035533	C	7.742103	-1.597664	-0.273797
C	9.286184	1.173854	0.001235	C	9.181043	1.171859	0.44908
C	6.733093	-0.779546	0.043034	C	6.667105	-0.747798	-0.133643
C	7.90381	1.497997	0.015036	C	7.793071	1.478843	0.44441
C	6.78486	0.695336	0.032593	C	6.692372	0.69082	0.200149
H	7.513511	-2.711339	0.044896	H	7.483868	-2.624278	-0.526005
H	7.700529	2.567022	0.010525	H	7.570475	2.518864	0.674647
C	5.341952	-1.155206	0.060571	C	5.286655	-1.121572	-0.294158
C	4.567331	0.034611	0.060752	C	4.490599	0.033613	-0.071703
C	5.423397	1.167404	0.043214	C	5.323707	1.142923	0.22886
C	3.290853	-2.382255	0.085323	C	3.261681	-2.331208	-0.681408
C	4.673905	-2.385529	0.073248	C	4.641313	-2.325796	-0.606437
C	4.842277	2.441375	0.036365	C	4.720984	2.381817	0.479013
H	2.765516	-3.331932	0.094076	H	2.754453	-3.260287	-0.92123
H	5.210839	-3.329784	0.072946	H	5.195247	-3.242511	-0.7875
H	5.443808	3.345853	0.022341	H	5.305371	3.266768	0.714389
C	3.462375	2.534274	0.046571	C	3.341971	2.464927	0.419044
H	3.004566	3.518241	0.039729	H	2.866794	3.421889	0.609791
C	15.874061	-1.633469	-0.069367	C	15.811463	-1.517495	0.17559
C	14.501145	-1.908024	-0.049743	C	14.446644	-1.794174	0.037356
C	15.964804	0.894706	-0.082756	C	15.854171	0.944571	0.757077
C	13.428657	-1.024919	-0.039949	C	13.357797	-0.941955	0.178996
C	14.615375	1.267567	-0.066814	C	14.498039	1.298241	0.766726
C	13.481811	0.463933	-0.048084	C	13.383236	0.508683	0.520516
H	16.527384	-2.501539	-0.073859	H	16.481009	-2.357689	0.013989
H	14.238741	-2.964417	-0.041132	H	14.204815	-2.824498	-0.217462
H	16.678858	1.713453	-0.09609	H	16.550992	1.74677	0.983527
H	14.429594	2.34012	-0.069605	H	14.291752	2.341085	1.000946
C	12.050743	-1.395214	-0.02014	C	11.989993	-1.311294	0.019009
C	11.277295	-0.202782	-0.016293	C	11.19447	-0.155139	0.247151
C	12.133833	0.931544	-0.032992	C	12.027389	0.955159	0.552055
C	10.000871	-2.625506	0.012636	C	9.966316	-2.523242	-0.372986
C	11.375063	-2.63318	-0.005079	C	11.338118	-2.521797	-0.299504
C	10.176082	2.304289	-0.015329	C	10.046966	2.278569	0.755241
C	11.547306	2.214514	-0.031929	C	11.418214	2.200292	0.811135

H	9.473033	-3.574209	0.024398	H	9.457138	-3.450629	-0.616897
H	11.9118	-3.577096	-0.007141	H	11.892198	-3.437233	-0.484274
H	9.717098	3.28816	-0.01468	H	9.569537	3.233411	0.953039
H	12.149742	3.11793	-0.043966	H	12.002801	3.083776	1.049766
H	17.600491	-0.430008	-0.09813	H	17.51225	-0.333051	0.545753
C	-7.000468	-0.82206	-0.088743	C	-6.91808	-0.843289	-0.034504
N	-3.945165	2.362731	-0.159183	N	-4.027914	2.145426	-0.388223
C	-11.678242	0.630389	0.036401	C	-11.59331	0.532616	-0.05435
C	-6.919928	1.707685	-0.043966	C	-6.887648	1.515729	-0.766171
C	-6.273776	0.409608	0.003435	C	-6.170176	0.314475	-0.416173
H	-11.05762	2.760811	0.125369	H	-11.069671	2.325826	-1.255378
C	-2.186885	0.271184	0.328758	C	-2.27126	0.218893	-0.384959
C	16.513299	-0.390923	-0.083895	C	16.425858	-0.302146	0.494467
C	-13.087377	0.795942	0.077156	C	-13.002873	0.68414	-0.009679
C	-11.388342	-1.91841	-0.102309	C	-11.184912	-1.602579	1.317011
C	-14.066703	-0.166254	0.05029	C	-13.933075	-0.112486	0.612907
C	-12.697558	-2.373532	-0.095977	C	-12.467946	-1.969756	1.694856
C	-13.898958	-1.645238	-0.030273	C	-13.696639	-1.348979	1.410348
C	-15.474915	0.082406	0.095324	C	-15.345808	0.108195	0.61299
C	-15.184271	-2.189556	-0.029255	C	-14.951461	-1.79125	1.835783
C	-16.135129	-1.134511	0.047194	C	-15.946851	-0.902024	1.347592
H	-13.429793	1.828831	0.138254	H	-13.39248	1.550907	-0.543336
H	-10.62736	-2.691717	-0.16019	H	-10.38918	-2.251444	1.673068
H	-12.820173	-3.454303	-0.149781	H	-12.540128	-2.870338	2.302892
H	-15.413157	-3.247246	-0.079063	H	-15.129185	-2.672367	2.440484
H	-15.926574	1.064575	0.156553	H	-15.8419	0.932758	0.116545
H	-17.210613	-1.268925	0.064736	H	-17.011195	-1.003545	1.525893
H	-5.152203	5.484483	-0.25674	H	-5.229692	5.246706	-0.87991
H	-2.433638	5.33948	-0.147854	H	-2.589671	5.163302	-0.139815
H	-5.512179	-4.7189	-0.215358	H	-5.5208	-4.662381	-0.435916
H	-2.792546	-4.773184	-0.058144	H	-2.837358	-4.681149	-1.00514
Zn	-4.205813	0.339663	0.16286	Ni	-4.159002	0.265793	-0.437859

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C	0.093196	-9.822777	4.216654	C	9.656435	-4.200707	0.031705
C	-0.178701	-11.148348	4.20599	C	11.010472	-4.194667	0.182517
C	-0.276439	-11.528974	2.787552	C	11.436243	-2.796567	0.157249
C	0.487033	-7.795847	-1.155977	C	7.551281	1.1468	-0.297234
C	0.487033	-7.795847	1.155977	C	7.551268	-1.146887	-0.297388
C	0.093196	-9.822777	-4.216654	C	9.656313	4.200696	0.032347
C	-0.178701	-11.148348	-4.20599	C	11.010333	4.194709	0.183203
C	0.173438	-9.40677	-2.806356	C	9.220642	2.809107	-0.095016

Mg-P_N-4A-A

C	-0.276439	-11.528974	-2.787552	C	11.436199	2.79663	0.15757
C	0.173438	-9.40677	2.806356	C	9.220687	-2.809121	-0.095279
N	-0.056526	-10.473148	1.978886	N	10.340904	-2.007298	-0.024541
N	-0.556423	-12.78775	2.407166	N	12.71026	-2.396247	0.31925
N	-0.556423	-12.78775	-2.407166	N	12.710227	2.396363	0.319594
N	0.395897	-8.14375	-2.453422	N	7.939657	2.443889	-0.209124
N	0.395897	-8.14375	2.453422	N	7.939659	-2.443951	-0.20943
C	0.435667	-6.393944	0.727774	C	6.136034	-0.731638	-0.261496
C	0.435667	-6.393944	-0.727774	C	6.136042	0.73157	-0.261453
C	0.374527	-5.330442	1.585393	C	5.067897	-1.585157	-0.219426
C	0.333998	-3.930126	1.30779	C	3.66658	-1.307346	-0.19344
C	0.316558	-3.309019	0	C	3.044372	-0.000031	-0.183618
C	0.333998	-3.930126	-1.30779	C	3.666588	1.30728	-0.193411
C	0.374527	-5.330442	-1.585393	C	5.067904	1.58509	-0.21936
H	0.362488	-5.606903	-2.637569	H	5.339921	2.638778	-0.20863
H	0.362488	-5.606903	2.637569	H	5.339912	-2.638847	-0.208762
C	0.113918	3.405539	0	C	-3.672489	-0.000013	-0.061732
C	0.132824	2.783673	1.305958	C	-3.050214	-1.305814	-0.072571
C	0.174845	1.386297	1.579537	C	-1.652637	-1.579492	-0.097187
C	0.132824	2.783673	-1.305958	C	-3.050208	1.305785	-0.07275
C	0.207115	0.300435	0.738947	C	-0.566272	-0.738812	-0.116466
C	0.174845	1.386297	-1.579537	C	-1.652633	1.579457	-0.097299
C	0.207115	0.300435	-0.738947	C	-0.566267	0.73877	-0.116486
H	0.182144	1.146014	2.641007	H	-1.412229	-2.640928	-0.101422
H	0.182144	1.146014	-2.641007	H	-1.41222	2.640891	-0.101589
C	0.248242	-1.078796	1.162779	C	0.813429	-1.162419	-0.141153
C	0.273168	-1.893129	0	C	1.628252	-0.000028	-0.156698
C	0.248242	-1.078796	-1.162779	C	0.813432	1.162367	-0.141164
C	0.306225	-3.085332	2.459936	C	2.821008	-2.459015	-0.174943
C	0.265314	-1.703406	2.415103	C	1.438462	-2.414383	-0.150312
C	0.265314	-1.703406	-2.415103	C	1.438474	2.41433	-0.15031
H	0.319037	-3.576995	3.42752	H	3.312584	-3.426724	-0.181851
H	0.246664	-1.133924	3.339937	H	0.869042	-3.33944	-0.138205
H	0.246664	-1.133924	-3.339937	H	0.869059	3.339389	-0.138202
C	0.306225	-3.085332	-2.459936	C	2.821018	2.458954	-0.174916
H	0.319037	-3.576995	-3.42752	H	3.312599	3.42666	-0.181801
C	-0.071245	9.49248	1.305626	C	-9.761199	-1.305579	0.043572
C	-0.028087	8.099162	1.579903	C	-8.367586	-1.579896	0.019378
C	-0.071245	9.49248	-1.305626	C	-9.761196	1.305588	0.043222
C	0.004893	7.009794	0.739955	C	-7.277753	-0.739888	0.000689
C	-0.028087	8.099162	-1.579903	C	-8.367587	1.579899	0.019005
C	0.004893	7.009794	-0.739955	C	-7.27775	0.739885	0.000536

H	-0.020464	7.859079	2.641526	H	-8.127394	-2.641503	0.015196
H	-0.020464	7.859079	-2.641526	H	-8.127393	2.641504	0.014579
C	0.046615	5.635418	1.163944	C	-5.903017	-1.16384	-0.022961
C	0.071134	4.820903	0	C	-5.088259	-0.000009	-0.037099
C	0.046615	5.635418	-1.163944	C	-5.903019	1.163826	-0.023188
C	0.107626	3.629385	2.461869	C	-3.896338	-2.461825	-0.057829
C	0.065838	5.00818	2.418923	C	-5.275469	-2.418817	-0.033801
C	0.107626	3.629385	-2.461869	C	-3.896334	2.461801	-0.058229
C	0.065838	5.00818	-2.418923	C	-5.275463	2.418802	-0.034241
H	0.122765	3.138475	3.43024	H	-3.405283	-3.430183	-0.066446
H	0.048801	5.577235	3.343794	H	-5.844655	-3.343724	-0.023888
H	0.122765	3.138475	-3.43024	H	-3.405276	3.430156	-0.066988
H	0.048801	5.577235	-3.343794	H	-5.844647	3.343712	-0.024515
H	0.728084	-9.649333	0	C	13.097087	-1.11583	0.344857
C	-0.649018	-13.138974	1.135628	N	10.340949	2.007341	-0.024507
N	-0.056526	-10.473148	-1.978886	C	13.097066	1.115932	0.345014
C	-0.649018	-13.138974	-1.135628	C	8.361046	-0.000029	-0.382292
C	0.596139	-8.588638	0	C	-10.382558	0.000005	0.054352
C	-0.090842	10.113558	0	H	11.679784	-5.033627	0.314868
H	-0.320607	-11.828329	5.034931	H	8.985073	-5.048543	0.012724
H	0.238095	-9.158671	5.05798	H	11.679573	5.033685	0.31582
H	-0.320607	-11.828329	-5.034931	H	8.984907	5.048503	0.013597
H	0.238095	-9.158671	-5.05798	C	-10.609794	2.46717	0.057613
C	-0.097308	10.340726	-2.467124	C	-11.799188	0.000009	0.079096
C	-0.135202	11.529743	0	C	-10.609793	-2.467156	0.058304
C	-0.097308	10.340726	2.467124	C	-12.614497	1.164978	0.093067
C	-0.160615	12.344786	-1.165014	C	-11.982941	2.426959	0.081659
C	-0.140447	11.71347	-2.426983	C	-12.614494	-1.164955	0.093408
C	-0.160615	12.344786	1.165014	C	-11.982941	-2.426938	0.08236
C	-0.140447	11.71347	2.426983	H	-12.553052	3.351015	0.091305
H	-0.158007	12.283394	-3.351038	H	-10.115528	3.433979	0.0486
H	-0.081405	9.846615	-3.433938	H	-10.115527	-3.433967	0.049561
H	-0.081405	9.846615	3.433938	H	-12.553053	-3.350991	0.092286
H	-0.158007	12.283394	3.351038	C	-13.977908	0.746071	0.116905
C	-0.203401	13.707768	-0.746121	C	-13.97791	-0.74604	0.117124
C	-0.203401	13.707768	0.746121	C	-15.08108	1.589015	0.13591
C	-0.237898	14.810502	-1.588999	C	-16.443959	1.265405	0.159853
C	-0.280987	16.173005	-1.265414	C	-17.037011	0.000023	0.170549
C	-0.299932	16.765774	0	C	-16.443961	-1.265358	0.160229
C	-0.280987	16.173005	1.265414	C	-15.081078	-1.588977	0.13638
C	-0.237898	14.810502	1.588999	H	-14.856989	2.654351	0.13174
H	-0.230686	14.586478	-2.654341	H	-17.128196	2.109177	0.171638

H	-0.302482	16.857007	-2.109181	H	-18.124983	0.000027	0.189605
H	-0.33431	17.853382	0	H	-17.128196	-2.109127	0.172266
H	-0.302482	16.857007	2.109181	H	-14.856988	-2.654314	0.132524
H	-0.230686	14.586478	2.654341	C	14.471061	0.681139	0.595911
C	-0.897556	-14.491775	-0.681683	C	14.471067	-0.681043	0.595848
C	-0.897556	-14.491775	0.681683	H	15.299455	1.356337	0.760614
H	-1.039355	-15.321074	-1.359561	H	15.299467	-1.356249	0.760488
H	-1.039355	-15.321074	1.359561	N	12.318877	0.000065	0.182703
N	-0.516755	-12.362954	0	Mg	10.375097	0.000018	-0.189568

Zn-P_N-4A-A

C	-0.041633	-9.242829	4.216845	C	0.000314	-9.279908	4.129761
C	-0.210794	-10.593121	4.20888	C	0.000551	-10.63457	4.10795
C	-0.240431	-11.005412	2.806053	C	0.000522	-11.032553	2.713349
C	0.328754	-7.190379	-1.144711	C	-0.000153	-7.227796	-1.13125
C	0.328754	-7.190379	1.144711	C	-0.000153	-7.227796	1.13125
C	-0.041633	-9.242829	-4.216845	C	0.000314	-9.279908	-4.129761
C	-0.210794	-10.593121	-4.20888	C	0.000551	-10.63457	-4.10795
C	0.047039	-8.81037	-2.820971	C	0.00022	-8.835763	-2.750295
C	-0.240431	-11.005412	-2.806053	C	0.000522	-11.032553	-2.713349
C	0.047039	-8.81037	2.820971	C	0.00022	-8.835763	2.750295
N	-0.094608	-9.913238	2.014086	N	0.000511	-9.925536	1.893366
N	-0.394831	-12.273099	2.397681	N	0.000595	-12.314558	2.367461
N	-0.394831	-12.273099	-2.397681	N	0.000595	-12.314558	-2.367461
N	0.215336	-7.543408	-2.444743	N	-0.000034	-7.554981	-2.427017
N	0.215336	-7.543408	2.444743	N	-0.000034	-7.554981	2.427017
C	0.284806	-5.778965	0.728048	C	-0.000328	-5.823573	0.722742
C	0.284806	-5.778965	-0.728048	C	-0.000328	-5.823573	-0.722742
C	0.236246	-4.713573	1.584703	C	-0.000552	-4.760601	1.585621
C	0.212238	-3.31261	1.307511	C	-0.000627	-3.360979	1.307848
C	0.202695	-2.690583	0	C	-0.000624	-2.738482	0
C	0.212238	-3.31261	-1.307511	C	-0.000627	-3.360979	-1.307848
C	0.236246	-4.713573	-1.584703	C	-0.000552	-4.760601	-1.585621
H	0.219682	-4.988402	-2.637414	H	-0.000596	-5.036975	-2.637634
H	0.219682	-4.988402	2.637414	H	-0.000596	-5.036975	2.637634
C	0.074192	4.025881	0	C	-0.000514	3.978768	0
C	0.086358	3.403668	1.305855	C	-0.000558	3.356328	1.305817
C	0.113192	2.006136	1.579501	C	-0.000631	1.958972	1.579543
C	0.086358	3.403668	-1.305855	C	-0.000558	3.356328	-1.305817
C	0.133776	0.919759	0.738847	C	-0.000653	0.871896	0.738897
C	0.113192	2.006136	-1.579501	C	-0.000631	1.958972	-1.579543

Ni-P_N-4A-A

C	0.133776	0.919759	-0.738847	C	-0.000653	0.871896	-0.738897
H	0.117756	1.76575	2.640949	H	-0.000651	1.718564	2.640997
H	0.117756	1.76575	-2.640949	H	-0.000651	1.718564	-2.640997
C	0.159516	-0.45979	1.162549	C	-0.000666	-0.507228	1.162493
C	0.175368	-1.274532	0	C	-0.000649	-1.322456	0
C	0.159516	-0.45979	-1.162549	C	-0.000666	-0.507228	-1.162493
C	0.193646	-2.46721	2.459435	C	-0.000701	-2.514529	2.460243
C	0.168911	-1.084805	2.414676	C	-0.000709	-1.132501	2.415053
C	0.168911	-1.084805	-2.414676	C	-0.000709	-1.132501	-2.415053
H	0.200327	-2.958961	3.427046	H	-0.000736	-3.006251	3.427874
H	0.156636	-0.515256	3.339632	H	-0.000744	-0.562589	3.339879
H	0.156636	-0.515256	-3.339632	H	-0.000744	-0.562589	-3.339879
C	0.193646	-2.46721	-2.459435	C	-0.000701	-2.514529	-2.460243
H	0.200327	-2.958961	-3.427046	H	-0.000736	-3.006251	-3.427874
C	-0.046514	10.114317	1.305596	C	0.000026	10.068196	1.305576
C	-0.018147	8.720756	1.579902	C	-0.000134	8.674516	1.57992
C	-0.046514	10.114317	-1.305596	C	0.000026	10.068196	-1.305576
C	0.00346	7.630985	0.739913	C	-0.000236	7.584339	0.739964
C	-0.018147	8.720756	-1.579902	C	-0.000134	8.674516	-1.57992
C	0.00346	7.630985	-0.739913	C	-0.000236	7.584339	-0.739964
H	-0.013156	8.480587	2.641515	H	-0.00016	8.434308	2.64154
H	-0.013156	8.480587	-2.641515	H	-0.00016	8.434308	-2.64154
C	0.030652	6.256333	1.163867	C	-0.000356	6.209691	1.163848
C	0.046556	5.441591	0	C	-0.000416	5.394748	0
C	0.030652	6.256333	-1.163867	C	-0.000356	6.209691	-1.163848
C	0.07017	4.249758	2.461867	C	-0.000517	4.202861	2.462096
C	0.043155	5.628826	2.41887	C	-0.000416	5.581921	2.41907
C	0.07017	4.249758	-2.461867	C	-0.000517	4.202861	-2.462096
C	0.043155	5.628826	-2.41887	C	-0.000416	5.581921	-2.41907
H	0.079973	3.758714	3.430226	H	-0.000561	3.711637	3.430414
H	0.03217	6.198015	3.34376	H	-0.000385	6.15129	3.343919
H	0.079973	3.758714	-3.430226	H	-0.000561	3.711637	-3.430414
H	0.03217	6.198015	-3.34376	H	-0.000385	6.15129	-3.343919
C	-0.407084	-12.630526	1.112964	C	0.000446	-12.671593	1.094702
N	-0.094608	-9.913238	-2.014086	N	0.000511	-9.925536	-1.893366
C	-0.407084	-12.630526	-1.112964	C	0.000446	-12.671593	-1.094702
C	0.456	-8.007954	0	C	-0.000112	-8.085901	0
C	-0.059437	10.735628	0	C	0.000103	10.689674	0
H	-0.317744	-11.268574	5.046552	H	0.000682	-11.3422	4.92465
H	0.028792	-8.575019	5.064709	H	0.000185	-8.601167	4.970836
H	-0.317744	-11.268574	-5.046552	H	0.000682	-11.3422	-4.92465
H	0.028792	-8.575019	-5.064709	H	0.000185	-8.601167	-4.970836

C	-0.0637	10.962859	-2.467161	C	0.000117	10.917022	-2.46725
C	-0.088733	12.152182	0	C	0.000267	12.106542	0
C	-0.0637	10.962859	2.467161	C	0.000117	10.917022	2.46725
C	-0.105539	12.967447	-1.164981	C	0.000361	12.921989	-1.16498
C	-0.092197	12.335929	-2.426969	C	0.000285	12.290277	-2.427051
C	-0.105539	12.967447	1.164981	C	0.000361	12.921989	1.16498
C	-0.092197	12.335929	2.426969	C	0.000285	12.290277	2.427051
H	-0.103786	12.906011	-3.351021	H	0.000345	12.860507	-3.351086
H	-0.053193	10.468615	-3.433971	H	0.000047	10.422631	-3.434044
H	-0.053193	10.468615	3.433971	H	0.000047	10.422631	3.434044
H	-0.103786	12.906011	3.351021	H	0.000345	12.860507	3.351086
C	-0.133843	14.330773	-0.746083	C	0.000537	14.285524	-0.746116
C	-0.133843	14.330773	0.746083	C	0.000537	14.285524	0.746116
C	-0.156683	15.433861	-1.588998	C	0.000672	15.388893	-1.589018
C	-0.18522	16.79668	-1.26539	C	0.000878	16.751977	-1.265392
C	-0.197768	17.38967	0	C	0.000982	17.34511	0
C	-0.18522	16.79668	1.26539	C	0.000878	16.751977	1.265392
C	-0.156683	15.433861	1.588998	C	0.000672	15.388893	1.589018
H	-0.151913	15.209787	-2.654338	H	0.000618	15.164784	-2.654364
H	-0.199458	17.480873	-2.109159	H	0.000973	17.436328	-2.109159
H	-0.220535	18.477575	0	H	0.001161	18.433253	0
H	-0.199458	17.480873	2.109159	H	0.000973	17.436328	2.109159
H	-0.151913	15.209787	2.654338	H	0.000618	15.164784	2.654364
C	-0.662069	-14.001018	-0.679346	C	0.000523	-14.064754	-0.677239
C	-0.662069	-14.001018	0.679346	C	0.000523	-14.064754	0.677239
H	-0.832114	-14.822911	-1.36078	H	0.000604	-14.894463	-1.369745
H	-0.832114	-14.822911	1.36078	H	0.000604	-14.894463	1.369745
N	-0.236	-11.839236	0	N	0.00032	-11.842172	0
Zn	0.225067	-9.930199	0	Ni	0.000341	-9.933732	0

P_N-2A-N-2A-N

C	-1.787572	-8.104185	0
C	-3.180245	-7.628453	0
C	-1.823512	-9.502044	0
C	-4.352903	-0.617027	0
C	-4.799815	-1.885148	0
C	-3.600392	-2.754712	0
C	1.333593	-0.35655	0
C	-0.833711	0.390915	0
C	3.48223	-3.319314	0
C	3.055334	-4.594452	0

C	2.263667	-2.491381	0
C	1.575462	-4.543634	0
C	-4.037594	-8.80362	0
C	-2.882254	-0.713376	0
N	-2.444429	-1.976875	0
N	-3.770531	-4.042821	0
N	0.919735	-5.664688	0
N	2.378182	-1.137168	0
N	-2.138716	0.422314	0
C	-0.631102	-7.334724	0
C	-3.596937	-6.328736	0
H	-4.666517	-6.143792	0
H	0.308239	-7.880958	0
C	0.021243	1.582874	0
C	1.394788	1.109826	0
C	-0.458051	2.850778	0
C	0.265516	4.101348	0
C	1.708611	4.256387	0
C	2.751014	3.246468	0
C	2.552423	1.814887	0
H	3.457197	1.211243	0
H	-1.542729	2.930986	0
C	3.914469	10.678134	0
C	2.476136	10.478747	0
C	1.760496	9.21225	0
C	4.926966	9.637235	0
C	2.19208	7.929051	0
C	4.713941	8.198067	0
C	3.585239	7.450435	0
H	0.679822	9.339426	0
H	5.645033	7.634975	0
C	1.330474	6.742881	0
C	2.168116	5.593206	0
C	3.535563	5.98499	0
C	-0.538426	5.257525	0
C	-0.041085	6.56663	0
C	4.508646	5.002371	0
H	-1.614823	5.114638	0
H	-0.730975	7.40501	0
H	5.568257	5.239342	0
C	4.095857	3.664045	0
H	4.856861	2.889543	0

C	3.468295	13.131089	0
C	4.383217	12.043484	0
C	5.773224	12.339665	0
C	1.635491	11.597475	0
C	2.114048	12.913601	0
C	6.277498	10.003665	0
C	6.708309	11.336174	0
H	0.562644	11.431032	0
H	1.415787	13.744791	0
H	7.021734	9.213194	0
H	7.769874	11.563159	0
H	-0.334631	-1.672881	0
C	-2.859419	-5.086781	0
N	1.141565	-3.217141	0
C	-3.166079	-9.954448	0
C	-0.439926	-5.930956	0
C	-1.463488	-4.937185	0
H	-1.107189	-3.914641	0
H	-0.953399	-10.14786	0
C	-3.515145	-11.33167	0
C	-5.445217	-8.769923	0
C	-4.763474	-11.900562	0
C	-6.3385	-9.826547	0
C	-6.088812	-11.212005	0
C	-5.033924	-13.305688	0
C	-7.054334	-12.215501	0
C	-6.406003	-13.484389	0
H	-2.672135	-12.022216	0
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H	-7.39227	-9.55212	0
H	-8.125087	-12.051792	0
H	-4.277486	-14.080174	0
H	-6.916613	-14.440542	0
H	3.617411	-5.517806	0
H	4.486691	-2.919515	0
H	-5.810714	-2.268053	0
H	-4.899301	0.315804	0
H	6.076092	13.38266	0
H	3.869941	14.140161	0
N	0	-0.704898	0