Supporting Information

Strong second order nonlinear optical properties of azulene-based porphyrin derivatives

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Supporting Information list:

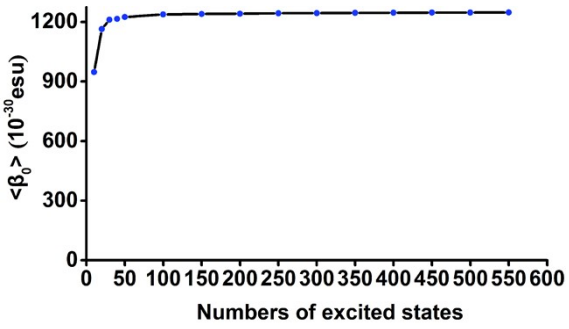

Figure S1 Evolution of the static first hyperpolarizability (<β_0>) with the numbers of excited states in Zn-APs-b.

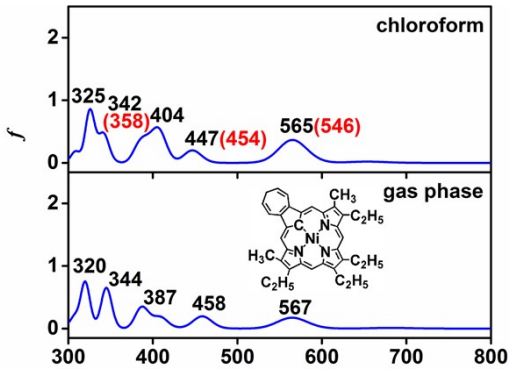

Figure S2 Electronic spectra of 6b[S1] predicted with TD-CAM-B3LYP/6-31++G(d,p) in gas phase and chloroform, respectively. The red numerbs are the measured wavelengths.

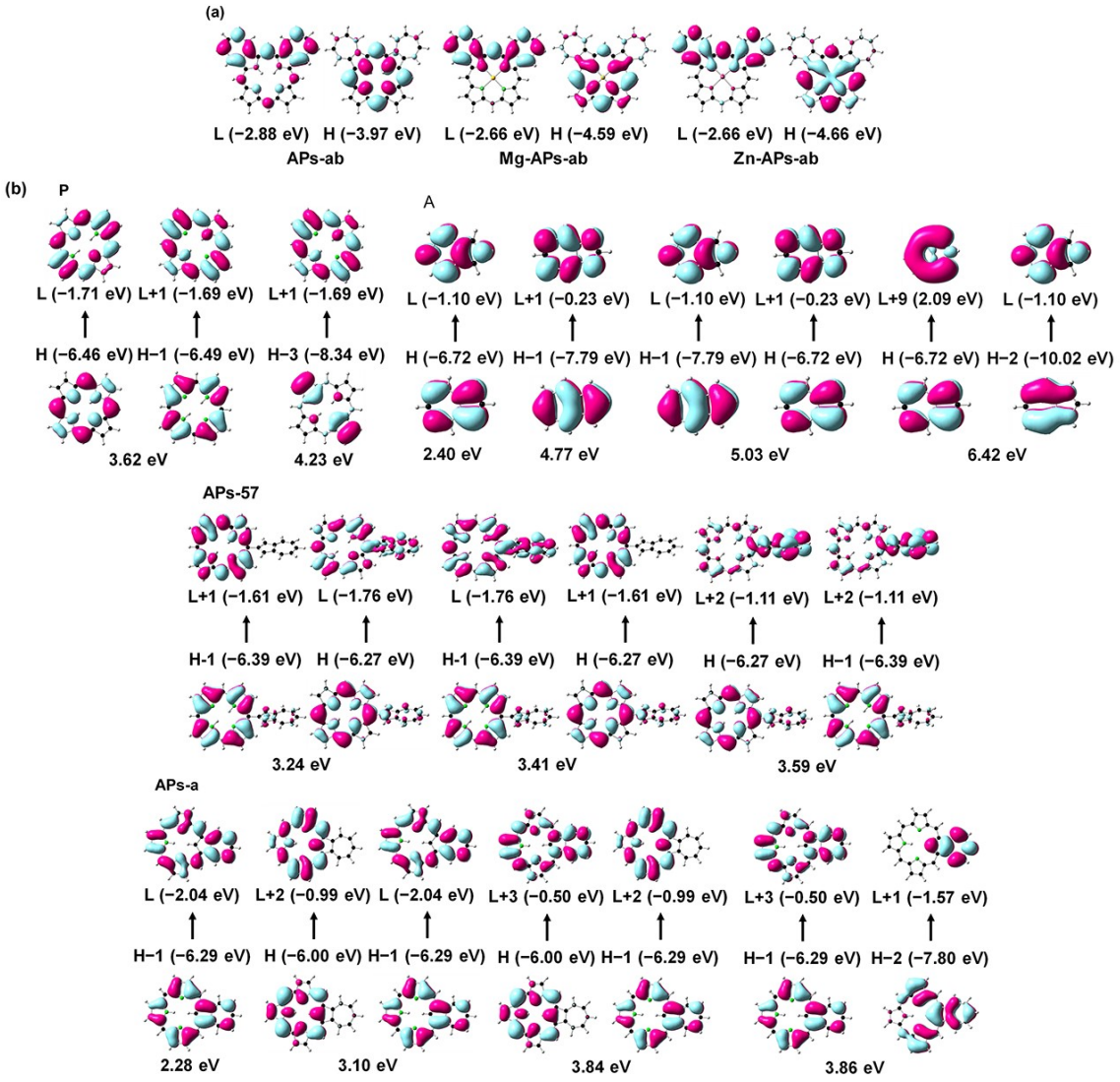

Figure S3 (a) Frontier molecular orbitals of three APs-ab molecules. (b) The transition nature of major electron excitations in porphyrin (P), azulene (A), APs-pen and APs-a.

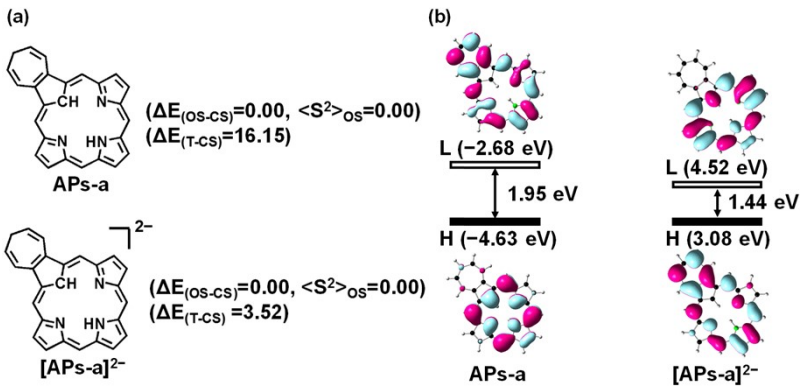

Figure S4 (a) Structures, electronic properties, and (b) frontier molecular orbitals, molecular orbital energy diagrams of APs-a and $[APs\text{-}a]^{2-}$. ΔE_{OS-CS} and ΔE_{T-CS} (in Kcal/mol) are the relative electronic energy differences between the open-shell singlet or triplet (T) and the closed-shell singlet (CS) (CS is taken as the reference).

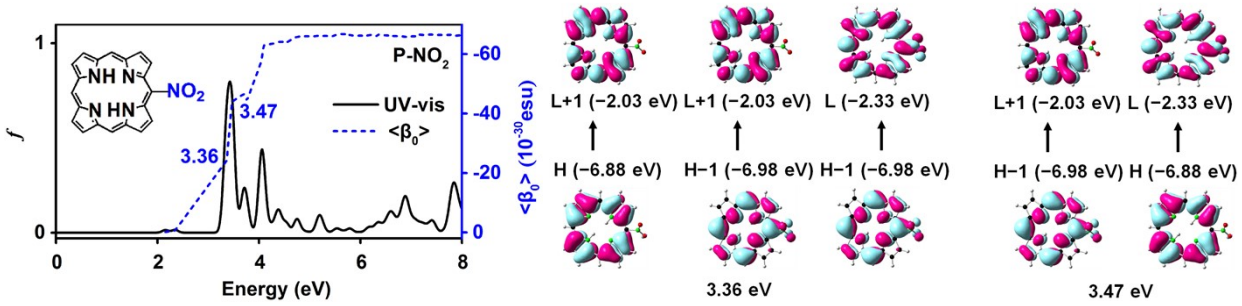

Figure S5 Evolution of the static first hyperpolarizability (<β_0>) with electron excitations in P-NO_2. *f* is the oscillator strength in arbitrary units. The electric spectra are plotted with the Lorentzian fitting function (half-height-width of 400 cm^{-1}). The molecular orbitals are predicted with the CAM-B3LYP/6-31++G(d,p).

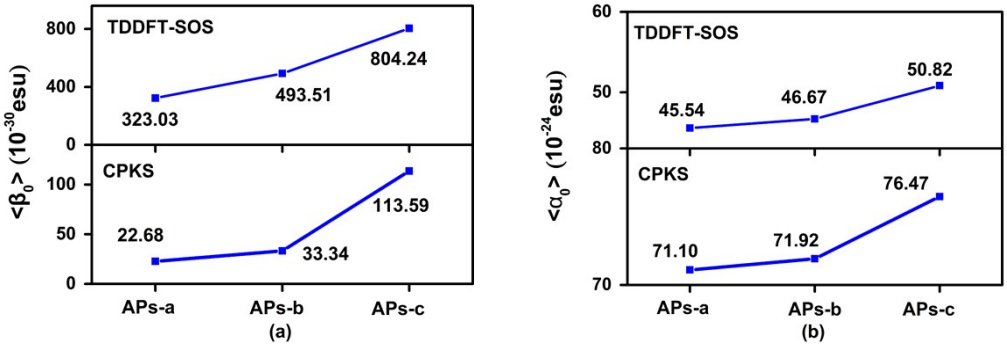

Figure S6 The predicted (a) <β_0> and (b) <α_0> of APs-a, APs-b and APs-c from TD-CAM-B3LYP/6-31++G(d,p)-SOS and coupled perturbed Kohn–Sham (CPKS) model at CAM-B3LYP/6-31++G(d,p) level, respectively.

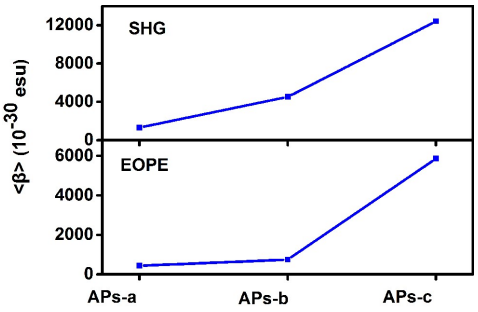

Figure S7 Second harmonic generation (SHG) and electro-optical Pockels effect (EOPE) of APs-a, APs-b and APs-c at 1064 nm predicted by TD-CAM-B3LYP/6-31++G(d,p)-SOS.

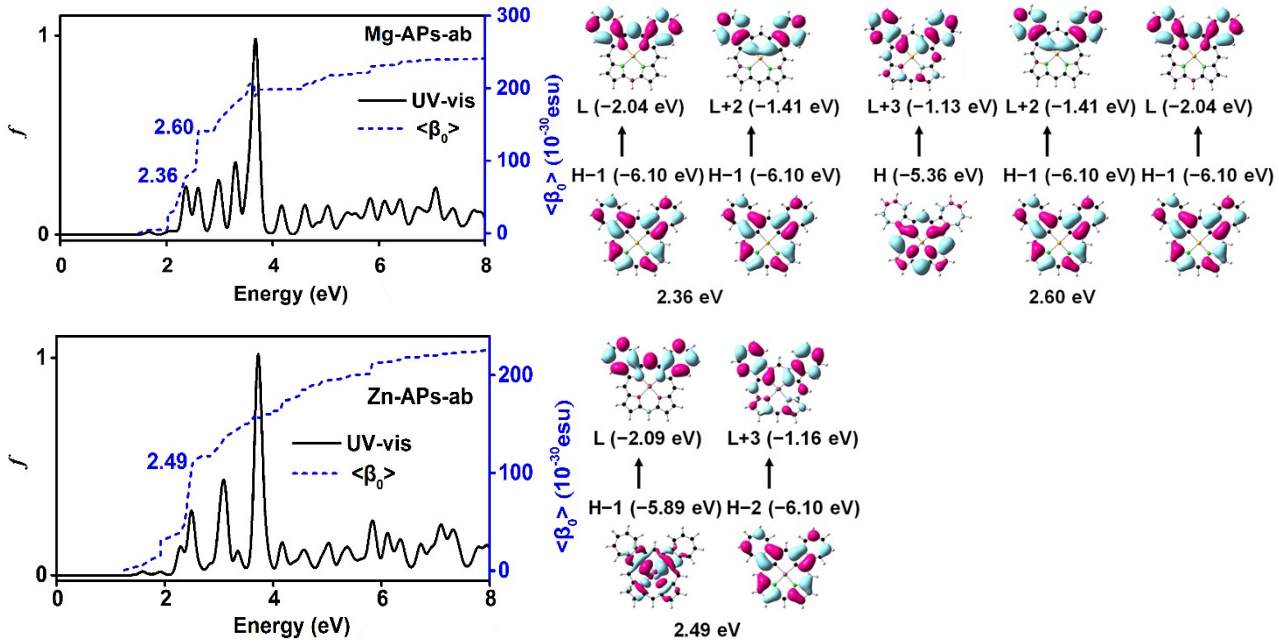

Figure S8 Evolution of the <β_0> with the electron excitations in Mg-APs-ab and Zn-APs-ab.

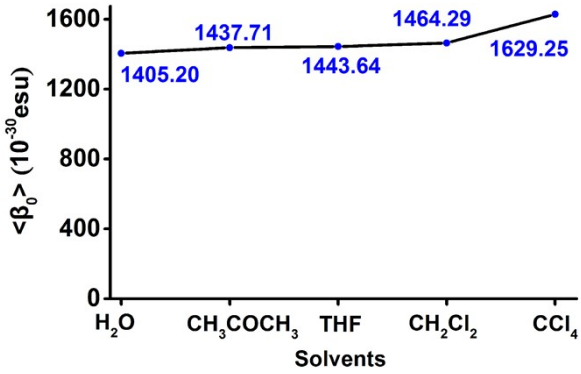

Figure S9 Variation of the <β_0> with different solvents. *e.g.*, water (H_2O), acetone (CH_3COCH_3), TetraHydroFuran (THF), Dichloromethane MethyleneChloride (CH_2Cl_2) and CarbonTetraChloride (CCl_4).

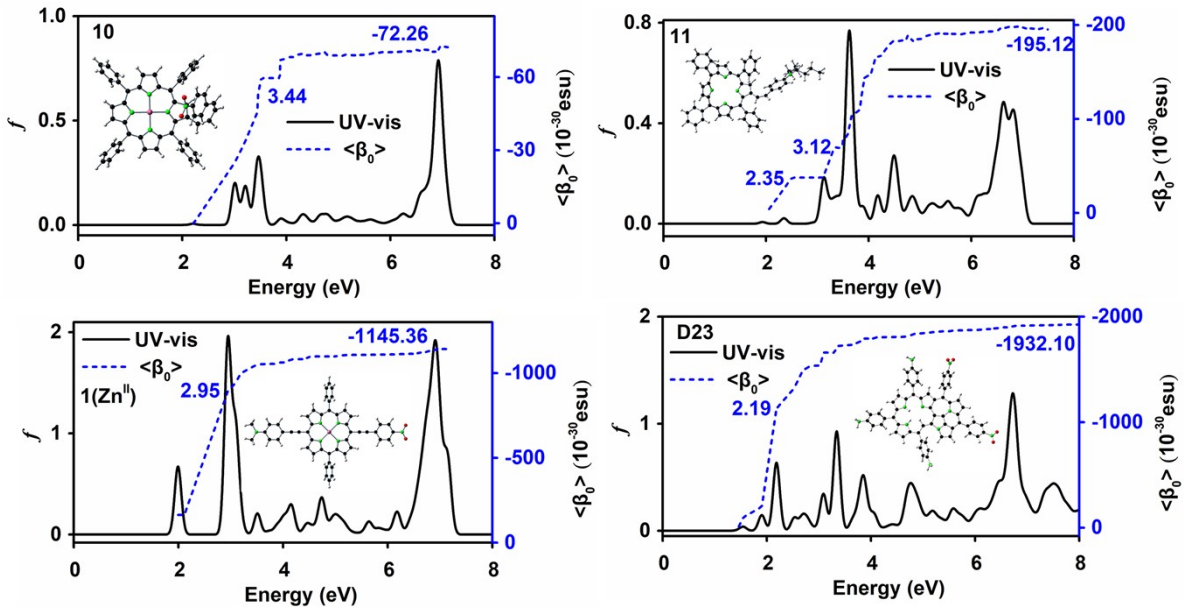

Figure S10 Evolution of the $<\beta_0>$ with the electron excitations in classical donor-acceptor porphyrin-based molecules [*e.g.*, compounds 10 and 11[S2], and 1(Zn^{II})[S3]] and the recently reported similar molecule D23[S4].

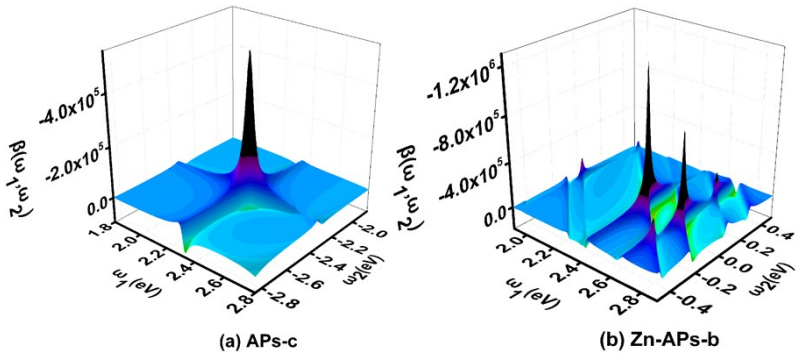

Figure S11 Two-dimensional second order NLO spectra of (a) APs-c and (b) Zn-APs-b scanned with step size of 0.005 eV [(a) ω_1 scanned from 1.80 eV to 2.80 eV and ω_2 scanned from –0.50 eV to 0.50 eV; (b) ω_1 scanned from 1.90 eV to 2.90 eV and ω_2 scanned from –0.50 eV to 0.50 eV].

Table S1 Major electron excitations with transition nature in porphyrin (P), azulene (A) and azulene-defected porphyrins (APs). *ƒ* is the oscillator strength, λ is the wavelength, TNMC to $<\beta_0>$ is the transition nature of electron excitation with major contribution to $<\beta_0>$.

Compounds	ƒ	λ/nm (eV)	Transition	TNMC to $<\beta_0>$	Contributions to $<\beta_0>$ (10^{-30} esu)
P	0.0015	568.93 (2.18)	$S_0 \rightarrow S_1$	H→L+1 (52.78%) H−1→L (47.30%)	0.00
	0.9024	352.29 (3.52)	$S_0 \rightarrow S_3$	H−1→L (47.98%) H→L+1 (47.30%)	0.00
	1.2030	342.35 (3.62)	$S_0 \rightarrow S_4$	H→L (51.08%) H−1→L+1 (50.24%)	0.00
	0.5181	293.14 (4.23)	$S_0 \rightarrow S_6$	H−3→L+1 (78.58%)	0.00
	0.0749	278.03 (4.46)	$S_0 \rightarrow S_8$	H−3→L (90.42%)	0.00
A	0.0081	516.86 (2.40)	$S_0 \rightarrow S_1$	H→L (97.14%)	1.94
	0.0809	260.12 (4.77)	$S_0 \rightarrow S_3$	H−1→L+1 (85.8%)	2.97
	1.1499	246.68 (5.03)	$S_0 \rightarrow S_5$	H−1→L (52.96%) H→L+1 (45.62%)	2.64
	0.3188	193.09 (6.42)	$S_0 \rightarrow S_{15}$	H→L+9 (55.22%) H−2→L (32.88%)	52.86
APs-hep	0.0017	578.09 (2.14)	$S_0 \rightarrow S_1$	H→L+1 (39.26%) H−1→L (33.92%)	0.00
	1.3332	366.13 (3.39)	$S_0 \rightarrow S_4$	H−1→L+1 (28.72%) H→L (27.56%)	−58.83
	0.8864	358.66 (3.46)	$S_0 \rightarrow S_5$	H−1→L (37.02%) H→L+1 (26.38%)	19.23
	0.2565	348.41 (3.56)	$S_0 \rightarrow S_6$	H→L+2 (21.70%) H−2→L+1 (18.40%)	26.66
	0.1851	342.41 (3.62)	$S_0 \rightarrow S_7$	H−2→L (73.44%)	19.46
	0.5917	298.79 (4.15)	$S_0 \rightarrow S_{12}$	H−5→L+1 (37.54%) H−5→L (32.10%)	8.05
	0.5564	247.61 (5.01)	$S_0 \rightarrow S_{28}$	H−3→L+2 (36.68%) H−2→L+3 (35.28%)	3.14
APs-pen	0.0098	584.80 (2.12)	$S_0 \rightarrow S_1$	H→L+1 (35.44%) H−1→L (29.90%)	0.12
	1.2875	383.08 (3.24)	$S_0 \rightarrow S_4$	H−1→L+1 (32.52%) H→L (32.14%)	245.13
	0.7452	363.80 (3.41)	$S_0 \rightarrow S_5$	H−1→L (50.22%) H→L+1 (41.26%)	12.31
	0.7105	344.99 (3.59)	$S_0 \rightarrow S_6$	H→L+2 (35.18%) H−1→L+1 (24.66%)	30.44
	0.5394	302.62 (4.10)	$S_0 \rightarrow S_{12}$	H−5→L (28.24%) H−5→L+1 (23.40%)	−4.88
	0.5099	244.09 (5.08)	$S_0 \rightarrow S_{30}$	H−3→L+2 (34.14%) H−2→L+3 (22.08%)	18.04
Mg-APs-hep	0.0034	547.15 (2.27)	$S_0 \rightarrow S_1$	H→L (48.86%) H−1→L+1 (44.70%)	0.01
	1.6636	363.22 (3.41)	$S_0 \rightarrow S_4$	H−1→L (43.70%) H→L+1 (38.24%)	−164.15
Zn-APs-hep	0.0070	534.36 (2.32)	$S_0 \rightarrow S_1$	H→L (46.70%) H−1→L+1 (34.42%)	0.13
	1.6842	358.57 (3.46)	$S_0 \rightarrow S_4$	H−1→L (47.60%)	−125.11

				H→L+1 (38.38%)	
Mg-APs-pen	0.0492	563.96 (2.20)	$S_0 \rightarrow S_1$	H→L (55.22%) H−1→L+1 (39.38%)	1.79
	1.3199	391.72 (3.17)	$S_0 \rightarrow S_4$	H→L (34.6%) H−1→L+1 (32.44%)	256.25
Zn-APs-pen	0.0063	539.15 (2.30)	$S_0 \rightarrow S_1$	H−1→L (47.32%) H→L+1 (39.74%)	0.06
	1.3006	377.57 (3.28)	$S_0 \rightarrow S_4$	H→L (41.30%) H−1→L+1 (29.50%)	231.62
APs-a	0.0254	683.05 (1.82)	$S_0 \rightarrow S_1$	H→L (90.78%)	7.54
	0.1614	543.39 (2.28)	$S_0 \rightarrow S_3$	H−1→L (64.06%)	36.01
	1.1468	400.15 (3.10)	$S_0 \rightarrow S_5$	H→L+2 (53.94%) H−1→L (28.04%)	189.44
	0.6523	322.79 (3.84)	$S_0 \rightarrow S_9$	H→L+3 (57.14%) H−1→L+2 (26.94%)	−1.25
	0.5585	321.26 (3.86)	$S_0 \rightarrow S_{10}$	H−1→L+3 (38.16%) H−2→L+1 (22.08%)	13.91
APs-b	0.0067	789.52 (1.57)	$S_0 \rightarrow S_1$	H−1→L+1 (40.86%) H→L+1 (38.74%)	11.50
	0.2273	517.66 (2.40)	$S_0 \rightarrow S_4$	H−1→L+1 (29.08%) H−1→L (20.78%)	139.33
	0.3287	454.54 (2.73)	$S_0 \rightarrow S_5$	H→L+2 (34.74%) H−2→L (21.88%) H−1→L (20.96%)	79.42
	0.5310	404.62 (3.06)	$S_0 \rightarrow S_6$	H−2→L (50.50%)	71.51
APs-c	0.0110	1096.80 (1.13)	$S_0 \rightarrow S_1$	H→L+1 (54.88%) H−1→L (43.02%)	17.4
	0.0170	978.48 (1.27)	$S_0 \rightarrow S_2$	H→L (82.80%) H−1→L+1 (15.22%)	86.18
	0.5587	533.78 (2.32)	$S_0 \rightarrow S_4$	H−1→L+1 (62.94%) H→L+2 (22.88%) H→L (13.16%)	257.24
	0.4245	428.76 (2.89)	$S_0 \rightarrow S_6$	H→L+2 (39.66%) H−2→L (36.62%)	158.30
	0.2548	416.49 (2.98)	$S_0 \rightarrow S_8$	H−2→L (48.68%) H→L+2 (24.88%)	84.26
Mg-APs-a	0.0178	761.28 (1.63)	$S_0 \rightarrow S_1$	H→L (89.92%)	6.34
	0.1617	469.75 (2.64)	$S_0 \rightarrow S_4$	H→L+1 (59.06%) H→L+2 (24.24%)	89.43
	1.2101	403.41 (3.07)	$S_0 \rightarrow S_7$	H→L+2 (52.20%) H−1→L (26.22%)	161.48
Zn-APs-a	0.0183	705.94 (1.76)	$S_0 \rightarrow S_1$	H→L (88.98%)	5.56
	0.1407	557.82 (2.22)	$S_0 \rightarrow S_3$	H−1→L (64.86%) H→L+1 (21.88%)	47.89
	0.1377	474.22 (2.61)	$S_0 \rightarrow S_5$	H→L+1 (69.48%)	83.27
	0.9603	399.81 (3.10)	$S_0 \rightarrow S_8$	H→L+2 (58.22%) H−1→L (21.30%)	124.96

Mg-APs-b	0.0230	896.50 (1.38)	$S_0 \rightarrow S_1$	H→L (64.16%)	66.60
	0.1297	516.13 (2.40)	$S_0 \rightarrow S_4$	H→L+2 (48.04%) H−1→L+1 (27.90%)	60.85
	0.4939	345.98 (2.64)	$S_0 \rightarrow S_5$	H−1→L+1 (42.64%) H→L+2 (23.60%)	127.83
Zn-APs-b	0.0120	830.63 (1.49)	$S_0 \rightarrow S_1$	H→L (50.08%) H−1→L+1 (22.70%) H−1→L (20.08%)	115.00
	0.0530	682.73 (1.82)	$S_0 \rightarrow S_2$	H→L+1 (87.52%)	126.17
	0.3048	511.39 (2.42)	$S_0 \rightarrow S_5$	H−1→L+1 (46.32%) H−1→L+2 (25.86%)	332.28
	0.2320	465.98 (2.66)	$S_0 \rightarrow S_6$	H−1→L+2 (34.82%) H−2→L+1 (25.10%)	209.57
Mg-APs-c	0.0332	1094.58 (1.13)	$S_0 \rightarrow S_1$	H→L+1 (86.02%)	56.10
	0.3193	563.49 (2.20)	$S_0 \rightarrow S_4$	H−1→L+1 (57.48%) H→L+2 (31.52%)	142.47
	0.8645	438.44 (2.83)	$S_0 \rightarrow S_7$	H→L+2 (55.96%) H−1→L+1 (30.54%)	188.08
Zn-APs-c	0.0239	977.32 (1.27)	$S_0 \rightarrow S_1$	H→L+1 (71.64%) H−1→L (24.16%)	28.10
	0.3943	543.77 (2.28)	$S_0 \rightarrow S_5$	H−1→L+1 (60.88%) H→L+2 (25.76%)	172.24
	0.7253	428.32 (2.89)	$S_0 \rightarrow S_8$	H→L+2 (58.76%) H−1→L+1 (24.56%)	155.47
Mg-APs-ab	0.0215	742.50 (1.67)	$S_0 \rightarrow S_1$	H→L+1 (75.38%)	4.85
	0.3652	524.32 (2.36)	$S_0 \rightarrow S_6$	H−1→L (54.12%) H−1→L+2 (27.70%)	46.89
	0.3297	477.26 (2.60)	$S_0 \rightarrow S_8$	H→L+3 (28.44%) H−1→L+2 (26.20%) H−1→L (21.58%)	54.37
Zn-APs-ab	0.0002	991.51 (1.25)	$S_0 \rightarrow S_1$	H→L (80.98%)	0.69
	0.4179	497.42 (2.49)	$S_0 \rightarrow S_9$	H−1→L (39.74%) H−2→L+3 (19.28%)	57.11

Table S2 Predicted major β_{ijk} [i, j, k∈(x, y, z)] (×10^{-30} esu) of APs-hep/pen and APs-a/b/c, and the related molecular properties with important contributions to the β_{ijk} according to the SOS model. [n=0 is the ground state; n>0 is the mth excited state]. $\triangle\mu_{0n}$: the dipole moment difference between the ground state and the *n*th excited state. μ_{0n}: the transition moment between the ground state and the *n*th excited state. E: the transition energy.

compounds	Transition	$\triangle\mu_{0n}$/Debye	μ_{0n}/Debye	E_t/(eV)	$\beta_{ijk}/10^{-30}$ esu
APs-hep	$S_0 \rightarrow S_4$	−2.82	−9.68	3.28	55.68 (β_{XXX})
	$S_0 \rightarrow S_5$	2.25	−5.38	3.46	−12.77 (β_{XXX})
	$S_0 \rightarrow S_6$	7.87	−4.27	3.56	−26.50 (β_{XXX})
	$S_0 \rightarrow S_7$	−0.25 23.31	−0.37 3.70	3.62	−19.05 (β_{XYY})
APs-pen	$S_0 \rightarrow S_4$	−10.45	−10.25	3.24	245.17 (β_{XXX})
APs-a	$S_0 \rightarrow S_5$	7.96	9.89	3.10	−189.45 (β_{ZZZ})
APs-b	$S_0 \rightarrow S_4$	−13.97	−5.01	2.40	142.64 (β_{XXX})
	$S_0 \rightarrow S_5$	−7.84	5.65	2.73	78.53 (β_{XXX})
	$S_0 \rightarrow S_6$	−5.89	−6.76	3.06	67.00 (β_{XXX})
APs-c	$S_0 \rightarrow S_2$	−16.71	1.88	1.27	86.17 (β_{YYY})
	$S_0 \rightarrow S_4$	−9.34	7.97	2.32	257.25 (β_{YYY})
	$S_0 \rightarrow S_6$	−14.59	−6.23	2.89	158.30 (β_{YYY})
	$S_0 \rightarrow S_8$	−14.11	4.76	2.98	84.27 (β_{YYY})
Mg-APs-b	$S_0 \rightarrow S_1$	12.72	2.10	1.38	−68.29 (β_{YYY})
	$S_0 \rightarrow S_4$	10.86	−3.78	2.40	−62.92 (β_{YYY})
	$S_0 \rightarrow S_5$	7.64	−7.03	2.64	−126.86 (β_{YYY})
	$S_0 \rightarrow S_1$	16.80	−2.56	1.49	−115.26 (β_{YYY})
Zn-APs-b	$S_0 \rightarrow S_2$	13.72 −1.27 13.82	−4.78 −2.31 −2.31	1.82	−69.74 (β_{YYX}) −51.72 (β_{YYY})
	$S_0 \rightarrow S_5$	15.73	7.30	2.42	−331.57 (β_{YYY})
	$S_0 \rightarrow S_6$	9.39	−8.23	2.66	−207.64 (β_{YYY})

(1) APs-hep:

β_{XXX} ($S_0 \rightarrow S_4$)

$$\beta_{XXX} = 6\frac{r_{04}^X\left(r_{44}^X - r_{00}^X\right)r_{40}^X}{E_4^2} = 6 \times \frac{-9.68 \times [-4.39 - (-1.47)] \times 9.68}{3.39^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 55.66 \times 10^{-30}\ esu$$

β_{XXX} ($S_0 \rightarrow S_5$)

$$\beta_{XXX} = 6\frac{r_{05}^X\left(r_{55}^X - r_{00}^X\right)r_{50}^X}{E_5^2} = 6 \times \frac{-5.38 \times [0.78 - (-1.47)] \times 5.38}{3.46^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -12.72 \times 10^{-30}\ esu$$

β_{XXX} ($S_0 \rightarrow S_6$)

$$\beta_{XXX} = 6\frac{r_{06}^X\left(r_{66}^X - r_{00}^X\right)r_{60}^X}{E_6^2} = 6 \times \frac{-4.27 \times [6.40 - (-1.47)] \times 4.27}{3.56^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -26.47 \times 10^{-30}\ esu$$

β_{XYY} ($S_0 \rightarrow S_7$)

$$\beta_{XYY} = 4\frac{r_{07}^{X}\left(r_{77}^{Y} - r_{00}^{Y}\right)r_{70}^{X}}{E_7^2} + 2\frac{r_{07}^{Y}\left(r_{77}^{X} - r_{00}^{X}\right)r_{70}^{Y}}{E_7^2} = 4 \times \frac{-0.37 \times [-0.30 - (-0.05)] \times 0.37}{3.62^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2}$$

$$+ 2 \times \frac{3.70 \times [21.84 - (-1.47)] \times (-3.70)}{3.62^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -18.97 \times 10^{-30}\ esu$$

(2) APs-pen:

β_{XXX} ($S_0 \rightarrow S_4$)

$$\beta_{XXX} = 6\frac{r_{04}^{X}\left(r_{44}^{X} - r_{00}^{X}\right)r_{40}^{X}}{E_4^2} = 6 \times \frac{-10.25 \times [-8.47 - 1.98] \times 10.25}{3.24^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 244.51 \times 10^{-30}\ esu$$

(3) APs-a:

β_{ZZZ} ($S_0 \rightarrow S_5$)

$$\beta_{ZZZ} = 6\frac{r_{05}^{Z}\left(r_{55}^{Z} - r_{00}^{Z}\right)r_{50}^{Z}}{E_5^2} = 6 \times \frac{9.89 \times [3.15 - (-4.81)] \times (-9.89)}{(3.10)^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -190.13 \times 10^{-30}\ esu$$

(4) APs-b:

β_{XXX} ($S_0 \rightarrow S_4$)

$$\beta_{XXX} = 6\frac{r_{04}^{X}\left(r_{44}^{X} - r_{00}^{X}\right)r_{40}^{X}}{E_4^2} = 6 \times \frac{-5.01 \times (-6.28 - 7.69) \times 5.01}{2.40^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 142.32 \times 10^{-30}\ esu$$

β_{XXX} ($S_0 \rightarrow S_5$)

$$\beta_{XXX} = 6\frac{r_{05}^{X}\left(r_{55}^{X} - r_{00}^{X}\right)r_{50}^{X}}{E_5^2} = 6 \times \frac{5.65 \times (-0.15 - 7.69) \times (-5.65)}{2.73^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 78.51 \times 10^{-30}\ esu$$

β_{XXX} ($S_0 \rightarrow S_6$)

$$\beta_{XXX} = 6\frac{r_{06}^{X}\left(r_{66}^{X} - r_{00}^{X}\right)r_{60}^{X}}{E_6^2} = 6 \times \frac{-6.76 \times (1.80 - 7.69) \times 6.76}{3.06^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 67.20 \times 10^{-30}\ esu$$

(5) APs-c:

β_{YYY} ($S_0 \rightarrow S_2$)

$$\beta_{YYY} = 6\frac{r_{02}^{Y}\left(r_{22}^{Y} - r_{00}^{Y}\right)r_{20}^{Y}}{E_2^2} = 6 \times \frac{1.88 \times (-6.70 - 10.01) \times -1.88}{1.27^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 85.61 \times 10^{-30}\ esu$$

β_{YYY} ($S_0 \rightarrow S_4$)

$$\beta_{YYY} = 6\frac{r_{04}^{Y}\left(r_{44}^{Y} - r_{00}^{Y}\right)r_{40}^{Y}}{E_4^2} = 6 \times \frac{7.97 \times (0.67 - 10.01) \times -7.97}{2.32^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 257.70 \times 10^{-30}\ esu$$

β_{YYY} ($S_0 \rightarrow S_6$)

$$\beta_{YYY} = 6\frac{r_{06}^{Y}\left(r_{66}^{Y} - r_{00}^{Y}\right)r_{60}^{Y}}{E_6^2} = 6 \times \frac{-6.23 \times (-4.58 - 10.01) \times 6.23}{2.89^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 157.64 \times 10^{-30}\ esu$$

β_{YYY} ($S_0 \rightarrow S_8$)

$$\beta_{YYY} = 6\frac{r_{08}^{Y}\left(r_{88}^{Y} - r_{00}^{Y}\right)r_{80}^{Y}}{E_8^2} = 6 \times \frac{4.76 \times (-4.10 - 10.01) \times (-4.76)}{2.98^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = 84.17 \times 10^{-30}\ esu$$

(6) Mg-APs-b:

$\beta_{YYY}(S_0 \rightarrow S_1)$

$$\beta_{YYY} = 6\frac{r_{01}^{Y}\left(r_{11}^{Y} - r_{00}^{Y}\right)r_{10}^{Y}}{E_1^2} = 6 \times \frac{2.10 \times [5.37 - (-7.35)] \times (-2.10)}{1.38^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -68.86 \times 10^{-30}\ esu$$

$\beta_{YYY}(S_0 \rightarrow S_4)$

$$\beta_{YYY} = 6\frac{r_{04}^{Y}\left(r_{44}^{Y} - r_{00}^{Y}\right)r_{40}^{Y}}{E_4^2} = 6 \times \frac{-3.78 \times [3.51 - (-7.35)] \times 3.78}{2.40^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -62.98 \times 10^{-30}\ esu$$

$\beta_{YYY}(S_0 \rightarrow S_5)$

$$\beta_{YYY} = 6\frac{r_{05}^{Y}\left(r_{55}^{Y} - r_{00}^{Y}\right)r_{50}^{Y}}{E_5^2} = 6 \times \frac{-7.03 \times [0.29 - (-7.35)] \times 7.03}{2.64^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -126.62 \times 10^{-30}\ esu$$

(7) Zn-APs-b:

$\beta_{YYY}(S_0 \rightarrow S_1)$

$$\beta_{YYY} = 6\frac{r_{01}^{Y}\left(r_{11}^{Y} - r_{00}^{Y}\right)r_{10}^{Y}}{E_1^2} = 6 \times \frac{-2.56 \times [9.13 - (-7.76)] \times 2.56}{1.49^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -116.56 \times 10^{-30}\ esu$$

$B_{YYX}(S_0 \rightarrow S_2)$

$$\beta_{YYX} = 4\frac{r_{02}^{Y}\left(r_{22}^{Y} - r_{00}^{Y}\right)r_{20}^{X}}{E_2^2} + 2\frac{r_{02}^{Y}\left(r_{22}^{X} - r_{00}^{X}\right)r_{20}^{Y}}{E_2^2} = 4 \times \frac{-2.31 \times [6.06 - (-7.67)] \times 4.78}{1.82^2} \times \frac{-2.31 \times [-2.78 - (-1.51)] \times 2.31}{1.82^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -69.74 \times 10^{-30}\ esu$$

$\beta_{YYY}(S_0 \rightarrow S_2)$

$$\beta_{YYY} = 6\frac{r_{02}^{Y}\left(r_{22}^{Y} - r_{00}^{Y}\right)r_{20}^{Y}}{E_2^2} = 6 \times \frac{-2.31 \times [6.06 - (-7.76)] \times 2.31}{1.82^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -52.05 \times 10^{-30}\ esu$$

$\beta_{YYY}(S_0 \rightarrow S_5)$

$$\beta_{YYY} = 6\frac{r_{05}^{Y}\left(r_{55}^{Y} - r_{00}^{Y}\right)r_{50}^{Y}}{E_5^2} = 6 \times \frac{7.30 \times [7.97 - (-7.76)] \times (-7.30)}{2.42^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -334.63 \times 10^{-30}\ esu$$

$\beta_{YYY}(S_0 \rightarrow S_6)$

$$\beta_{YYY} = 6\frac{r_{06}^{Y}\left(r_{66}^{Y} - r_{00}^{Y}\right)r_{60}^{Y}}{E_6^2} = 6 \times \frac{-8.23 \times [1.63 - (-7.76)] \times 8.23}{2.66^2} \times \frac{\left(10^{-18}\right)^3}{\left(1.602 \times 10^{-12}\right)^2} = -210.15 \times 10^{-30}\ esu$$

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

APs-hep

C	0.28052500	3.48952200	0.13199600
C	1.28123500	2.55349600	0.10011700
C	-0.97622000	2.80275700	0.08207300
C	-5.72993600	2.52822300	0.10084300
C	-4.75622600	3.47175100	0.12601600
C	-3.48750900	2.74836100	0.09208100
C	-4.73083300	-3.48434200	-0.11056000
C	-5.72363300	-2.53817700	-0.06995600
C	-3.46695700	-2.80453900	-0.08832400
C	-5.10044000	-1.24754200	-0.02279500
C	0.30330100	-3.46483700	-0.17909500
C	1.28895200	-2.53532100	-0.14909400
C	-0.95451300	-2.73227200	-0.10929700
C	0.62176500	-1.23685000	-0.05267100
C	0.67160800	1.25490400	0.01938000
C	1.30432000	0.00013100	-0.01577500
C	-2.19729000	-3.37620300	-0.12442600
C	-2.24244600	3.38507800	0.10983400
C	-5.04482700	1.24011600	0.05322600
C	-5.70555400	0.00700800	0.01996000
H	-2.17625900	-4.46064300	-0.17571200
H	-6.79087400	0.01999400	0.02605500
H	-2.25171900	4.46992200	0.15631200
N	-3.69050300	1.40277900	0.04756800
N	-0.68742600	1.46204000	0.01205800
N	-0.73594100	-1.38734600	-0.03627600
N	-3.74524800	-1.46336300	-0.03313700
H	-4.86303200	4.54836700	0.16329800
H	-6.80331900	2.66789100	0.11380500
H	-6.79257100	-2.70091500	-0.07419300
H	-4.84350500	-4.55891800	-0.15353100
H	0.39874200	-4.54082400	-0.25002000
H	2.35613200	-2.69538100	-0.19542600
H	2.34574500	2.72860500	0.13248400
H	0.38509400	4.56401600	0.19349500
C	2.80923200	-0.00472800	-0.00815800
C	3.42464500	-0.49766100	1.15716600
C	3.44230500	0.48757600	-1.16406600
C	4.78151400	-0.62687200	1.46370200
H	2.73960400	-0.81787200	1.93690400
C	4.80378700	0.61275400	-1.45245000
H	2.76928500	0.80887100	-1.95384800
C	5.89976200	-0.30117800	0.70215400
H	4.99568300	-1.03950400	2.44907200
C	5.91025500	0.28480600	-0.67530800
H	5.03248200	1.02425700	-2.43505000
C	7.24323300	-0.45910200	1.08190800
C	7.25953700	0.44020000	-1.03578600
H	7.58211800	-0.86083900	2.02860700
C	8.05746200	-0.01015800	0.02881900
H	7.61272500	0.84098500	-1.97765600
H	9.14176000	-0.01126100	0.03667400
H	-1.36517200	0.70705200	-0.01822300
H	-3.06140500	-0.71397900	-0.00361900

APs-pen

C	0.24050000	-3.45894300	-0.25718800
C	1.23309400	-2.53697000	-0.22362200
C	-1.00976900	-2.72042200	-0.14825500
C	-5.78416400	-2.53769600	-0.08620000
C	-4.78616500	-3.47816100	-0.13819000
C	-3.52579800	-2.79233800	-0.11048400
C	-4.80997800	3.46839400	0.15705200
C	-5.78908400	2.53041700	0.12352900
C	-3.54520100	2.73854000	0.11631200
C	-5.11103800	1.23937500	0.06464400
C	0.22021600	3.48157300	0.20310000
C	1.22820600	2.55351400	0.16592100
C	-1.02991500	2.78829400	0.11564600
C	0.63068400	1.25382900	0.03713200
C	0.57875100	-1.23670300	-0.07827700
C	1.27272900	-0.00100800	-0.01973800
C	-2.29738100	3.36854600	0.14570100
C	-2.25458700	-3.35962000	-0.16234000
C	-5.16737900	-1.24489800	-0.02654900
C	-5.77502700	0.00819300	0.02477800
H	-2.30418600	4.45262800	0.21003900
H	-6.86030100	0.02150300	0.03195300
H	-2.23411700	-4.44319500	-0.23167400
N	-3.81090500	-1.45360100	-0.03904900
N	-0.77892500	-1.37823400	-0.04685000
N	-0.72942600	1.45145500	0.01543000
N	-3.75583900	1.39506400	0.05880600
H	-4.89316700	-4.55279000	-0.19344600
H	-6.85225500	-2.70595800	-0.09192200
H	-6.86169100	2.67597200	0.13858800
H	-4.91096600	4.54522700	0.20428500
H	0.31552700	4.55453000	0.29824000
H	2.28972700	2.73315900	0.23282500
H	2.29704000	-2.70069200	-0.30334100
H	0.32664400	-4.53318100	-0.36013500
C	7.97947300	-0.00896200	0.03275900
C	7.37696000	-0.79439200	1.02053200
C	7.39524400	0.77666200	-0.96552200
C	6.01732400	-1.00353100	1.26215000
H	8.05896500	-1.31621100	1.68731300
C	6.04006100	0.98690700	-1.23113500
H	8.08929000	1.29745000	-1.62059100
C	4.91608000	-0.47973600	0.58667100
H	5.78067100	-1.67054000	2.09024200
C	4.92685900	0.46511500	-0.57445700
H	5.81885300	1.65321300	-2.06410700
C	3.57002900	-0.73568100	0.88199200
C	3.58597400	0.72289100	-0.89229800
H	3.21183700	-1.36155200	1.68915400
C	2.75226100	-0.00637900	-0.01241200
H	3.24351200	1.34580900	-1.70873700
H	9.06779400	-0.00947000	0.04234100
H	-3.13509100	-0.69685200	-0.00058400
H	-1.39616900	0.68729300	-0.03631100

Mg-APs-hep

C	0.00000000	3.49675300	-0.40388400

Zn-APs-hep

C	-0.07629800	3.48392300	-0.54527600

C	-0.01142300	2.54520700	-1.38074400
C	0.02636100	2.80359400	0.86180200
C	0.02797200	2.53075200	5.61430200
C	0.03740200	3.49382100	4.64720900
C	0.03078300	2.81020800	3.37266000
C	-0.03740200	-3.49382100	4.64720900
C	-0.02797200	-2.53075200	5.61430200
C	-0.03078300	-2.81020800	3.37266000
C	-0.01470000	-1.25260600	4.93707900
C	0.00000000	-3.49675300	-0.40388400
C	0.01142300	-2.54520700	-1.38074400
C	-0.02636100	-2.80359400	0.86180200
C	-0.01705800	-1.25550500	-0.71888000
C	0.01705800	1.25550500	-0.71888000
C	0.00000000	0.00000000	-1.36726100
C	-0.03244100	-3.42570300	2.11633100
C	0.03244100	3.42570300	2.11633100
C	0.01470000	1.25260600	4.93707900
C	0.00000000	0.00000000	5.56167100
H	-0.03422200	-4.51179200	2.11133400
H	0.00000000	0.00000000	6.64768500
H	0.03422200	4.51179200	2.11133400
N	0.01740400	1.45410100	3.57941600
N	0.03500400	1.44705800	0.64249700
N	-0.03500400	-1.44705800	0.64249700
N	-0.01740400	-1.45410100	3.57941600
H	0.04795100	4.56815500	4.77714700
H	0.02914800	2.66543200	6.68812300
H	-0.02914800	-2.66543200	6.68812300
H	-0.04795100	-4.56815500	4.77714700
H	0.01648700	-4.57206000	-0.52476100
H	0.04183700	-2.69836900	-2.44934400
H	-0.04183700	2.69836900	-2.44934400
H	-0.01648700	4.57206000	-0.52476100
C	0.00000000	0.00000000	-2.87404400
C	1.19230100	0.40907900	-3.49852700
C	-1.19230100	-0.40907900	-3.49852700
C	1.49855500	0.51396000	-4.85772300
H	1.99688100	0.67648900	-2.81935100
C	-1.49855500	-0.51396000	-4.85772300
H	-1.99688100	-0.67648900	-2.81935100
C	0.70805100	0.24230300	-5.97018200
H	2.50933400	0.85518500	-5.07920800
C	-0.70805100	-0.24230300	-5.97018200
H	-2.50933400	-0.85518500	-5.07920800
C	1.08869600	0.37152200	-7.31667600
C	-1.08869600	-0.37152200	-7.31667600
H	2.05960500	0.70344400	-7.66262800
C	0.00000000	0.00000000	-8.12279100
H	-2.05960500	-0.70344400	-7.66262800
H	0.00000000	0.00000000	-9.20713000
Mg	0.00000000	0.00000000	2.11261500

Mg-APs-pen

C	2.11665300	1.38638200	5.66564000
C	2.92316100	1.91155800	4.69770200
C	1.04660300	0.68674700	4.98937900
C	-2.92316100	-1.91155800	4.69770200
C	-2.11665300	-1.38638200	5.66564000
C	-1.04660300	-0.68674700	4.98937900
C	-2.17488500	-1.33017200	-1.32861900
C	-2.96670700	-1.85371500	-0.34943300
C	-1.05399700	-0.68558300	-0.67287400
C	-2.35178400	-1.52367400	0.91253800

C	-0.06357000	2.53281000	-1.51996400
C	-0.03950000	2.79112500	0.71879100
C	-0.03969800	2.51958500	5.45004300
C	-0.05429100	3.48177800	4.48478600
C	-0.04214200	2.79749700	3.21222500
C	0.05429100	-3.48177800	4.48478600
C	0.03969800	-2.51958500	5.45004300
C	0.04214200	-2.79749700	3.21222500
C	0.01940000	-1.24420900	4.77076300
C	0.07629800	-3.48392300	-0.54527600
C	0.06357000	-2.53281000	-1.51996400
C	0.03950000	-2.79112500	0.71879100
C	0.01040400	-1.24685600	-0.85548000
C	-0.01040400	1.24685600	-0.85548000
C	0.00000000	0.00000000	-1.50824100
C	0.05194000	-3.41880500	1.96468400
C	-0.05194000	3.41880500	1.96468400
C	-0.01940000	1.24420900	4.77076300
C	0.00000000	0.00000000	5.40044500
H	0.07592700	-4.50430000	1.95986800
H	0.00000000	0.00000000	6.48613700
H	-0.07592700	4.50430000	1.95986800
N	-0.02163700	1.43939800	3.41122500
N	0.00000000	1.43323700	0.50804900
N	0.00000000	-1.43323700	0.50804900
N	0.02163700	-1.43939800	3.41122500
H	-0.07109000	4.55636600	4.61102100
H	-0.04256400	2.64938500	6.52435500
H	0.04256400	-2.64938500	6.52435500
H	0.07109000	-4.55636600	4.61102100
H	0.11513900	-4.55888600	-0.66301700
H	0.09276100	-2.68040200	-2.58928100
H	-0.09276100	2.68040200	-2.58928100
H	-0.11513900	4.55888600	-0.66301700
Zn	0.00000000	0.00000000	1.96126800
C	0.00000000	0.00000000	-3.01517100
C	1.19361500	0.40591300	-3.63839700
C	-1.19361500	-0.40591300	-3.63839700
C	1.50030500	0.51004900	-4.99767200
H	1.99826900	0.67192700	-2.95871200
C	-1.50030500	-0.51004900	-4.99767200
H	-1.99826900	-0.67192700	-2.95871200
C	0.70880600	0.24046200	-6.10983500
H	2.51180300	0.84900400	-5.21924300
C	-0.70880600	-0.24046200	-6.10983500
H	-2.51180300	-0.84900400	-5.21924300
C	1.08966100	0.36869500	-7.45635400
C	-1.08966100	-0.36869500	-7.45635400
H	2.06142600	0.69805500	-7.80232400
C	0.00000000	0.00000000	-8.26243100
H	-2.06142600	-0.69805500	-7.80232400
H	0.00000000	0.00000000	-9.34676500

Zn-APs-pen

C	-2.14306300	1.32477600	5.49789500
C	-2.96170700	1.83013400	4.53215400
C	-1.05798100	0.65414800	4.81917200
C	2.96170700	-1.83013400	4.53215400
C	2.14306300	-1.32477600	5.49789500
C	1.05798100	-0.65414800	4.81917200
C	2.18801600	-1.28473800	-1.47116400
C	2.99221700	-1.78815000	-0.49424000
C	1.05961300	-0.65974600	-0.81246200
C	2.37413900	-1.46433600	0.76631700

C	2.17488500	1.33017200	-1.32861900
C	2.96670700	1.85371500	-0.34943300
C	1.05399700	0.68558300	-0.67287400
C	2.35178400	1.52367400	0.91253800
C	2.34997400	1.53668700	3.42414100
C	2.86981400	1.86472900	2.16765200
C	0.00000000	0.00000000	-1.32901300
C	0.00000000	0.00000000	5.61498100
C	-2.34997400	-1.53668700	3.42414100
C	-2.86981400	-1.86472900	2.16765200
H	-3.78760800	-2.44564200	2.16284400
H	0.00000000	0.00000000	6.70100300
H	3.78760800	2.44564200	2.16284400
N	-1.21385800	-0.79619800	3.63144900
N	1.21385800	0.79619800	3.63144900
N	1.19599700	0.81330300	0.68832900
N	-1.19599700	-0.81330300	0.68832900
H	-2.22989000	-1.46045200	6.73942700
H	-3.82335800	-2.49838700	4.82646900
H	-3.89293400	-2.40112700	-0.46663900
H	-2.33637000	-1.36391900	-2.39524400
H	2.33637000	1.36391900	-2.39524400
H	3.89293400	2.40112700	-0.46663900
H	3.82335800	2.49838700	4.82646900
H	2.22989000	1.46045200	6.73942700
C	0.00000000	0.00000000	-2.81132700
C	0.02272800	1.14790400	-3.63674800
C	-0.02272800	-1.14790400	-3.63674800
H	0.01379400	2.17181000	-3.28542000
H	-0.01379400	-2.17181000	-3.28542000
C	0.01070200	0.74869100	-4.98060300
C	-0.01070200	-0.74869100	-4.98060300
C	-0.00759100	-1.59520900	-6.08780200
C	0.00000000	-1.26611400	-7.44536600
C	0.00000000	0.00000000	-8.03876300
C	0.00000000	1.26611400	-7.44536600
C	0.00759100	1.59520900	-6.08780200
H	0.01551800	2.66025100	-5.85892700
H	-0.00122300	2.10790000	-8.13345400
H	0.00000000	0.00000000	-9.12715300
H	0.00122300	-2.10790000	-8.13345400
H	-0.01551800	-2.66025100	-5.85892700
Mg	0.00000000	0.00000000	2.15738400

C	-2.18801600	1.28473800	-1.47116400
C	-2.99221700	1.78815000	-0.49424000
C	-1.05961300	0.65974600	-0.81246200
C	-2.37413900	1.46433600	0.76631700
C	-2.37839600	1.47087900	3.26031300
C	-2.90775400	1.79347100	2.01234600
C	0.00000000	0.00000000	-1.47302300
C	0.00000000	0.00000000	5.44937100
C	2.37839600	-1.47087900	3.26031300
C	2.90775400	-1.79347100	2.01234600
H	3.83795400	-2.35363000	2.00685300
H	0.00000000	0.00000000	6.53507800
H	-3.83795400	2.35363000	2.00685300
N	1.22331200	-0.75668300	3.45941600
N	-1.22331200	0.75668300	3.45941600
N	-1.20232300	0.77666700	0.55102000
N	1.20232300	-0.77666700	0.55102000
H	2.25413200	-1.39265600	6.57220600
H	3.87629800	-2.39475000	4.65775500
H	3.92811700	-2.31927500	-0.60841600
H	2.34241900	-1.31806700	-2.53870200
H	-2.34241900	1.31806700	-2.53870200
H	-3.92811700	2.31927500	-0.60841600
H	-3.87629800	2.39475000	4.65775500
H	-2.25413200	1.39265600	6.57220600
Zn	0.00000000	0.00000000	2.00606700
C	0.00000000	0.00000000	-2.95594500
C	-0.02171100	1.14803200	-3.78037200
C	0.02171100	-1.14803200	-3.78037200
H	-0.01337900	2.17178800	-3.42871700
H	0.01337900	-2.17178800	-3.42871700
C	-0.01031700	0.74868300	-5.12447100
C	0.01031700	-0.74868300	-5.12447100
C	0.00733100	-1.59517900	-6.23152700
C	0.00000000	-1.26612500	-7.58915100
C	0.00000000	0.00000000	-8.18245400
C	0.00000000	1.26612500	-7.58915100
C	-0.00733100	1.59517900	-6.23152700
H	-0.01480200	2.66021700	-6.00263400
H	0.00124600	2.10790600	-8.27722300
H	0.00000000	0.00000000	-9.27084000
H	-0.00124600	-2.10790600	-8.27722300
H	0.01480200	-2.66021700	-6.00263400

APs-a

C	0.00000000	0.68170700	5.32543600
C	0.00000000	-0.68170700	5.32543600
C	0.00000000	1.13498200	3.95340400
C	0.00000000	4.31180600	0.41659100
C	0.00000000	4.30493800	1.77233800
C	0.00000000	2.89441500	2.16991900
C	0.00000000	0.00000000	-6.25292700
C	0.00000000	-1.25925900	-5.64974500
C	0.00000000	-1.58098200	-4.28850000
C	0.00000000	1.25925900	-5.64974500
C	0.00000000	-0.73694700	-3.18176100
C	0.00000000	1.58098200	-4.28850000
C	0.00000000	0.73694700	-3.18176100
H	0.00000000	0.00000000	-7.34053400
H	0.00000000	-2.10730600	-6.32992800
H	0.00000000	-2.64562800	-4.06831600
H	0.00000000	2.10730600	-6.32992800
H	0.00000000	2.64562800	-4.06831600
C	0.00000000	-1.16266000	-1.80481800

APs-b

C	-0.47187500	-4.20133800	-0.00105100
C	-1.83417200	-4.20588100	-0.00178300
C	-0.01790100	-2.82674000	-0.00746200
C	3.23730700	0.72449000	0.00566900
C	3.22134500	-0.74392800	-0.00077700
C	1.81712000	-1.09854400	0.00107300
C	-1.74199300	4.27614700	-0.03855600
C	-0.38787600	4.28706700	-0.03555300
C	-2.20974900	2.86913100	0.01359700
C	0.08314400	2.88754900	0.01568700
C	-5.41766700	0.73162100	0.00388200
C	-5.44294200	-0.62695700	0.00147500
C	-4.00909000	1.11938800	0.00617900
C	-4.04424700	-1.05286700	-0.00061400
C	-2.29190400	-2.83679200	-0.00849900
C	-3.60441100	-2.39895800	-0.00599200
C	-3.55526300	2.43666500	0.00760700
C	1.30491400	-2.42157900	-0.00439200
C	1.85957200	1.11456700	0.01040700

C	0.00000000	1.16266000	-1.80481800
C	0.00000000	-4.31180600	0.41659100
C	0.00000000	-4.30493800	1.77233800
C	0.00000000	-2.90970800	-0.00370600
C	0.00000000	-2.89441500	2.16991900
C	0.00000000	-1.13498200	3.95340400
C	0.00000000	-2.44765700	3.51292800
C	0.00000000	-2.50187400	-1.32869400
C	0.00000000	2.44765700	3.51292800
C	0.00000000	2.90970800	-0.00370600
C	0.00000000	2.50187400	-1.32869400
H	0.00000000	-3.30255600	-2.06381900
H	0.00000000	3.30255600	-2.06381900
H	0.00000000	3.20818000	4.28765400
H	0.00000000	-3.20818000	4.28765400
N	0.00000000	2.08169500	1.09873200
N	0.00000000	0.00000000	3.17272800
N	0.00000000	-2.08169500	1.09873200
H	0.00000000	-5.16589100	-0.24919700
H	0.00000000	-5.15074100	2.44834600
H	0.00000000	-1.34356500	6.18077300
H	0.00000000	1.34356500	6.18077300
H	0.00000000	5.15074100	2.44834600
H	0.00000000	5.16589100	-0.24919700
C	0.00000000	0.00000000	-1.01371700
H	0.00000000	0.00000000	0.05887300
H	0.00000000	0.00000000	2.15844800

C	1.39536900	2.46649400	0.00636200
H	-4.32581300	3.20571500	-0.00513900
H	2.16102200	3.23812600	-0.01828500
H	2.02403900	-3.23356300	-0.00385400
H	-4.36501100	-3.17372500	-0.00515600
N	1.04857700	0.01477000	0.00853500
N	-1.15629100	-2.04930100	-0.01272600
N	-3.20897000	0.00201900	0.00224100
H	-6.25676700	1.41621300	0.00618500
H	-6.30473700	-1.28247800	-0.00137200
H	-2.49292000	-5.06364200	0.00474800
H	0.19242400	-5.05495600	0.00593300
C	-1.08040500	2.06249500	0.05365900
H	-1.07929400	0.99498400	0.11555500
H	-1.19175100	-1.03622100	-0.03397000
C	4.29700000	-1.61159000	-0.00845900
C	5.67125200	-1.31063800	-0.00883300
C	6.28102800	-0.06054100	-0.00213600
C	5.70319100	1.21848400	0.00617700
C	4.35141300	1.56182000	0.01010600
H	4.05714500	-2.67234400	-0.01460400
H	6.34060800	-2.16655700	-0.01474400
H	7.36907800	-0.07452100	-0.00364700
H	6.40202800	2.05046200	0.01014700
H	4.14552700	2.62939000	0.01796900
H	0.25994000	5.15471400	-0.07401000
H	-2.39769900	5.13859200	-0.07876400

APs-c

C	-0.00109100	-0.42592200	4.31244100
C	0.00355300	-1.78435600	4.29943900
C	-0.00199600	-0.01559400	2.91050700
C	-0.00814500	3.14656800	-0.73279300
C	-0.00814500	3.14656800	0.73279300
C	-0.01398700	1.77626300	1.15059100
C	0.00355300	-1.78435600	-4.29943900
C	-0.00109100	-0.42592200	-4.31244100
C	0.00910200	-2.18550100	-2.89352700
C	-0.00199600	-0.01559400	-2.91050700
C	-0.04189700	-5.38681900	-0.67698300
C	-0.04189700	-5.38681900	0.67698300
C	0.02419900	-3.98096800	-1.14455300
C	0.02419900	-3.98096800	1.14455300
C	0.00910200	-2.18550100	2.89352700
C	0.01020100	-3.53030500	2.46482700
C	0.01020100	-3.53030500	-2.46482700
C	-0.01069100	1.31210500	2.47006000
C	-0.01398700	1.77626300	-1.15059100
C	-0.01069100	1.31210500	-2.47006000
H	-0.01431700	-4.27726900	-3.25648700
H	-0.01322900	2.07137700	-3.24459700
H	-0.01322900	2.07137700	3.24459700
H	-0.01431700	-4.27726900	3.25648700
N	-0.01862000	1.00583400	0.00000000
N	0.00424400	-1.09354100	2.08262600
H	-0.09208100	-6.25082100	-1.32915000
H	-0.09208100	-6.25082100	1.32915000
H	0.00554800	-2.46121200	5.14476100
H	-0.00654700	0.23811800	5.16769800
C	-0.00147700	4.25438700	1.58289400
C	0.00491900	5.61254700	1.26174900
C	0.00767300	6.21533100	0.00000000
C	0.00491900	5.61254700	-1.26174900
C	-0.00147700	4.25438700	-1.58289400

APs-ab

C	0.01361700	-3.53331300	3.92324600
C	0.00810500	-2.52730400	4.82842200
C	0.02814600	-2.88856000	2.60134300
C	-0.14478800	-2.53695800	-2.20039500
C	-0.13680400	-3.58285800	-1.17288800
C	0.00000000	-2.93588700	0.10693300
C	0.13680400	3.58285800	-1.17288800
C	0.14478800	2.53695800	-2.20039500
C	0.00000000	2.93588700	0.10693300
C	0.01360500	1.25936000	-1.52186700
C	-0.01361700	3.53331300	3.92324600
C	-0.00810500	2.52730400	4.82842200
C	-0.02814600	2.88856000	2.60134300
C	-0.01673700	1.27002700	4.05495800
C	0.01673700	-1.27002700	4.05495800
C	0.00000000	0.00000000	4.65798100
C	-0.01262100	3.56284200	1.38336200
C	0.01262100	-3.56284200	1.38336200
C	-0.01360500	-1.25936000	-1.52186700
C	0.00000000	0.00000000	-2.15607100
H	0.01075900	4.64796700	1.42943500
H	0.00000000	0.00000000	-3.24163500
H	-0.01075900	-4.64796700	1.42943500
H	0.00000000	0.00000000	5.74567900
N	0.03524800	-1.52800400	2.73110500
N	-0.03524800	1.52800400	2.73110500
H	-0.00759100	-2.59998500	5.90922800
H	0.00641800	-4.60092100	4.10663500
C	-0.26583000	-2.70662900	-3.57499400
C	-0.38204900	-3.88930500	-4.31794200
C	-0.42587600	-5.20704000	-3.86742300
C	-0.36800000	-5.68289000	-2.55267100
C	-0.24682800	-4.96195000	-1.36462900
H	-0.26998800	-1.79474900	-4.16612100
H	-0.45089000	-3.75739700	-5.39506800

H	-0.00131800	4.03392200	2.64676500
H	0.00861100	6.29261100	2.10935200
H	0.01313800	7.30275800	0.00000000
H	0.00861100	6.29261100	-2.10935200
H	-0.00131800	4.03392200	-2.64676500
H	-0.00654700	0.23811800	-5.16769800
H	0.00554800	-2.46121200	-5.14476100
C	0.07610400	-3.16914100	0.00000000
N	0.00424400	-1.09354100	-2.08262600
H	0.15159800	-2.10229100	0.00000000
H	-0.04209900	-0.01117700	0.00000000

H	-0.52201400	-5.96697200	-4.63943400
H	-0.42832100	-6.76271500	-2.44078700
H	-0.23376500	-5.56174300	-0.45851600
H	-0.00641800	4.60092100	4.10663500
H	0.00759100	2.59998500	5.90922800
C	0.26583000	2.70662900	-3.57499400
C	0.38204900	3.88930500	-4.31794200
C	0.42587600	5.20704000	-3.86742300
C	0.36800000	5.68289000	-2.55267100
C	0.24682800	4.96195000	-1.36462900
H	0.23376500	5.56174300	-0.45851600
H	0.42832100	6.76271500	-2.44078700
H	0.52201400	5.96697200	-4.63943400
H	0.45089000	3.75739700	-5.39506800
H	0.26998800	1.79474900	-4.16612100
C	-0.09659400	1.55304600	-0.14097500
C	0.09659400	-1.55304600	-0.14097500
H	0.25019900	-0.86472400	0.67225700
H	-0.25019900	0.86472400	0.67225700

Mg-APs-a

C	0.00000000	0.68003100	5.30861200
C	0.00000000	-0.68003100	5.30861200
C	0.00000000	1.10902700	3.91825400
C	0.00000000	4.28617900	0.36688400
C	0.00000000	4.28375800	1.73032500
C	0.00000000	2.89349100	2.14654100
C	0.00000000	0.00000000	-6.33909200
C	0.00000000	-1.25825400	-5.73306200
C	0.00000000	-1.58024400	-4.37233700
C	0.00000000	1.25825400	-5.73306200
C	0.00000000	-0.73508800	-3.26375600
C	0.00000000	1.58024400	-4.37233700
C	0.00000000	0.73508800	-3.26375600
H	0.00000000	0.00000000	-7.42655000
H	0.00000000	-2.10692900	-6.41319200
H	0.00000000	-2.64513100	-4.15190300
H	0.00000000	2.10692900	-6.41319200
H	0.00000000	2.64513100	-4.15190300
C	0.00000000	-1.14709700	-1.87747100
C	0.00000000	1.14709700	-1.87747100
C	0.00000000	-4.28617900	0.36688400
C	0.00000000	-4.28375800	1.73032500
C	0.00000000	-2.90161300	-0.06745400
C	0.00000000	-2.89349100	2.14654100
C	0.00000000	-1.10902700	3.91825400
C	0.00000000	-2.43414500	3.48185900
C	0.00000000	-2.48559200	-1.39816500
C	0.00000000	2.43414500	3.48185900
C	0.00000000	2.90161300	-0.06745400
C	0.00000000	2.48559200	-1.39816500
H	0.00000000	-3.29630900	-2.12379100
H	0.00000000	3.29630900	-2.12379100
H	0.00000000	3.19751200	4.25426700
H	0.00000000	-3.19751200	4.25426700
N	0.00000000	2.08542600	1.05212500
N	0.00000000	0.00000000	3.10686200
N	0.00000000	-2.08542600	1.05212500
H	0.00000000	-5.14375800	-0.29412400
H	0.00000000	-5.13600500	2.39754300
H	0.00000000	-1.34542900	6.16232200
H	0.00000000	1.34542900	6.16232200
H	0.00000000	5.13600500	2.39754300
H	0.00000000	5.14375800	-0.29412400

Zn-APs-a

C	0.00000000	0.67857000	5.15713100
C	0.00000000	-0.67857000	5.15713100
C	0.00000000	1.10690900	3.76933600
C	0.00000000	4.31701600	0.28067100
C	0.00000000	4.31460100	1.64251600
C	0.00000000	2.92061600	2.05281700
C	0.00000000	0.00000000	-6.36645800
C	0.00000000	-1.25796100	-5.76079000
C	0.00000000	-1.57842300	-4.39951800
C	0.00000000	1.25796100	-5.76079000
C	0.00000000	-0.73340900	-3.29169400
C	0.00000000	1.57842300	-4.39951800
C	0.00000000	0.73340900	-3.29169400
H	0.00000000	0.00000000	-7.45402200
H	0.00000000	-2.10708700	-6.44011500
H	0.00000000	-2.64333000	-4.18091600
H	0.00000000	2.10708700	-6.44011500
H	0.00000000	2.64333000	-4.18091600
C	0.00000000	-1.14681100	-1.90722100
C	0.00000000	1.14681100	-1.90722100
C	0.00000000	-4.31701600	0.28067100
C	0.00000000	-4.31460100	1.64251600
C	0.00000000	-2.92882500	-0.14734400
C	0.00000000	-2.92061600	2.05281700
C	0.00000000	-1.10690900	3.76933600
C	0.00000000	-2.44042300	3.37391100
C	0.00000000	-2.49430400	-1.46546800
C	0.00000000	2.44042300	3.37391100
C	0.00000000	2.92882500	-0.14734400
C	0.00000000	2.49430400	-1.46546800
H	0.00000000	-3.28537400	-2.21098900
H	0.00000000	3.28537400	-2.21098900
H	0.00000000	3.18071800	4.16826700
H	0.00000000	-3.18071800	4.16826700
N	0.00000000	2.11210100	0.96552500
N	0.00000000	0.00000000	2.94483800
N	0.00000000	-2.11210100	0.96552500
H	0.00000000	-5.17280400	-0.38269200
H	0.00000000	-5.16510700	2.31220700
H	0.00000000	-1.34842000	6.00696900
H	0.00000000	1.34842000	6.00696900
H	0.00000000	5.16510700	2.31220700
H	0.00000000	5.17280400	-0.38269200

C	0.00000000	0.00000000	-1.04197500
Mg	0.00000000	0.00000000	1.05751500

Mg-APs-b

C	-4.25616000	0.43441100	0.00000000
C	-4.23330500	1.79458800	0.00000000
C	-2.87319200	-0.01580500	0.00000000
C	0.70146000	-3.25349500	0.00000000
C	-0.76735400	-3.24841300	0.00000000
C	-1.14550800	-1.84739100	0.00000000
C	4.33922600	1.66160100	0.00000000
C	4.33604800	0.30710800	0.00000000
C	2.92725600	2.13246500	0.00000000
C	2.92216600	-0.13894900	0.00000000
C	0.75966100	5.32071600	0.00000000
C	-0.60921900	5.34935300	0.00000000
C	1.15935400	3.93194200	0.00000000
C	-1.04949400	3.97288900	0.00000000
C	-2.83920400	2.20296500	0.00000000
C	-2.38874900	3.52172500	0.00000000
C	2.48963200	3.46897200	0.00000000
C	-2.46604900	-1.35093500	0.00000000
C	1.10197400	-1.88850100	0.00000000
C	2.46431700	-1.44187500	0.00000000
H	3.24614500	4.25313900	0.00000000
H	3.21088500	-2.23293500	0.00000000
H	-3.26728000	-2.08214100	0.00000000
H	-3.15588000	4.29084100	0.00000000
N	-0.01825000	-1.07611300	0.00000000
N	-2.04341500	1.07662800	0.00000000
N	0.03181300	3.14301200	0.00000000
H	1.43897900	6.16380400	0.00000000
H	-1.25685700	6.21651600	0.00000000
H	-5.07674100	2.47311800	0.00000000
H	-5.12115300	-0.21636600	0.00000000
C	2.06825100	1.01579500	0.00000000
C	-1.62954200	-4.32542100	0.00000000
C	-1.32556300	-5.70426400	0.00000000
C	-0.08084600	-6.31043600	0.00000000
C	1.20243800	-5.72283800	0.00000000
C	1.54096400	-4.37823000	0.00000000
H	-2.69078300	-4.08932200	0.00000000
H	-2.18280200	-6.37211400	0.00000000
H	-0.08940400	-7.39838400	0.00000000
H	2.03577000	-6.42010000	0.00000000
H	2.60802100	-4.17188600	0.00000000
H	5.20377700	-0.34376800	0.00000000
H	5.21491000	2.30281600	0.00000000
Mg	0.00000000	1.05785300	0.00000000

Mg-APs-c

C	0.00000000	0.73215400	-3.22562600
C	0.00000000	-0.73215400	-3.22562600
C	0.00000000	1.12592900	-1.84156300
C	0.00000000	4.27437100	1.73605400
C	0.00000000	4.29292100	0.37041600
C	0.00000000	2.90952000	-0.06032100
C	0.00000000	-1.13283400	3.95863100
C	0.00000000	1.13283400	3.95863100
C	0.00000000	-4.27437100	1.73605400
C	0.00000000	-4.29292100	0.37041600
C	0.00000000	-2.88577900	2.15048200
C	0.00000000	-2.90952000	-0.06032100
C	0.00000000	-1.12592900	-1.84156300

C	0.00000000	0.00000000	-1.06671800
Zn	0.00000000	0.00000000	0.92413900

Zn-APs-b

C	-4.19359900	0.20531300	0.00000000
C	-4.21802000	1.56145700	0.00000000
C	-2.79859000	-0.19851400	0.00000000
C	0.80869800	-3.36015700	0.00000000
C	-0.66027900	-3.40184800	0.00000000
C	-1.07371100	-2.01483400	0.00000000
C	4.19904100	1.71983700	0.00000000
C	4.24075500	0.36853700	0.00000000
C	2.77660500	2.14439600	0.00000000
C	2.84685300	-0.12555400	0.00000000
C	0.57202800	5.30767300	0.00000000
C	-0.79445400	5.28856700	0.00000000
C	1.01670800	3.92826000	0.00000000
C	-1.18232400	3.89237400	0.00000000
C	-2.84100400	2.01978300	0.00000000
C	-2.48548600	3.36636000	0.00000000
C	2.34355300	3.48279900	0.00000000
C	-2.39584600	-1.52822800	0.00000000
C	1.15665500	-1.97718800	0.00000000
C	2.48464400	-1.45576800	0.00000000
H	3.10402700	4.26208600	0.00000000
H	3.28566000	-2.19133700	0.00000000
H	-3.19870600	-2.25788900	0.00000000
H	-3.30647000	4.07721300	0.00000000
N	0.01883000	-1.20888000	0.00000000
N	-1.99373900	0.92610300	0.00000000
N	-0.07859000	3.10328700	0.00000000
H	1.22300100	6.17290600	0.00000000
H	-1.47336900	6.13146000	0.00000000
H	-5.08088500	2.21480900	0.00000000
H	-5.03147900	-0.47977200	0.00000000
C	1.95012800	1.00223000	0.00000000
C	-1.48794900	-4.50696500	0.00000000
C	-1.13605100	-5.87164500	0.00000000
C	0.13289300	-6.43403600	0.00000000
C	1.39327700	-5.80729700	0.00000000
C	1.68693600	-4.44817900	0.00000000
H	-2.55656000	-4.30473800	0.00000000
H	-1.96771100	-6.57096500	0.00000000
H	0.16016000	-7.52176900	0.00000000
H	2.24948100	-6.47622100	0.00000000
H	2.74604900	-4.20251400	0.00000000
H	5.12479400	-0.25942700	0.00000000
H	5.04772700	2.39584200	0.00000000
Zn	0.00000000	1.01075000	0.00000000

Zn-APs-c

C	0.00000000	0.72973400	-3.26485100
C	0.00000000	-0.72973400	-3.26485100
C	0.00000000	1.12350700	-1.88214300
C	0.00000000	4.30717200	1.63450200
C	0.00000000	4.32466300	0.27087100
C	0.00000000	2.93686600	-0.15238500
C	0.00000000	-1.13265300	3.79909500
C	0.00000000	1.13265300	3.79909500
C	0.00000000	-4.30717200	1.63450200
C	0.00000000	-4.32466300	0.27087100
C	0.00000000	-2.91424900	2.04463100
C	0.00000000	-2.93686600	-0.15238500
C	0.00000000	-1.12350700	-1.88214300

C	0.00000000	-2.45924200	-1.38288100
C	0.00000000	-2.45197200	3.50090500
C	0.00000000	2.45924200	-1.38288100
C	0.00000000	2.88577900	2.15048200
C	0.00000000	2.45197200	3.50090500
H	0.00000000	-3.25562000	4.23634900
H	0.00000000	3.25562000	4.23634900
H	0.00000000	3.23616600	-2.13990800
H	0.00000000	-3.23616600	-2.13990800
N	0.00000000	2.08683100	1.03827700
N	0.00000000	0.00000000	-1.04425700
N	0.00000000	-2.08683100	1.03827700
H	0.00000000	-5.12218600	2.40951200
H	0.00000000	-5.15478800	-0.28442600
H	0.00000000	5.15478800	-0.28442600
H	0.00000000	5.12218600	2.40951200
C	0.00000000	0.00000000	3.10667700
Mg	0.00000000	0.00000000	1.03718000
C	0.00000000	1.58333100	-4.32858600
C	0.00000000	1.26239200	-5.68886300
C	0.00000000	0.00000000	-6.28902500
C	0.00000000	-1.26239200	-5.68886300
C	0.00000000	-1.58333100	-4.32858600
H	0.00000000	2.64746600	-4.10757500
H	0.00000000	2.10897600	-6.37025100
H	0.00000000	0.00000000	-7.37671800
H	0.00000000	-2.10897600	-6.37025100
H	0.00000000	-2.64746600	-4.10757500
C	0.00000000	0.67601100	5.37910000
C	0.00000000	-0.67601100	5.37910000
H	0.00000000	1.32423200	6.24908300
H	0.00000000	-1.32423200	6.24908300

C	0.00000000	-2.46591900	-1.45962400
C	0.00000000	-2.46175700	3.38189100
C	0.00000000	2.46591900	-1.45962400
C	0.00000000	2.91424900	2.04463100
C	0.00000000	2.46175700	3.38189100
H	0.00000000	-3.24224900	4.14086300
H	0.00000000	3.24224900	4.14086300
H	0.00000000	3.22339900	-2.23537100
H	0.00000000	-3.22339900	-2.23537100
N	0.00000000	2.11488800	0.94052700
N	0.00000000	0.00000000	-1.07146500
N	0.00000000	-2.11488800	0.94052700
H	0.00000000	-5.15364700	2.30960200
H	0.00000000	-5.18437100	-0.38685100
H	0.00000000	5.18437100	-0.38685100
H	0.00000000	5.15364700	2.30960200
C	0.00000000	0.00000000	2.94152000
C	0.00000000	1.58071400	-4.36836400
C	0.00000000	1.26130500	-5.72883700
C	0.00000000	0.00000000	-6.33030700
C	0.00000000	-1.26130500	-5.72883700
C	0.00000000	-1.58071400	-4.36836400
H	0.00000000	2.64492200	-4.14988200
H	0.00000000	2.10901600	-6.40883300
H	0.00000000	0.00000000	-7.41796400
H	0.00000000	-2.10901600	-6.40883300
H	0.00000000	-2.64492200	-4.14988200
C	0.00000000	0.67534500	5.21327800
C	0.00000000	-0.67534500	5.21327800
H	0.00000000	1.32850300	6.07915100
H	0.00000000	-1.32850300	6.07915100
Zn	0.00000000	0.00000000	0.98431400

Mg-APs-ab

C	0.00000000	3.50887200	3.83186700
C	0.00000000	2.54500500	4.79029300
C	0.00000000	2.83923500	2.53693200
C	0.00000000	2.54695600	-2.30535400
C	0.00000000	3.58021000	-1.25857200
C	0.00000000	2.89422100	0.01077600
C	0.00000000	-3.58021000	-1.25857200
C	0.00000000	-2.54695600	-2.30535400
C	0.00000000	-2.89422100	0.01077600
C	0.00000000	-1.26631200	-1.61518700
C	0.00000000	-3.50887200	3.83186700
C	0.00000000	-2.54500500	4.79029300
C	0.00000000	-2.83923500	2.53693200
C	0.00000000	-1.25927000	4.10131600
C	0.00000000	1.25927000	4.10131600
C	0.00000000	0.00000000	4.72702300
C	0.00000000	-3.49529400	1.31164500
C	0.00000000	3.49529400	1.31164500
C	0.00000000	1.26631200	-1.61518700
C	0.00000000	0.00000000	-2.24507200
H	0.00000000	-4.58103500	1.38027300
H	0.00000000	0.00000000	-3.33443000
H	0.00000000	4.58103500	1.38027300
H	0.00000000	0.00000000	5.81283800
N	0.00000000	1.46879900	2.75489500
N	0.00000000	-1.46879900	2.75489500
H	0.00000000	2.67489900	5.86505000
H	0.00000000	4.58271300	3.97237700
C	0.00000000	2.74026700	-3.68098800
C	0.00000000	3.93803800	-4.41370500

Zn-APs-ab

C	0.13288200	3.48784200	3.72346600
C	0.12783600	2.52514300	4.67929800
C	0.08656400	2.81273900	2.43371600
C	-0.09177400	2.52608300	-2.37155100
C	-0.07514500	3.54831600	-1.32451700
C	-0.10277800	2.85627100	-0.06055300
C	0.07514500	-3.54831600	-1.32451700
C	0.09177400	-2.52608300	-2.37155100
C	0.10277800	-2.85627100	-0.06055300
C	0.12523000	-1.24526200	-1.68551400
C	-0.13288200	-3.48784200	3.72346600
C	-0.12783600	-2.52514300	4.67929800
C	-0.08656400	-2.81273900	2.43371600
C	-0.08547900	-1.24349900	3.98630300
C	0.08547900	1.24349900	3.98630300
C	0.00000000	0.00000000	4.62080100
C	0.00000000	-3.47004000	1.21973400
C	0.00000000	3.47004000	1.21973400
C	-0.12523000	1.24526200	-1.68551400
C	0.00000000	0.00000000	-2.32649300
H	-0.03597500	-4.55482800	1.27876400
H	0.00000000	0.00000000	-3.41447100
H	0.03597500	4.55482800	1.27876400
H	0.00000000	0.00000000	5.70625800
N	0.09184500	1.44213800	2.63803300
N	-0.09184500	-1.44213800	2.63803300
H	0.14037400	2.64832300	5.75471400
H	0.14682200	4.56225500	3.85752400
C	-0.08440800	2.72085900	-3.74653600
C	-0.11178000	3.92206400	-4.47436300

C	0.00000000	5.24928100	-3.95006200
C	0.00000000	5.70577300	-2.62424300
C	0.00000000	4.96771000	-1.44307300
H	0.00000000	1.83693200	-4.28642400
H	0.00000000	3.82106500	-5.49511600
H	0.00000000	6.02256400	-4.71474500
H	0.00000000	6.78642000	-2.50129800
H	0.00000000	5.55871900	-0.53016500
H	0.00000000	-4.58271300	3.97237700
H	0.00000000	-2.67489900	5.86505000
C	0.00000000	-2.74026700	-3.68098800
C	0.00000000	-3.93803800	-4.41370500
C	0.00000000	-5.24928100	-3.95006200
C	0.00000000	-5.70577300	-2.62424300
C	0.00000000	-4.96771000	-1.44307300
H	0.00000000	-5.55871900	-0.53016500
H	0.00000000	-6.78642000	-2.50129800
H	0.00000000	-6.02256400	-4.71474500
H	0.00000000	-3.82106500	-5.49511600
H	0.00000000	-1.83693200	-4.28642400
Mg	0.00000000	0.00000000	1.30139500
C	0.00000000	1.49573800	-0.20291800
C	0.00000000	-1.49573800	-0.20291800

P

C	0.00000000	4.25627100	0.67803300
C	0.00000000	4.25627100	-0.67803300
C	0.00000000	2.85383200	1.08464300
C	0.00000000	-0.68600900	4.26081400
C	0.00000000	0.68600900	4.26081400
C	0.00000000	1.12956000	2.89636700
C	0.00000000	-4.25627100	-0.67803300
C	0.00000000	-4.25627100	0.67803300
C	0.00000000	-2.85383200	-1.08464300
C	0.00000000	-2.85383200	1.08464300
C	0.00000000	-0.68600900	-4.26081400
C	0.00000000	0.68600900	-4.26081400
C	0.00000000	-1.12956000	-2.89636700
C	0.00000000	1.12956000	-2.89636700
C	0.00000000	2.85383200	-1.08464300
C	0.00000000	2.44014700	-2.42195500
C	0.00000000	-2.44014700	-2.42195500
C	0.00000000	2.44014700	2.42195500
C	0.00000000	-1.12956000	2.89636700
C	0.00000000	-2.44014700	2.42195500
H	0.00000000	-3.21860100	-3.17869700
H	0.00000000	-3.21860100	3.17869700
H	0.00000000	3.21860100	3.17869700
N	0.00000000	0.00000000	2.11733800
N	0.00000000	2.02764600	0.00000000
N	0.00000000	0.00000000	-2.11733800
N	0.00000000	-2.02764600	0.00000000
H	0.00000000	1.34668800	5.11682100
H	0.00000000	-1.34668800	5.11682100
H	0.00000000	-5.10422500	1.35102800
H	0.00000000	-5.10422500	-1.35102800
H	0.00000000	-1.34668800	-5.11682100
H	0.00000000	1.34668800	-5.11682100
H	0.00000000	5.10422500	-1.35102800
H	0.00000000	5.10422500	1.35102800
H	0.00000000	3.21860100	-3.17869700
H	0.00000000	0.00000000	1.10284300
H	0.00000000	0.00000000	-1.10284300
C	-0.11402800	5.23037400	-4.00499600
C	-0.08794400	5.68137000	-2.67605200
C	-0.06352600	4.93825600	-1.49970500
H	-0.07111300	1.82015500	-4.35518400
H	-0.13050500	3.80930400	-5.55602500
H	-0.13239100	6.00729100	-4.76572700
H	-0.08096300	6.76140400	-2.54852200
H	-0.03548200	5.52492800	-0.58485800
H	-0.14682200	-4.56225500	3.85752400
H	-0.14037400	-2.64832300	5.75471400
C	0.08440800	-2.72085900	-3.74653600
C	0.11178000	-3.92206400	-4.47436300
C	0.11402800	-5.23037400	-4.00499600
C	0.08794400	-5.68137000	-2.67605200
C	0.06352600	-4.93825600	-1.49970500
H	0.03548200	-5.52492800	-0.58485800
H	0.08096300	-6.76140400	-2.54852200
H	0.13239100	-6.00729100	-4.76572700
H	0.13050500	-3.80930400	-5.55602500
H	0.07111300	-1.82015500	-4.35518400
C	-0.23812400	1.46128400	-0.27543000
C	0.23812400	-1.46128400	-0.27543000
Zn	0.00000000	0.00000000	1.12563000

A

C	0.00000000	0.00000000	-2.50330100
C	0.00000000	1.26606900	-1.91074000
C	0.00000000	1.59455300	-0.55209300
C	0.00000000	-1.26606900	-1.91074000
C	0.00000000	0.75015800	0.55448600
C	0.00000000	-1.59455300	-0.55209300
C	0.00000000	-0.75015800	0.55448600
H	0.00000000	0.00000000	-3.59182800
H	0.00000000	2.10778000	-2.59892400
H	0.00000000	2.65988600	-0.32354100
H	0.00000000	-2.10778000	-2.59892400
H	0.00000000	-2.65988600	-0.32354100
C	0.00000000	1.14991500	1.90181000
H	0.00000000	2.17598300	2.24794000
C	0.00000000	0.00000000	2.70782700
H	0.00000000	0.00000000	3.79217700
C	0.00000000	-1.14991500	1.90181000
H	0.00000000	-2.17598300	2.24794000

1(Zn)^{II}

C	-3.41237800	2.52044600	0.03074600
C	-2.45173300	3.48666300	0.03499100
C	-2.73095000	1.25535200	-0.00655900
C	-2.45175000	-3.48664500	0.03489200
C	-3.41238500	-2.52042000	0.03063800
C	-2.73095100	-1.25533000	-0.00654900
C	3.55309200	-2.52386200	-0.03864100
C	2.59422400	-3.48909300	-0.04724100
C	2.86907600	-1.25639900	-0.00118600
C	1.31604800	-2.81632800	-0.00470500
C	3.55309700	2.52387600	-0.03846600
C	2.59422500	3.48910400	-0.04707300
C	2.86907700	1.25641000	-0.00115900
C	1.31605000	2.81633500	-0.00467800
C	-1.17691800	2.81265500	-0.00911200
C	0.07251300	3.46522300	-0.00832300
C	3.52221000	0.00000500	0.00043700
C	-3.38687600	0.00001000	-0.00542200
C	-1.17692400	-2.81264300	-0.00908500
C	0.07250700	-3.46521900	-0.00830900
N	-1.37267800	-1.44825700	-0.02853900
N	-1.37268200	1.44827000	-0.02864600
N	1.51405600	1.44824100	0.01724200
N	1.51405400	-1.44823600	0.01730900
H	-4.48486800	-2.64152800	0.05955600
H	-2.59026800	-4.55639300	0.07342700
H	2.73354100	-4.55872600	-0.08751100
H	4.62549800	-2.64601900	-0.06546600
H	2.73353900	4.55874100	-0.08726900
H	-2.59022900	4.55641200	0.07360700
H	-4.48485700	2.64155500	0.05977200
Zn	0.07080400	0.00000400	-0.00632000
H	4.62550600	2.64603000	-0.06516500
C	0.07049200	-4.96392900	-0.01040600
C	-0.37184400	-5.67836400	-1.13450900
C	0.51113500	-5.68292500	1.11134100
C	-0.37161100	-7.07340900	-1.13733300
C	0.50941400	-7.07810600	1.10916800
C	0.06860400	-7.77756400	-0.01534600
C	0.07048700	4.96394000	-0.01038600
C	-0.37153600	5.67837600	-1.13460900
C	0.51079300	5.68292700	1.11149500
C	0.50905100	7.07811000	1.10933600
C	-0.37132600	7.07342300	-1.13741800
C	0.06855500	7.77757300	-0.01529700
H	-0.70900300	5.13257500	-2.01054000
H	-0.71131000	7.60961400	-2.01872700
H	0.06812200	8.86359300	-0.01736600
H	0.84877700	7.61781300	1.98859000
H	0.84849500	5.14056700	1.98946500
H	-0.71184000	-7.60959900	-2.01854900
H	-0.70956600	-5.13255700	-2.01033700
H	0.06819500	-8.86358400	-0.01742600
H	0.84939700	-7.61781700	1.98831700
H	0.84908000	-5.14056400	1.98921700
C	-4.80593200	0.00001300	0.00765800
C	4.94152600	0.00000700	-0.00589500
C	-6.02605100	0.00002100	0.01718300
C	6.16131600	0.00002200	-0.00765600
C	-7.44402300	0.00004500	0.03048400
C	-8.17796500	-1.20444100	0.03629200
C	-8.17801300	1.20449300	0.03513900
C	-9.56286000	-1.20996500	0.05053300

D23

C	-5.74481800	-1.78890000	-0.27639500
C	-4.77780600	-2.80932300	-0.09758000
C	-4.90414100	-4.13696800	0.39012100
C	-3.63272900	-4.68680400	0.50919100
C	-2.68436900	-3.71559700	0.10528200
N	-3.41955600	-2.60726100	-0.27706700
C	-1.26360900	-3.66834700	0.20728600
C	-0.68600900	-2.39942300	0.14684700
C	0.60582200	-1.87937200	0.10303000
N	1.86901400	-2.55647800	0.03788300
C	2.54806700	-3.74295800	-0.26388000
H	2.02669000	-4.67764500	-0.38741300
C	3.90962000	-3.48329000	-0.34734100
H	4.65679900	-4.23390000	-0.56130100
C	4.11788700	-2.06882700	-0.11319700
C	2.83094100	-1.61040000	0.11213200
C	2.31202100	-0.34291000	0.16466800
C	0.89872400	-0.45587900	0.16540300
C	0.03353200	0.69530500	0.16174200
N	-1.28791200	0.66365900	0.05190700
C	-1.73626700	1.99967900	0.01777600
C	-3.08383500	2.39284500	-0.19520700
C	-4.17570100	1.51563500	-0.33767900
N	-4.15403300	0.14640000	-0.13661400
C	-5.40158500	-0.42283700	-0.37899100
C	-6.23961800	0.66289600	-0.78624200
H	-7.26529000	0.54923700	-1.10311800
C	-5.50741800	1.82568800	-0.75804800
H	-5.84286900	2.81201700	-1.03989800
C	-0.64166000	2.87261700	0.16729600
C	0.52816300	2.10108400	0.24395100
C	1.84017500	2.65527200	0.32582000
C	3.08205600	2.01470700	0.25945800
N	3.25897000	0.63291900	0.12801500
C	4.63766400	0.29913800	0.02224300
C	5.10084500	-1.03422200	-0.14603000
C	6.53037200	-1.33347100	-0.34959100
C	7.10142900	-2.46084000	0.27650900
C	8.43782200	-2.78836100	0.09049900
C	9.21949400	-1.98217400	-0.73624900
C	8.68888300	-0.86595800	-1.38162500
C	7.34994500	-0.55044000	-1.18772600
C	5.32396800	1.54783900	0.14763500
C	4.40580300	2.55986800	0.29037600
C	1.92017000	4.14819500	0.46341400
C	1.55481800	4.76872700	1.66911100
C	2.35932600	4.94457600	-0.60607900
C	1.63376800	6.15021100	1.81243400
C	2.07512200	6.91097600	0.73139700
C	2.43757400	6.32878200	-0.48063700
H	-5.83755700	-4.59388300	0.68386000
H	-3.38174000	-5.65545000	0.91641500
H	4.62672600	3.60962500	0.40907700
H	6.39775000	1.65580400	0.15094400
H	-0.69824700	3.94858700	0.18637800
H	-3.04343200	-1.86976600	-0.85225000
H	-3.34900600	-0.29401600	0.28607000
H	-1.38043400	-1.56955500	0.15788300
N	10.63223100	-2.32014900	-0.93631600
N	2.16177300	8.37250600	0.87380700
H	6.48836800	-3.06820500	0.93356900
H	8.88749100	-3.64461700	0.57708700
H	9.32363400	-0.27629600	-2.03096200

H	-7.64340800	-2.14907300	0.02669600
C	-9.56291300	1.20996200	0.04936900
H	-7.64351400	2.14914900	0.02458100
C	-10.30005900	-0.00000900	0.06573600
H	-10.07685300	-2.16283700	0.04930400
H	-10.07694900	2.16280900	0.04716300
C	7.57874900	0.00001800	-0.00803300
C	8.29936200	-1.21657600	-0.00812100
C	8.29938700	1.21659500	-0.00765200
C	9.68596200	-1.21928400	-0.00765100
H	7.75540800	-2.15461300	-0.00829600
C	9.68598600	1.21927200	-0.00718100
H	7.75545300	2.15464400	-0.00746700
C	10.36524200	-0.00001300	-0.00713400
H	10.25253300	-2.14178700	-0.00762200
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N	11.82985900	-0.00002700	-0.00633400
C	-12.40955900	-1.25365100	0.00692900
H	-13.47877600	-1.05183600	0.07681200
H	-12.22292700	-1.77943900	-0.94082400
H	-12.14498300	-1.93165100	0.82750700
C	-12.40963200	1.25347800	0.00611200
H	-13.47880800	1.05171400	0.07679800
H	-12.14461500	1.93223700	0.82591600
H	-12.22354000	1.77839800	-0.94223400
O	12.40416700	-1.09077500	-0.00625700
O	12.40418800	1.09071000	-0.00568600
H	6.92195400	0.29365100	-1.71653000
H	1.20747100	4.15970300	2.49684400
H	1.36253100	6.64424300	2.73672600
H	2.63419400	4.47293200	-1.54376800
H	2.76868200	6.95836600	-1.29673200
O	11.30078800	-1.58361800	-1.66361500
O	11.06858500	-3.32106500	-0.36504500
O	2.54426500	9.02029900	-0.10099500
O	1.84885100	8.86124700	1.95913200
C	-7.17451000	-2.18133600	-0.32284100
C	-7.61295100	-3.23833500	-1.14199600
C	-8.14778400	-1.53232800	0.45947800
C	-8.94706300	-3.62443900	-1.18493200
H	-6.89133000	-3.75614500	-1.76607300
C	-9.48491600	-1.90880900	0.42169800
H	-7.84261100	-0.73053200	1.12440100
C	-9.91122200	-2.96376700	-0.40378700
H	-9.25379800	-4.43580500	-1.84061900
H	-10.20960500	-1.38941200	1.04415100
C	-0.53295000	-4.92691000	0.49472900
C	0.25949000	-5.05154700	1.64932800
C	-0.63822000	-6.05118400	-0.34165600
C	0.92688200	-6.23349400	1.94954800
H	0.34233600	-4.20621900	2.32579600
C	0.03098300	-7.23711000	-0.05413200
H	-1.24866700	-5.98836200	-1.23765600
C	0.82691900	-7.34986500	1.09958500
H	1.53051000	-6.29983300	2.85139300
H	-0.05817600	-8.08575200	-0.72797600
C	-3.38202600	3.85195200	-0.31431200
C	-2.82104100	4.63818900	-1.33488300
C	-4.24844700	4.49239700	0.58700100
C	-3.10431800	5.99488500	-1.44985000
H	-2.15954000	4.17117700	-2.05828200
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H	-4.69631000	3.91424000	1.38982800
C	-3.96874400	6.62698000	-0.53906500
H	-2.65684100	6.57466500	-2.25362600
H	-5.20370200	6.31692500	1.20473100
N	-11.25902200	-3.30820400	-0.48766300
H	-11.44718200	-4.25169900	-0.79691900
H	-11.82288400	-3.05062200	0.31041600
N	1.54305100	-8.51582500	1.36408300
H	1.79871600	-8.65702600	2.33157900
H	1.17375300	-9.35692400	0.94279500
N	-4.20784500	7.99836200	-0.61305600
H	-4.06306300	8.41581900	-1.52178500
H	-5.06608000	8.31307000	-0.18245700

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