

Supplementary material

Theoretical Design of Higher Performance Catalysts for Ethylene Polymerization Based on Nickel- α -diimine

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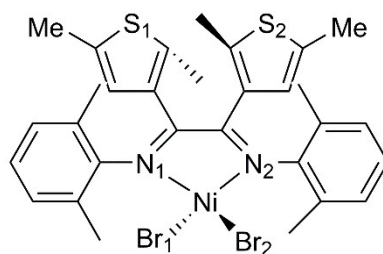
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Table S1. Comparison of experimental activities of Ni(II) and Pd(II) catalysts for ethylene polymerization with different backbones.

Entry	Metals	Backbone substituent	Polymerization Conditions	Activity ($10^6 \text{ g mol}^{-1} \text{ h}^{-1}$)	References
1	Pd(II) α -diimine	Acenaphthylene backbone Bulky 8- <i>p</i> -tolyl naphthyl	25 °C, CH_2Cl_2	TOF: 56-202 h^{-1}	[20]
2	Pd(II) α -diimine	Bulky dibenzobarrelene (axial pentiptycenyl)	70 °C, toluene, ethylene (8 bar)	2.19	[21]
3	Ni(II) α -diimine	Dibenzobarrelene backbone (axial cycloalkyl)	30 °C, toluene, ethylene (6 atm)	2.05	[22]
	Pd(II) α -diimine		30 °C, toluene ethylene (4 atm)	0.306	
4	Ni(II) α -diimine	Brookhart-type (monoarylmethyl)	70 °C, toluene	7.38	[23]
		Acenaphthene backbone (monoarylmethyl)	30 °C, toluene	11.34	
5	Ni(II) α -diimine	Dibenzobarrelene backbone (dibenzhydrylanilines)	50 °C, toluene	6.98	[24]
6	Ni(II) α -diimine	Brookhart-type (naphthylamine)	30 °C, toluene, ethylene (6 atm)	13.02	[25]
	Pd(II) α -diimine		70 °C, toluene, ethylene (4 atm)	0.0251	
7	Ni(II) α -diimine	Acenaphthene backbone (8-cyclohexylnaphthyl)	30 °C, toluene, ethylene (6 bar)	1.97	[26]
	Pd(II) α -diimine		50 °C, toluene, ethylene (4 bar)	0.0127	
8	Ni(II) α -diimine	Thiophene backbone (2,5-dimethyl-thien-3-yl)	20 °C, toluene, 8 atm ethylene pressure	10.38	[19]

Table S2. Comparison of bond lengths, bond angles, torsion, and Mean Absolute Error (MAE) obtained from different theoretical methods.



Parameters	X-ray [19]	B3LYP/ 6-31G(d)	B3LYP- D3/ 6-31G(d)	M06-2X/ 6-31G(d)	M06L/ 6-31G(d)	ω B97XD/ 6-31G(d)	ω B97XD/ 6-31G(d)	ω B97XD/ 6-31G(d,p)
		LANL2DZ				SDD		
Ni-N ₁	1.99	2.07	2.05	2.09	2.03	2.07	2.06	2.06
Ni-Br ₁	2.33	2.39	2.37	2.39	2.36	2.36	2.34	2.34
N ₁ -C ₁	1.29	1.29	1.30	1.28	1.31	1.28	1.28	1.28
C ₁ -C ₂	1.52	1.52	1.51	1.52	1.49	1.51	1.51	1.51
N ₁ -C _{Ph}	1.45	1.43	1.43	1.43	1.42	1.43	1.43	1.43
C _S -S ₁	1.71	1.74	1.74	1.73	1.73	1.73	1.73	1.73
Ni-C _{Me}	3.87	3.88	3.74	3.71	3.67	3.82	3.82	3.83
N ₁ -Ni-N ₂	81.19	79.43	79.66	78.03	79.72	79.00	79.14	79.13
Br ₁ -Ni-Br ₂	131.81	125.31	129.95	135.29	130.28	131.71	130.93	130.94
N ₁ -Ni-Br ₁	111.34	113.30	116.12	115.60	116.79	113.61	113.69	113.44
N ₁ -C ₁ -C ₂ -N ₂	-12.19	-16.34	-15.66	-17.15	-17.25	-16.28	-16.12	-16.02
C ₁ -N ₁ -Ni-N ₂	-3.57	-4.63	-4.46	-4.93	-4.92	-4.63	-4.60	-4.58
MAE (bond length)		0.03	0.04	0.05	0.05	0.03	0.03	0.03
MAE (bond angle)		3.41	2.72	3.63	2.82	1.52	1.76	1.68
MAE (torsion)		2.61	2.18	3.16	3.21	2.58	2.48	2.42

Table S3. Results of the coordination free energy (G_{c1}), activation free energy ($\Delta G_x^\ddagger$) and reaction free energy (ΔG_{rx}) in kcal mol⁻¹ for ethylene (ET) in gas phase and in toluene solvent.

Ni- α -diimine catalyst	In gas phase						
	G_{cl}	$\Delta G_1^\ddagger$	ΔG_{r1}	$\Delta G_2^\ddagger$	ΔG_{r2}	$\Delta G_3^\ddagger$	ΔG_{r3}
6-31G(d), SDD (Ni)	-16.4	14.2	-15.7	10.4	-20.7	9.7	-19.6
6-311G(d,p), SDD (Ni)	-15.7	14.2	-14.9	11.3	-19.4	10.9	-18.9

Ni- α -diimine catalyst	In toluene						
	G_{cl}	$\Delta G_1^\ddagger$	ΔG_{r1}	$\Delta G_2^\ddagger$	ΔG_{r2}	$\Delta G_3^\ddagger$	ΔG_{r3}
6-31G(d), SDD (Ni)	-11.3	15.1	-19.1	9.0	-20.4	9.7	-19.4
6-311G(d,p), SDD (Ni)	-13.1	16.1	-16.2	7.7	-20.3	12.6	-17.3

Table S4. Comparison of coordination free energy (G_{cl}), activation free energy ($\Delta G_1^\ddagger$), and reaction energy (ΔG_{r1}) in kcal mol⁻¹ with different metal (M) substitutions.

M =	G_{cl}	$\Delta G_1^\ddagger$	ΔG_{r1}
Mn(II)	-13.8	12.4	-11.5
Fe(II)	-6.2	5.0	-15.2
Co(II)	-31.0	14.3	-13.4
Ni(II)	-16.4	14.2	-15.7
Cu(II)	-2.6	14.4	-16.8
Zn(II)	1.4	37.5	-16.9
Ru(II)	-13.0	14.7	-11.2
Rh(II)	-14.3	11.1	-11.6
Pd(II)	-18.4	9.5	-15.0
Ag(I)	4.1	41.0	-17.6
Cd(II)	1.7	45.8	-17.3

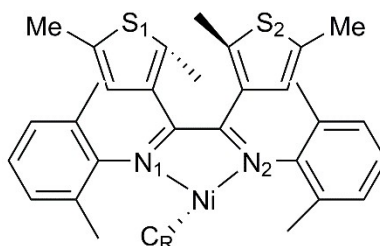
Table S5. Comparison of activation free energy ($\Delta G_1^\ddagger$) obtained from DFT calculation.

Metals	Backbone types	$\Delta G_1^\ddagger$ (kcal mol ⁻¹)	Activities (10 ⁶ g mol ⁻¹ h ⁻¹)	References
Ni	E ^a	14.2	10.38	19
Pd		9.5		
Pd	C ^b	18.1	0.0453	66

^a2,5-dimethyl-thien-3-yl

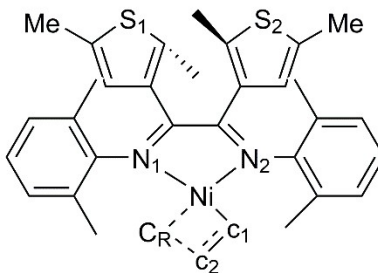
^b1,5-cyclooctadiene (axial isopropyl groups)

Table S6. Values of the coordination free energy (G_{c1}), bond distances, NBO charges, and %V_{Bur} of M- α -diimine catalysts of the active complexes (A₁).



Metals (M)	G_{c1} (kcal mol ⁻¹)	Bond distance (Å)			NBO charges				%V _{Bur} (A ₁)
		M-N ₁	M-N ₂	M-C _R	M	N ₁	N ₂	C _R	
Group I (Mn(II),Ni(II),Rh(II),Pd(II))									
Mn(II)	-13.8	1.89	1.96	2.00	1.30	-0.54	-0.62	-1.10	55.0
Ni(II)	-16.4	1.86	1.95	1.86	0.80	-0.42	-0.50	-0.99	53.0
Rh(II)	-14.3	2.01	2.17	2.02	0.76	-0.39	-0.47	-0.92	47.8
Pd(II)	-18.4	2.03	2.14	1.99	0.64	-0.41	-0.47	-0.82	47.6
R^2		0.11	0.06	0.11	0.52	0.25	0.35	0.58	0.21
Group II (Fe(II),Co(II),Ru(II))									
Fe(II)	-6.2	1.89	1.90	1.91	0.80	-0.42	-0.42	-1.00	53.5
Co(II)	-31.0	2.01	2.01	1.98	1.03	-0.52	-0.52	-1.17	50.4
Ru(II)	-13.0	1.94	1.95	2.01	0.56	-0.34	-0.35	-0.81	51.9
R^2		0.97	0.96	0.23	0.48	0.56	0.59	0.46	0.93
Group III (Cu(II),Zn(II),Ag(I),Cd(II))									
Cu(II)	-2.6	2.02	1.99	1.91	0.95	-0.48	-0.54	-1.06	50.7
Zn(II)	1.4	2.06	2.06	1.92	1.21	-0.57	-0.57	-1.28	49.5
Ag(I)	4.1	2.81	2.25	2.08	0.37	-0.40	-0.47	-1.15	40.0
Cd(II)	1.7	2.30	2.30	2.11	1.17	-0.55	-0.55	-1.20	43.3
R^2		0.68	0.60	0.50	0.22	0.07	0.29	0.27	0.72

Table S7. Values of the activation free energy ($\Delta G_1^\ddagger$), bond distances, NBO charges, and %V_{Bur} of M- α -diimine catalysts of the transition-state complexes (TS₁).



Metals (M)	$\Delta G_{T^\ddagger}$ (kcal mol ⁻¹)	Bond distance (Å)					NBO charges						%V _{Bur} (TS ₁)
		M- N ₁	M- N ₂	M- C ₁	M- C _R	C ₂ - C _R	M	N ₁	N ₂	C ₁	C ₂	C _R	
Group I (Mn(II),Ni(II),Rh(II),Pd(II))													
Mn(II)	12.4	1.95	1.97	2.10	2.12	2.22	1.07	-0.57	-0.58	-0.64	-0.35	-0.89	50.4
Ni(II)	14.2	1.93	2.01	1.93	2.00	2.08	0.47	-0.42	-0.43	-0.56	-0.41	-0.79	50.2
Rh(II)	11.1	2.08	2.16	2.04	2.21	2.00	0.47	-0.42	-0.44	-0.58	-0.42	-0.81	46.4
Pd(II)	9.5	2.08	2.17	2.03	2.19	2.04	0.38	-0.42	-0.44	-0.51	-0.43	-0.77	46.5
<i>R</i> ²		0.81	0.66	0.24	0.82	0.16	0.09	0.04	0.02	0.21	0.17	0.08	0.72
Group II (Fe(II),Co(II),Ru(II))													
Fe(II)	5.1	1.91	1.94	1.94	1.98	2.01	0.48	-0.38	-0.38	-0.57	-0.42	-0.78	51.3
Co(II)	14.4	2.03	2.04	2.04	2.11	2.12	0.90	-0.49	-0.49	-0.76	-0.39	-0.94	49.4
Ru(II)	14.7	2.00	1.97	2.03	2.19	2.01	0.33	-0.37	-0.32	-0.48	-0.43	-0.77	49.7
<i>R</i> ²		0.93	0.50	0.98	0.88	0.22	0.05	0.16	0.02	0.03	0.06	0.18	0.97
Group III (Cu(II),Zn(II),Ag(I),Cd(II))													
Cu(II)	14.4	2.05	2.08	2.04	2.10	2.10	0.72	-0.49	-0.49	-0.57	-0.48	-0.81	48.7
Zn(II)	37.5	2.04	2.02	2.00	2.16	2.15	1.23	-0.53	-0.54	-0.94	-0.37	-1.06	49.4
Ag(I)	41.0	2.22	2.36	2.18	2.42	2.16	0.52	-0.48	-0.45	-0.80	-0.42	-0.93	43.3
Cd(II)	45.9	2.26	2.25	2.19	2.37	2.24	1.17	-0.51	-0.51	-0.90	-0.35	-1.06	43.8
<i>R</i> ²		0.51	0.29	0.37	0.63	0.74	0.13	0.09	0.00	0.79	0.78	0.71	0.42

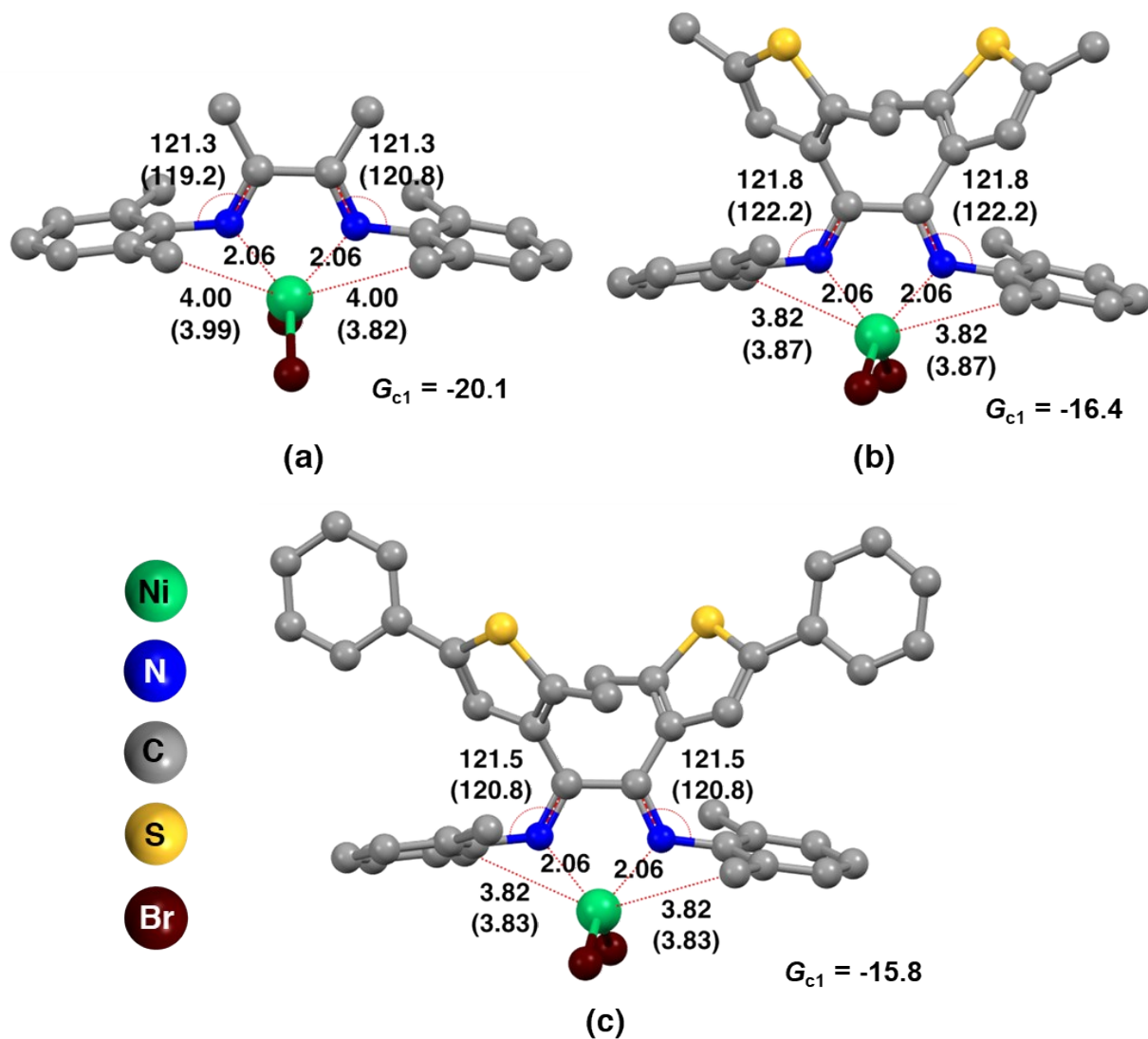


Fig. S1. Optimized pre-catalyst structures of a) Ni-A, b) Ni-Me, and c) Ni-Ph. Distances and angles are shown in black. The coordination free energy (G_{c1}) in kcal mol⁻¹. The results from X-ray data are given in parenthesis. H atoms were omitted for clarity.

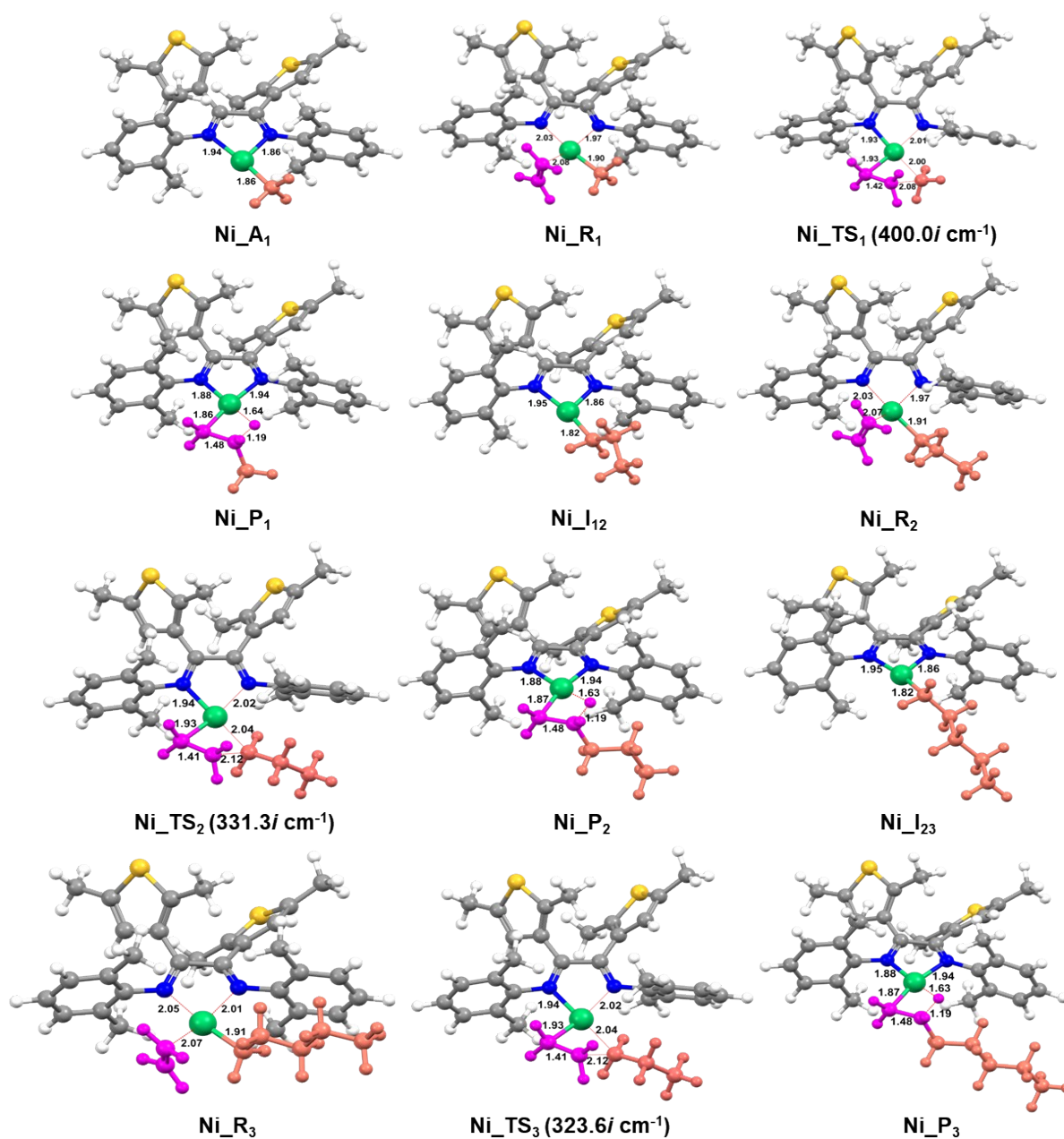


Fig. S2. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Ni- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

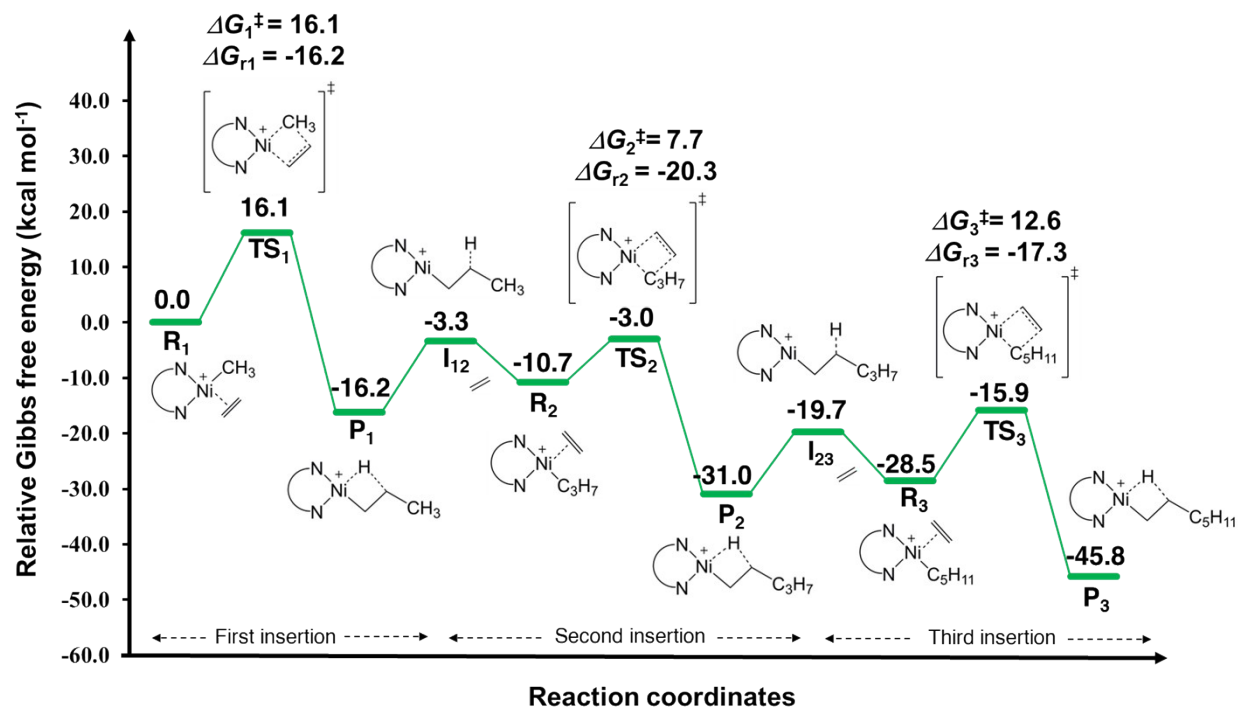


Fig. S3. The relative Gibbs free energies profile for ET polymerization catalyzed by Ni- α -diimine at 6-311G(d,p) levels in toluene. The coordination free energy (G_{cx}), activation free energy ($\Delta G_x^\ddagger$) and reaction energy (ΔG_r) were shown in kcal mol⁻¹.

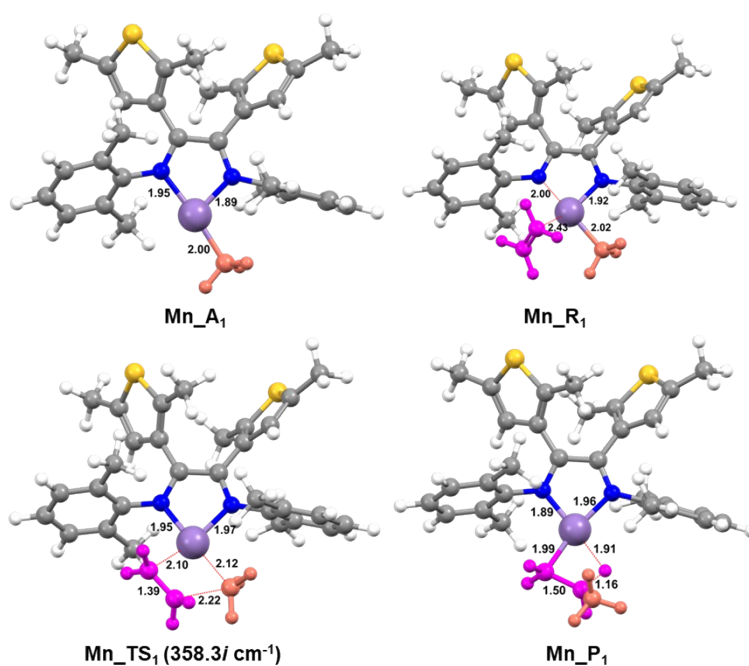


Fig. S4. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Mn- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

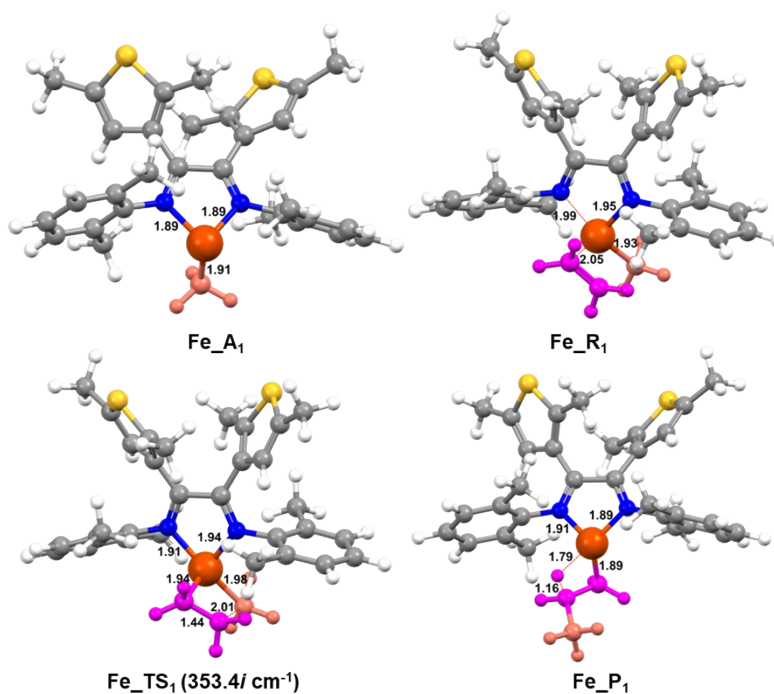


Fig. S5. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Fe- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

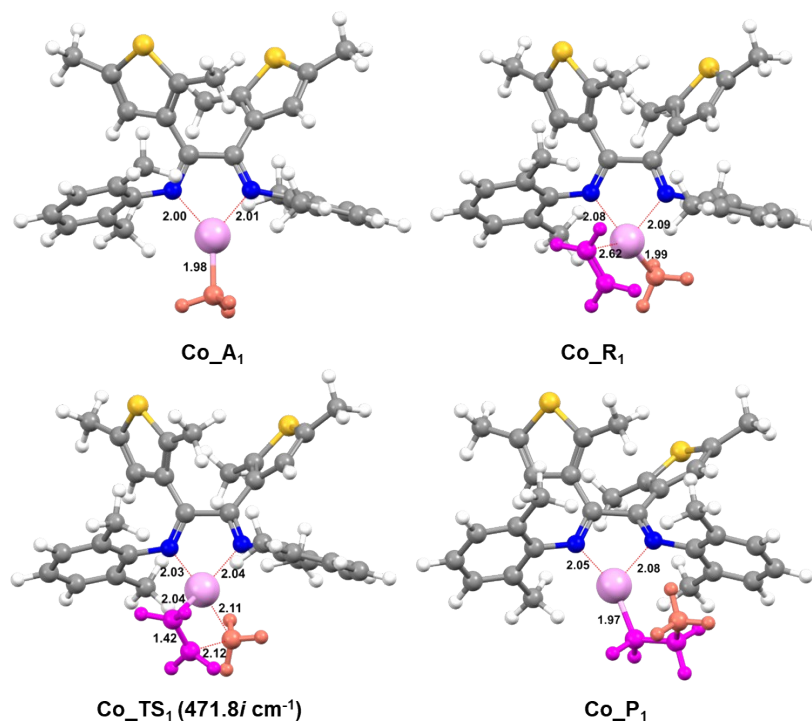


Fig. S6. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Co- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

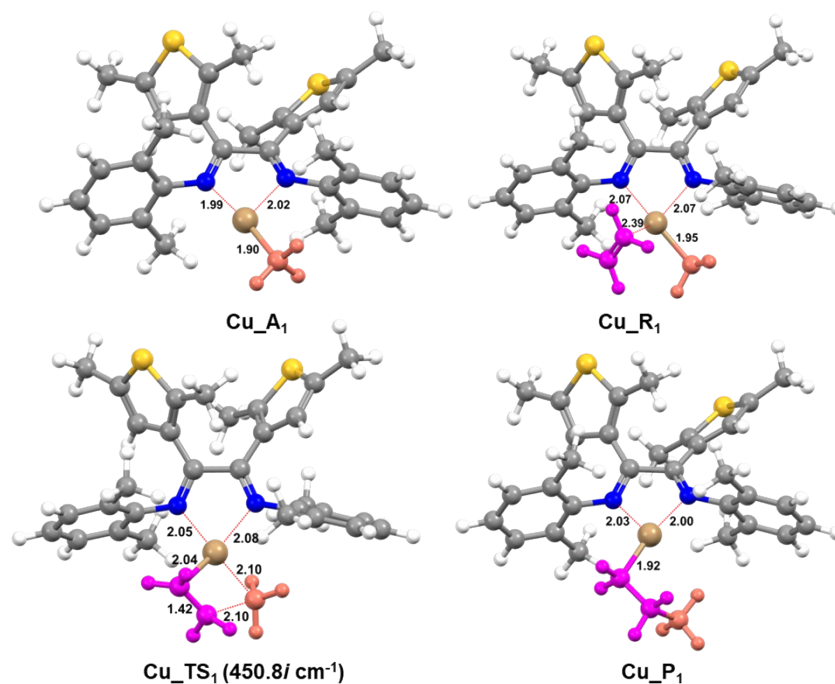


Fig. S7. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Cu- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

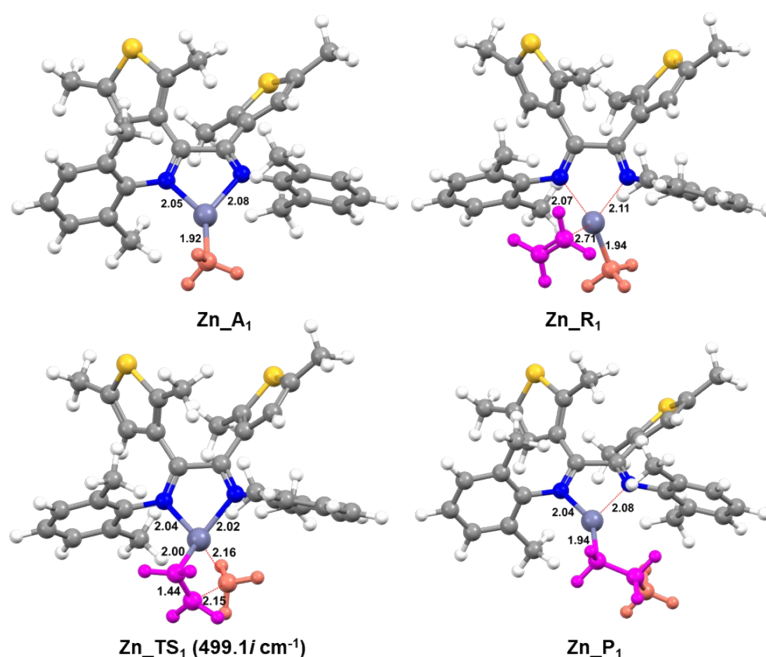


Fig. S8. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Zn- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

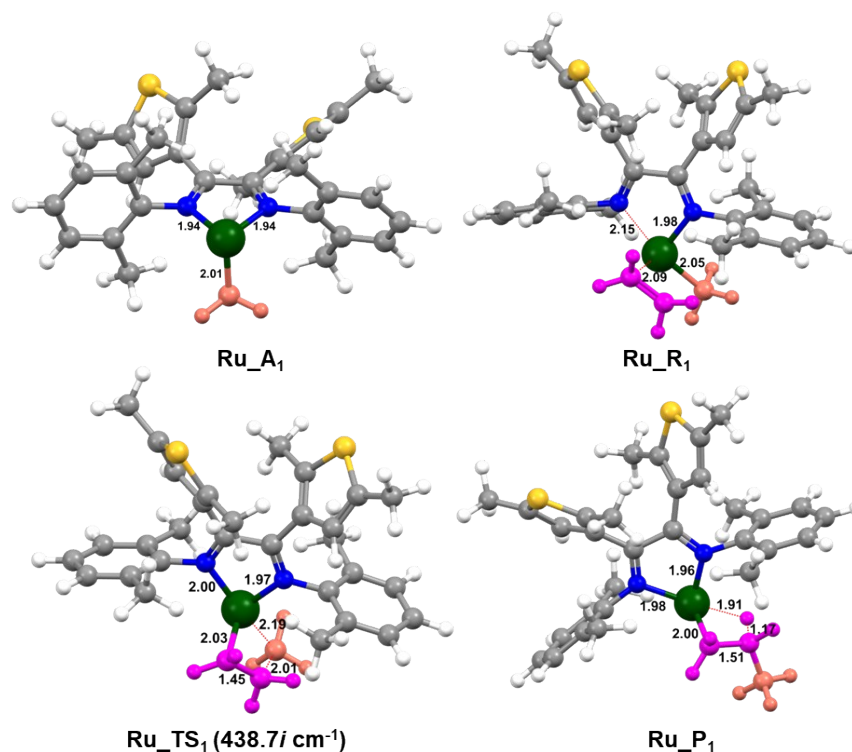


Fig. S9. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Ru- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

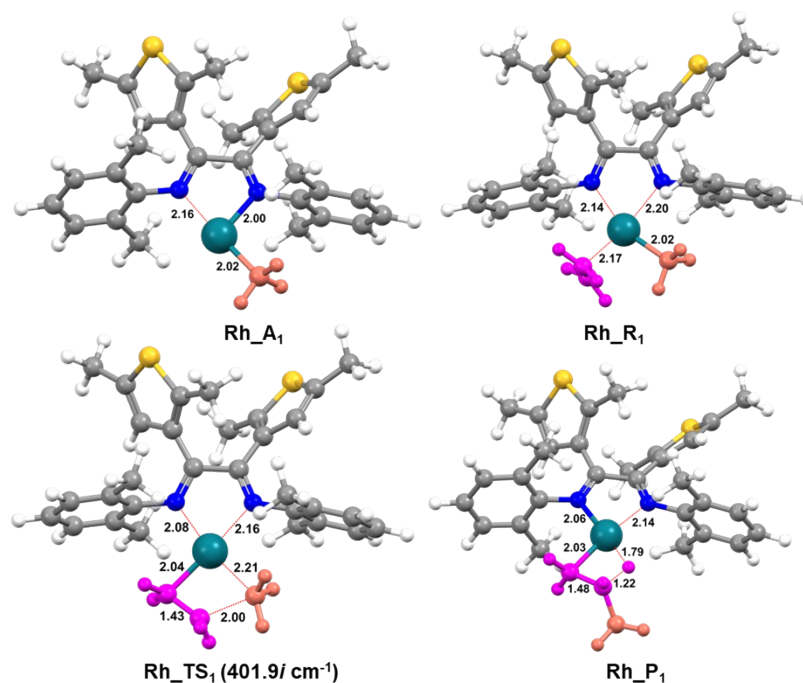


Fig. S10. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Rh- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

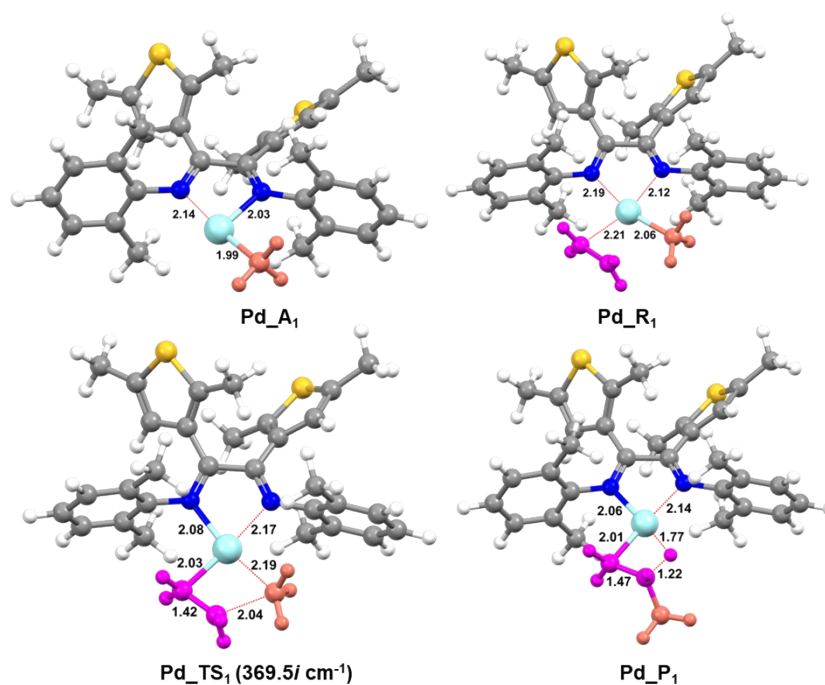


Fig. S11. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Pd- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

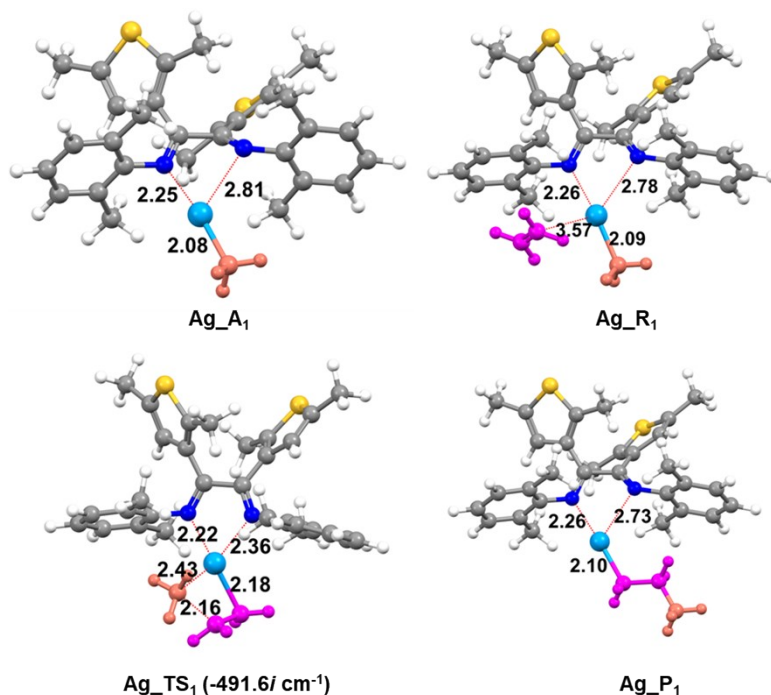


Fig. S12. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Ag- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

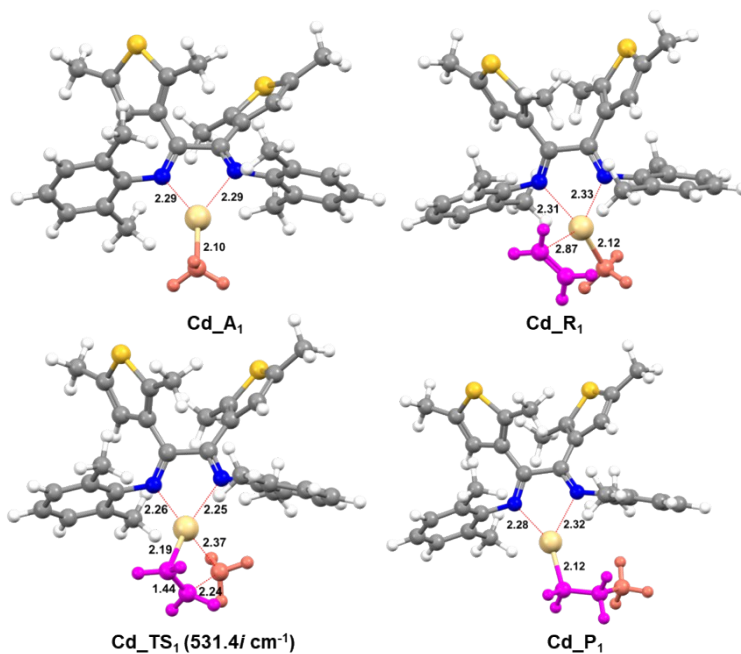


Fig. S13. Optimized structures of intermediates and transition states for ET polymerization catalyzed by Cd- α -diimine catalyst in gas phase. Bond distances are displayed in black color. Bond distances are given in Å.

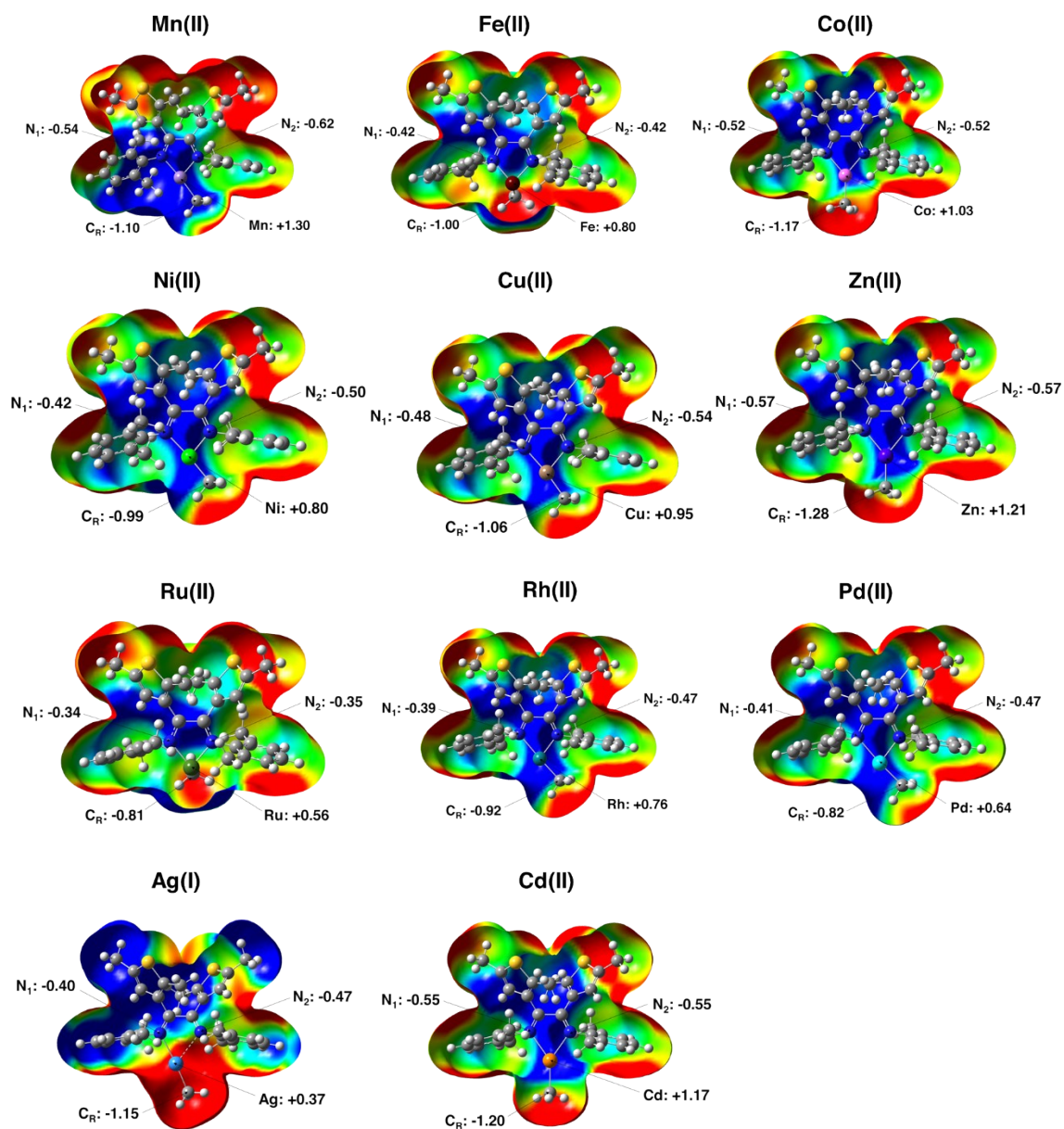


Fig. S14. The molecular electrostatic potential (MEP) maps and NBO charges of the active complex (A_1) structures with different metal substitutions. NBO charges are shown in black.

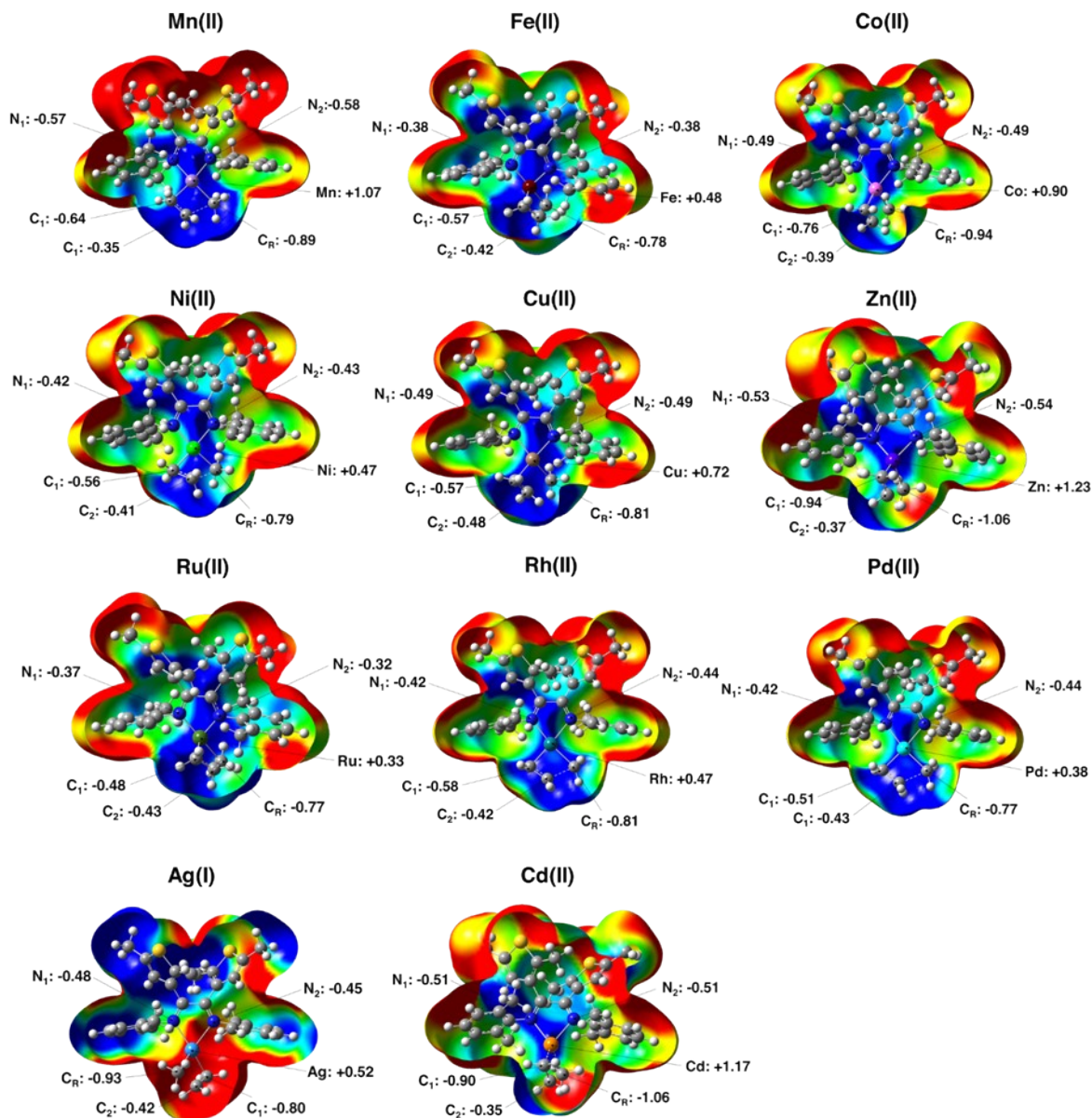


Fig. S15. The molecular electrostatic potential (MEP) maps and NBO charges of the transition-state (TS₁) complexes with different metal substitutions. NBO charges are shown in black.

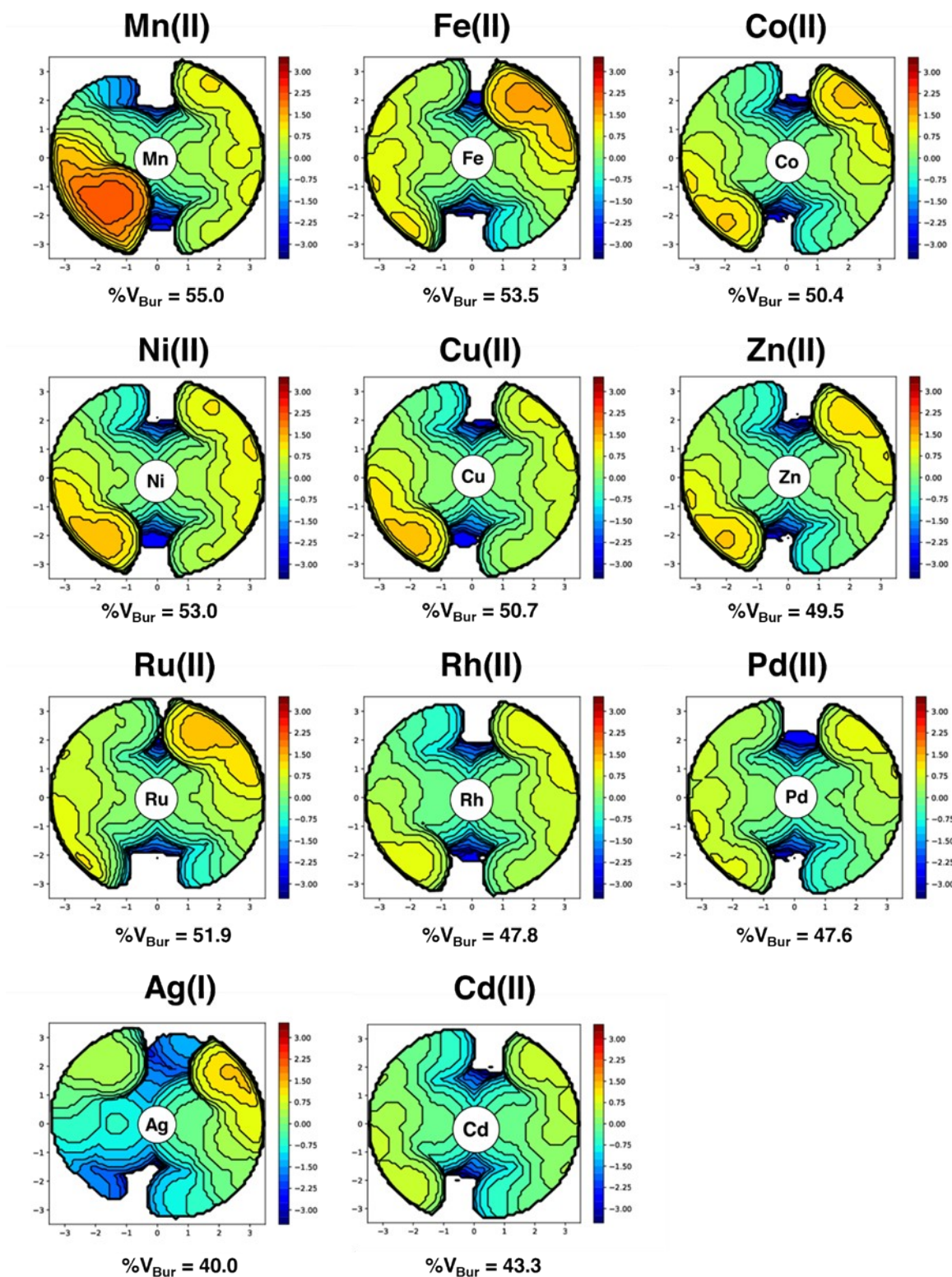


Fig. S16. Structures and topographic steric maps of active (A_1) complexes of M- α -diimine catalysts. Values on plots are given in Å, with a radius of 3.5 Å.

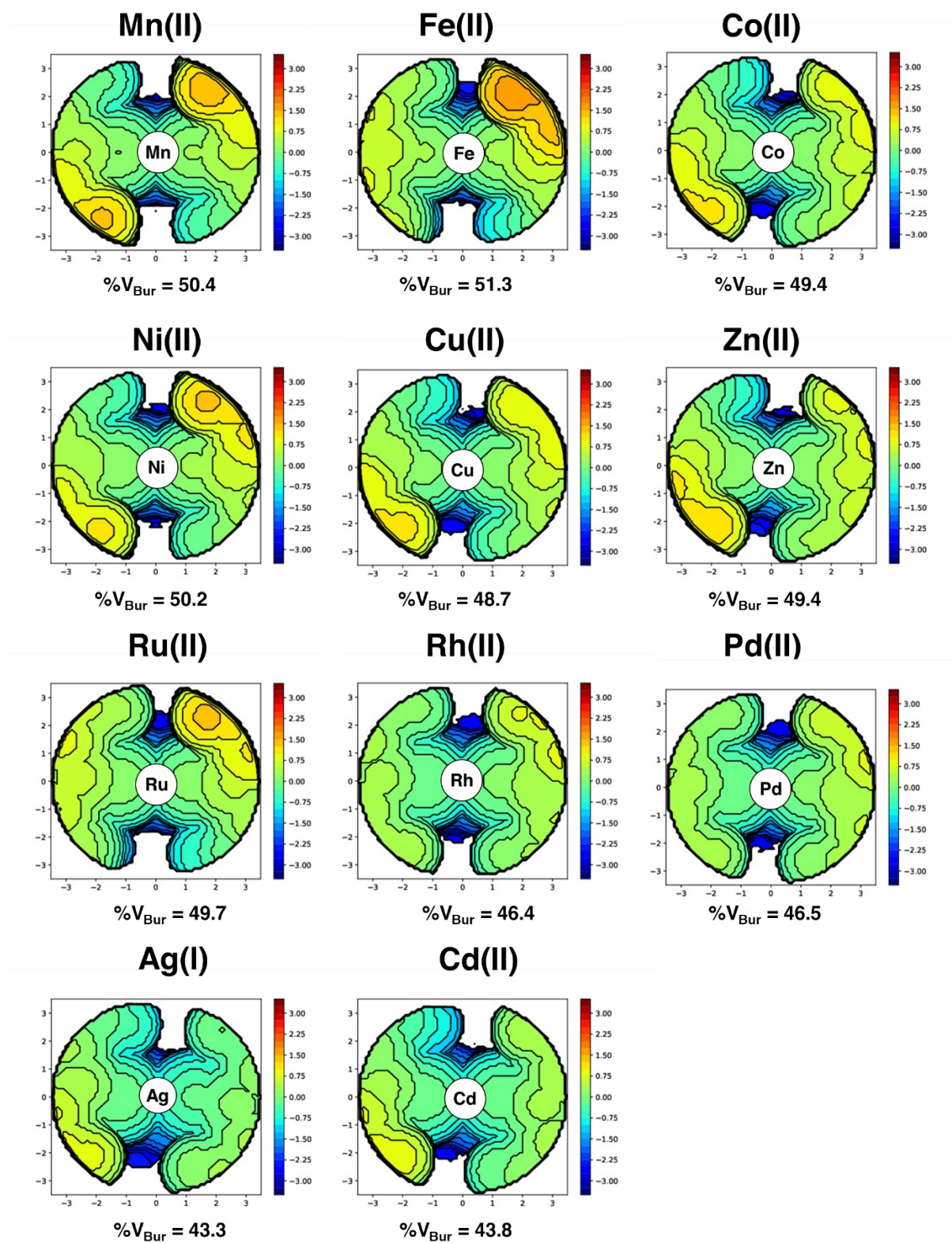


Fig. S17. Structures and topographic steric maps of transition-state (TS₁) complexes of M- α -diimine catalysts. Values on plots are given in Å, with a radius of 3.5 Å.

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Atomic coordinates of the optimized M- α -diimine catalysts

Ni-Me_pre-reaction											
Ni	-0.001000	2.150300	0.000200	C	0.372300	-2.596500	2.367700	C	-3.259700	-2.059800	-1.084000
Br	-0.591500	3.124500	-2.050100	H	-0.018300	-1.578000	2.449300	C	-4.596300	-2.439800	-1.002200
Br	0.588500	3.124100	2.050900	H	0.891400	-2.819000	3.305200	H	-5.085300	-2.855300	-1.878400
N	-1.299800	0.562000	0.181500	H	-0.476700	-3.281500	2.274200	C	-5.302700	-2.298300	0.188500
S	-2.385900	-4.058600	-1.083400	C	4.226900	-4.192800	-1.060700	H	-6.341500	-2.607500	0.241300
C	-0.755000	-0.589500	0.010700	H	3.903300	-5.184800	-1.394300	C	-4.677600	-1.775900	1.313300
C	-1.301900	-2.716900	-1.200100	H	5.093300	-4.326000	-0.404100	H	-5.229100	-1.685100	2.244600
C	-1.506000	-1.848400	-0.157900	H	4.554100	-3.628800	-1.938500	C	-3.343900	-1.364900	1.277200
C	-2.556100	-2.269900	0.726200	C	2.720200	0.736300	-0.175800	C	-2.482100	-2.195600	-2.369800
H	-2.870000	-1.704900	1.596000	C	3.328400	1.058100	-1.399900	H	-1.610200	-2.855300	-2.258400
C	-3.120200	-3.453600	0.372100	C	4.704400	1.272100	-1.408400	H	-2.103400	-1.228100	-2.721200
C	-0.369600	-2.596900	-2.367500	H	5.193800	1.512200	-2.348300	H	-3.107400	-2.618000	-3.159800
H	0.019800	-1.578000	-2.449300	C	5.447900	1.189100	-0.236200	C	-2.687100	-0.804300	2.512200
H	-0.888200	-2.820300	-3.305100	H	6.517600	1.374100	-0.256500	H	-2.741800	0.290300	2.522000
H	0.480300	-3.280800	-2.273500	C	4.820000	0.871100	0.959100	H	-1.630200	-1.084200	2.582200
C	-4.222900	-4.196900	1.060500	H	5.399500	0.807400	1.876100	H	-3.189000	-1.170600	3.411200
H	-3.898300	-5.188600	1.394000	C	3.445900	0.628300	1.018600	N	1.250200	-1.126500	0.059400
H	-5.089200	-4.331000	0.403900	C	2.528900	1.111300	-2.675000	S	2.277400	3.546300	-1.067100
H	-4.550800	-3.633300	1.938300	H	2.027500	0.154900	-2.876400	C	0.707300	0.048500	-0.025100
C	-2.720900	0.734100	0.175600	H	3.177800	1.332200	-3.526700	C	1.180400	2.221200	-1.166000
C	-3.329600	1.055200	1.399600	H	1.743400	1.873100	-2.633200	C	1.462600	1.295600	-0.183100
C	-4.705800	1.268000	1.407800	C	2.818600	0.241900	2.332800	C	2.583400	1.672500	0.634600
H	-5.195600	1.507600	2.347600	H	2.881000	-0.843100	2.481300	H	2.961800	1.077200	1.455400
C	-5.449000	1.184700	0.235400	H	1.772100	0.547500	2.398900	C	3.118700	2.874100	0.296800
H	-6.518900	1.368700	0.255400	H	3.347000	0.725900	3.158600	C	0.165300	2.179900	-2.269800
C	-4.820500	0.867400	-0.959900	Ni_A1				H	-0.223800	1.168200	-2.414200
H	-5.399700	0.803400	-1.877000	Ni	0.077100	-2.568400	-0.020100	H	0.612500	2.494400	-3.217600
C	-3.446300	0.625700	-1.019100	N	-1.278900	-1.171300	-0.040400	H	-0.681800	2.840800	-2.059200
C	-2.530500	1.108900	2.674800	S	-2.583700	3.485700	0.868200	C	4.269100	3.589700	0.934600
H	-2.028100	0.153100	2.876200	C	-0.804000	0.026000	0.034400	H	3.968500	4.564200	1.333100
H	-3.179700	1.329000	3.526500	C	-1.391500	2.253800	1.051400	H	5.082600	3.755900	0.221100
H	-1.745700	1.871500	2.633400	C	-1.616300	1.238700	0.147300	H	4.661800	2.990700	1.760300
C	-2.818100	0.240300	-2.333100	C	-2.772400	1.466700	-0.676900	C	2.671800	-1.312600	0.036600
H	-2.879300	-0.844700	-2.481900	H	-3.110600	0.778600	-1.442900	C	3.312200	-1.560500	1.256400
H	-1.772000	0.547100	-2.398900	C	-3.392000	2.648600	-0.424000	C	4.689700	-1.768600	1.228600
H	-3.346800	0.723900	-3.159000	C	-0.370200	2.362100	2.143800	H	5.216300	-1.954900	2.160100
N	1.299200	0.563100	-0.181500	H	0.087600	1.391200	2.351800	C	5.388900	-1.749100	0.026200
S	2.389800	-4.056400	1.083300	H	-0.832100	2.710800	3.072300	H	6.460600	-1.918700	0.021100
C	0.755400	-0.588800	-0.010700	H	0.428700	3.062300	1.878800	C	4.717200	-1.527100	-1.170200
C	1.304500	-2.715700	1.200100	C	-4.597500	3.229600	-1.095700	H	5.265200	-1.529000	-2.107900
C	1.507500	-1.847100	0.157700	H	-4.370700	4.187500	-1.575100	C	3.340100	-1.307200	-1.191200
C	2.558000	-2.267600	-0.726400	H	-5.411900	3.396300	-0.383200	C	2.535800	-1.585700	2.547200
H	2.871100	-1.702300	-1.596200	H	-4.957400	2.541100	-1.864700	H	2.038800	-0.627700	2.747600
C	3.123400	-3.450600	-0.372300	C	-2.662600	-1.503100	0.059200	H	3.192700	-1.801300	3.393100
								H	1.750800	-2.351600	2.524600

C	2.598300	-1.087900	-2.482900
H	2.235800	-0.056500	-2.565300
H	1.729200	-1.753200	-2.562200
H	3.247300	-1.281000	-3.340200
C	1.262200	-4.002000	-0.001100
H	1.919800	-4.014800	-0.877300
H	1.868900	-4.104000	0.903300
H	0.555000	-4.853900	-0.060200

Ni_R_i

Ni	0.056200	-2.529700	-0.011400
C	-1.302200	-3.859500	-0.104000
H	-0.945000	-4.892900	-0.108200
H	-1.922700	-3.699900	0.787200
H	-1.916500	-3.691700	-0.993700
N	-1.257400	-1.063400	-0.088200
S	-2.469300	3.499000	1.302000
C	-0.781500	0.131800	0.032300
C	-1.326000	2.209200	1.297300
C	-1.583700	1.344400	0.256000
C	-2.723400	1.738900	-0.525400
H	-3.092500	1.187800	-1.380400
C	-3.297700	2.894300	-0.099900
C	-0.291800	2.125400	2.380900
H	0.135400	1.119800	2.442100
H	-0.731900	2.349600	3.357200
H	0.525900	2.831900	2.205500
C	-4.480200	3.608700	-0.677700
H	-4.219600	4.618700	-1.010800
H	-5.292000	3.695500	0.051700
H	-4.859600	3.053400	-1.539600
C	-2.677900	-1.263100	-0.075800
C	-3.319300	-1.449100	-1.305600
C	-4.694700	-1.742200	-1.290500
H	-5.219000	-1.815500	-2.231300
C	-5.394400	-1.727900	-0.089800
H	-6.464200	-1.909400	-0.094100
C	-4.723700	-1.564600	1.116400
H	-5.270800	-1.623000	2.052900
C	-3.348600	-1.332300	1.148600
C	-2.547300	-1.381300	-2.598500
H	-1.674700	-2.045300	-2.582400
H	-2.172100	-0.368800	-2.797400
H	-3.176700	-1.669600	-3.443900
C	-2.611300	-1.167700	2.451500
H	-2.293500	-0.129000	2.599800
H	-1.712800	-1.796700	2.487700
H	-3.247800	-1.444000	3.295500
N	1.306800	-0.932200	0.119400
S	2.121000	3.709100	-1.297200
C	0.726200	0.209100	-0.022500
C	1.084600	2.331100	-1.293300
C	1.412300	1.489200	-0.253900
C	2.519500	1.971400	0.525200
H	2.931000	1.450200	1.380200
C	2.999500	3.169800	0.101000
C	0.063500	2.162100	-2.378800
H	-0.277100	1.124300	-2.441100
H	0.485700	2.422300	-3.354200
H	-0.810800	2.797800	-2.206700
C	4.119700	3.977800	0.679500
H	3.775400	4.959700	1.020600
H	4.918100	4.138600	-0.052200
H	4.548500	3.451300	1.536200
C	2.733300	-1.032800	0.108500
C	3.374500	-1.222100	1.341600
C	4.758400	-1.388400	1.337700
H	5.278100	-1.529600	2.281000
C	5.473600	-1.376200	0.144700
H	6.549700	-1.514600	0.156600

C	4.811300	-1.190700	-1.062500
H	5.373300	-1.182700	-1.992200
C	3.427600	-1.011300	-1.107600
C	2.594800	-1.182800	2.632800
H	2.285900	-0.159100	2.882000
H	3.198600	-1.552800	3.465100
H	1.677800	-1.781400	2.582900
C	2.723900	-0.777800	-2.420600
H	2.562600	0.293700	-2.586400
H	1.742400	-1.264300	-2.460000
H	3.321900	-1.156200	-3.253600
C	1.431400	-3.901600	-0.776000
C	1.440300	-3.981000	0.589400
H	2.176300	-3.298500	-1.289000
H	0.852600	-4.584600	-1.389100
H	2.202200	-3.454000	1.155600
H	0.866800	-4.732100	1.123300

Ni_TS_i

Ni	0.046200	-2.482600	0.053900
N	-1.282700	-0.976800	0.019900
S	-2.426900	3.732100	0.825600
C	-0.759500	0.202300	0.031600
C	-1.312900	2.433100	1.046800
C	-1.529600	1.454400	0.104200
C	-2.614000	1.766000	-0.785900
H	-2.938600	1.119100	-1.591700
C	-3.189200	2.971700	-0.538400
C	-0.350100	2.463100	2.195900
H	0.070600	1.470900	2.381700
H	-0.851200	2.782700	3.114800
H	0.480200	3.150700	2.005300
C	-4.320600	3.628000	-1.267500
H	-4.020500	4.587800	-1.700700
H	-5.172200	3.811700	-0.604500
H	-4.659500	2.979600	-2.079800
C	-2.700900	-1.152500	0.091000
C	-3.358300	-1.562000	-1.077700
C	-4.730100	-1.791100	-1.009100
H	-5.262700	-2.094800	-1.905800
C	-5.417800	-1.641900	0.191600
H	-6.485400	-1.831400	0.232000
C	-4.736200	-1.262400	1.339800
H	-5.272600	-1.160400	2.278900
C	-3.362800	-1.009500	1.315500
C	-2.599400	-1.727600	-2.369000
H	-1.817500	-2.490600	-2.276100
H	-2.097800	-0.800700	-2.673600
H	-3.267600	-2.027900	-3.179700
C	-2.641000	-0.590500	2.570700
H	-2.539600	0.499900	2.616300
H	-1.632300	-1.015400	2.632000
H	-3.193500	-0.910000	3.457900
N	1.271000	-0.985400	0.019000
S	2.424700	3.698600	-0.918000
C	0.749300	0.196100	-0.032800
C	1.311600	2.394200	-1.106500
C	1.526100	1.440900	-0.137300
C	2.607600	1.777400	0.747800
H	2.929700	1.153500	1.572300
C	3.182900	2.976000	0.468800
C	0.350200	2.393900	-2.257400
H	-0.072100	1.397700	-2.416500
H	0.853000	2.687500	-3.184000
H	-0.479100	3.087800	-2.086400
C	4.311600	3.652600	1.183200
H	4.009900	4.624100	1.588500
H	5.165500	3.818000	0.518200
H	4.647900	3.027000	2.014300
C	2.693900	-1.158500	-0.017800

C	3.328300	-1.521000	1.177300
C	4.705800	-1.725900	1.145400
H	5.223200	-1.993500	2.062300
C	5.417500	-1.599800	-0.043400
H	6.489300	-1.769000	-0.054100
C	4.754800	-1.274100	-1.219800
H	5.309600	-1.196600	-2.150400
C	3.377200	-1.047600	-1.233200
C	2.539100	-1.668200	2.452200
H	2.012200	-0.743400	2.719400
C	3.191000	-1.934300	3.287800
H	1.774700	-2.450500	2.356800
C	2.660600	-0.713400	-2.515900
H	2.458400	0.361300	-2.587300
H	1.698900	-1.235200	-2.592400
H	3.266100	-0.995000	-3.380900
C	-1.311600	-3.834500	0.622800
H	-1.097100	-4.748400	1.171400
H	-1.469100	-3.051700	1.383100
H	-2.215000	-3.935100	0.020500
C	0.117700	-4.387700	-0.788100
C	1.355500	-3.848300	-0.350700
H	-0.232500	-4.127700	-1.787000
H	-0.195300	-5.381300	-0.494300
H	2.025200	-3.395900	-1.077300
H	1.852100	-4.312200	0.500400

Ni_P_i

Ni	-0.044100	-2.311500	-0.151200
N	-1.304500	-0.832300	-0.144600
S	-2.293200	3.833800	1.074100
C	-0.751900	0.325600	-0.002600
C	-1.195900	2.506700	1.167300
C	-1.484600	1.581600	0.188600
C	-2.611600	1.957000	-0.621300
H	-2.992700	1.356700	-1.438600
C	-3.146200	3.158600	-0.281600
C	-0.174100	2.460600	2.264000
H	0.207200	1.445300	2.404100
H	-0.611800	2.778400	3.215200
H	0.676900	3.114300	2.047000
C	-4.300800	3.874000	-0.912200
H	-4.002400	4.847900	-1.313900
H	-5.109400	4.041800	-0.193400
H	-4.699500	3.274400	-1.734700
C	-2.715600	-1.044600	-0.066700
C	-3.374500	-1.403200	-1.251600
C	-4.740200	-1.667400	-1.183100
H	-5.276100	-1.930200	-2.090700
C	-5.416700	-1.603600	0.031200
H	-6.479500	-1.818800	0.071200
C	-4.730700	-1.278300	1.194600
H	-5.259200	-1.247100	2.143200
C	-3.364700	-0.991800	1.173400
C	-2.623200	-1.468400	-2.556700
H	-1.801600	-2.195700	-2.514500
H	-2.172800	-0.502600	-2.817700
H	-3.285900	-1.760200	-3.375000
C	-2.628700	-0.652100	2.443900
H	-2.474400	0.429300	2.533600
H	-1.643500	-1.131500	2.485500
H	-3.197900	-0.980000	3.317200
N	1.229300	-0.938600	0.005500
S	2.537300	3.704500	-0.963000
C	0.760200	0.266200	-0.051600
C	1.360900	2.452900	-1.111000
C	1.584800	1.474500	-0.166700
C	2.726000	1.750000	0.663000
H	3.066000	1.100200	1.459400
C	3.335600	2.928300	0.371200

C	0.341800	2.516300	-2.209800
H	-0.102800	1.534100	-2.393500
H	0.801600	2.845900	-3.146400
H	-0.467200	3.212400	-1.965200
C	4.528500	3.545200	1.033500
H	4.290000	4.521000	1.469300
H	5.351600	3.686600	0.325600
H	4.882000	2.891600	1.835300
C	2.634300	-1.217400	-0.029500
C	3.250900	-1.581200	1.173700
C	4.608000	-1.895700	1.135900
H	5.114300	-2.170200	2.056900
C	5.312200	-1.867900	-0.063400
H	6.367400	-2.120600	-0.077800
C	4.664000	-1.529700	-1.245300
H	5.213800	-1.524100	-2.182100
C	3.308700	-1.198800	-1.254400
C	2.470300	-1.605500	2.462200
H	2.084700	-0.612300	2.726400
H	3.094100	-1.949600	3.290700
H	1.601100	-2.271000	2.390300
C	2.595900	-0.849600	-2.534400
H	2.351600	0.218300	-2.575200
H	1.656500	-1.407700	-2.635700
H	3.219700	-1.081100	-3.401100
C	-0.942300	-5.213800	0.918500
H	-0.436000	-6.181400	0.974100
H	-0.765800	-4.682900	1.859300
H	-2.016500	-5.391400	0.818700
C	-0.387100	-4.422200	-0.263600
C	0.982700	-3.872300	-0.136900
H	-0.577600	-4.908400	-1.225000
H	1.637200	-3.948500	-1.006700
H	1.506900	-4.071400	0.799300
H	-1.151600	-3.509000	-0.375400

Ni_A₂

Ni	0.654000	-2.205200	-0.209500
N	1.315800	-0.473900	-0.027800
S	0.820400	4.315500	-1.013500
C	0.434700	0.475700	-0.067300
C	0.186000	2.718000	-1.139800
C	0.761200	1.900600	-0.189800
C	1.727300	2.585500	0.625200
H	2.288600	2.116000	1.422600
C	1.857700	3.902200	0.318000
C	-0.792100	2.391700	-2.229300
H	-0.849900	1.313100	-2.400500
H	-0.489000	2.855200	-3.172900
H	-1.797700	2.748500	-1.983700
C	2.744200	4.921900	0.963400
H	2.166100	5.746200	1.393700
H	3.452800	5.348400	0.246100
H	3.318500	4.453200	1.766900
C	2.724500	-0.213900	-0.051900
C	3.413100	-0.286000	1.164600
C	4.789300	-0.064600	1.140900
H	5.348700	-0.105200	2.071000
C	5.447300	0.194600	-0.056900
H	6.520000	0.358600	-0.060300
C	4.736900	0.232600	-1.251300
H	5.257400	0.422900	-2.185400
C	3.357500	0.027200	-1.274800
C	2.680200	-0.584700	2.446300
H	2.127000	-1.529000	2.373500
H	1.948800	0.195500	2.693500
H	3.376200	-0.664400	3.284700
C	2.578000	0.056900	-2.562500
H	1.922800	0.934700	-2.610200
H	1.946000	-0.833900	-2.668500

H	3.250100	0.096500	-3.422900
N	-1.079400	-1.300700	-0.119300
S	-3.722200	2.691300	1.029100
C	-0.993500	-0.019600	0.004800
C	-2.207600	1.874100	1.137400
C	-2.135800	0.880200	0.186700
C	-3.326800	0.781900	-0.613000
H	-3.459500	0.057500	-1.407900
C	-4.270000	1.705900	-0.294700
C	-1.238000	2.242800	2.220200
H	-0.506200	1.446200	2.380100
H	-1.758900	2.402400	3.169000
H	-0.691500	3.159100	1.974600
C	-5.612100	1.919800	-0.923200
H	-5.700400	2.921200	-1.357100
H	-6.420100	1.798200	-0.194500
H	-5.764700	1.188600	-1.721400
C	-2.298300	-2.034300	-0.013600
C	-2.750300	-2.681800	-1.174500
C	-3.912900	-3.442600	-1.086800
H	-4.292300	-3.937500	-1.976100
C	-4.583100	-3.578200	0.125200
H	-5.483200	-4.181600	0.181700
C	-4.094100	-2.954800	1.265900
H	-4.610500	-3.079200	2.213300
C	-2.941800	-2.167700	1.224800
C	-2.014500	-2.519800	-2.481000
H	-1.938100	-1.466900	-2.779100
H	-2.522300	-3.059500	-3.283800
H	-0.988200	-2.908000	-2.423900
C	-2.426700	-1.505100	2.476500
H	-2.786900	-0.472600	2.551000
H	-1.331700	-1.477400	2.507800
H	-2.772400	-2.042300	3.363300
C	2.087700	-3.315000	-0.390200
H	1.331700	-4.024300	-0.522800
H	2.602600	-3.180700	-1.351000
C	3.046700	-3.729300	0.705100
H	2.508600	-3.876300	1.649800
H	3.754600	-2.905600	0.861700
C	3.828900	-5.002500	0.360900
H	4.526400	-5.259300	1.163900
H	3.154200	-5.853200	0.215300
H	4.406500	-4.868100	-0.560000

Ni_R₂

Ni	0.730900	-2.162600	-0.147300
C	2.430100	-2.867900	-0.671200
H	2.176300	-3.587800	-1.463800
H	2.928800	-2.019500	-1.148400
C	3.378500	-3.501200	0.339900
H	3.004600	-4.484200	0.655700
H	3.442100	-2.880700	1.242300
C	4.789300	-3.658100	-0.235100
H	5.457800	-4.141300	0.484700
H	4.778800	-4.264500	-1.147600
H	5.209600	-2.677100	-0.484500
N	1.351400	-0.285400	-0.099400
S	0.727000	4.522100	-0.880900
C	0.441900	0.631400	-0.090700
C	0.164300	2.906000	-1.097300
C	0.715400	2.077400	-0.146200
C	1.605500	2.767600	0.746600
H	2.140400	2.290000	1.557400
C	1.703100	4.098700	0.492200
C	-0.735300	2.578400	-2.251800
H	-0.760700	1.501000	-2.438400
H	-0.380600	3.058800	-3.168800
H	-1.761200	2.913300	-2.067500
C	2.513600	5.125000	1.221700

H	1.882300	5.912100	1.647000
H	3.244400	5.602600	0.561000
H	3.060000	4.648100	2.039700
C	2.738800	0.072500	-0.069000
C	3.403300	-0.061400	1.156600
C	4.768600	0.214800	1.187500
H	5.306800	0.124300	2.126700
C	5.444300	0.596200	0.032600
H	6.509300	0.800800	0.070700
C	4.759800	0.704900	-1.171800
H	5.293000	0.989600	-2.074300
C	3.391400	0.442700	-1.248700
C	2.652300	-0.457600	2.402300
H	2.072600	-1.375600	2.248600
H	1.938100	0.317200	2.711400
H	3.339100	-0.624800	3.235600
C	2.649300	0.532500	-2.556000
H	2.021000	1.429700	-2.593800
H	1.996900	-0.336200	-2.707900
H	3.347000	0.578800	-3.395500
N	-1.048300	-1.184600	-0.050700
S	-3.779400	2.771200	0.917700
C	-0.973100	0.100900	-0.014800
C	-2.269300	1.952400	1.085500
C	-2.135000	0.996600	0.056000
C	-3.273500	0.927800	-0.768700
H	-3.356300	0.236400	-1.598600
C	-4.239600	1.836100	-0.472900
C	-1.364300	2.282800	2.234200
H	-0.610200	1.503700	2.376800
H	-1.932000	2.362100	3.166400
H	-0.841700	3.231100	2.072700
C	-5.542200	2.068200	-1.174300
H	-5.611500	3.085800	-1.572700
H	-6.392800	1.913200	-0.502700
H	-5.639800	1.369100	-2.009100
C	-2.308100	-1.855100	0.018000
C	-2.772000	-2.453900	-1.165000
C	-3.964800	-3.169500	-1.111700
H	-4.347700	-3.631600	-2.017100
C	-4.662500	-3.300900	0.086000
H	-5.586200	-3.869400	0.115600
C	-4.174500	-2.709600	1.242700
H	-4.719100	-2.817400	2.176500
C	-2.989400	-1.968800	1.235100
C	-2.005600	-2.296600	-2.454000
H	-1.917100	-1.243900	-2.750400
H	-2.497800	-2.832200	-3.269300
H	-0.981700	-2.684800	-2.368400
C	-2.506700	-1.306900	2.501400
H	-2.966000	-0.318400	2.615600
H	-1.421100	-1.163400	2.515000
H	-2.780500	-1.902300	3.376900
C	0.262100	-3.638300	1.232700
C	-0.014800	-4.149500	-0.005000
H	-0.524100	-3.174300	1.823600
H	1.187400	-3.868300	1.751400
H	-1.024900	-4.112000	-0.403700
H	0.682500	-4.814900	-0.502500

Ni_TS₂

Ni	0.589500	-2.211500	0.067100
N	1.326400	-0.325100	0.030300
S	0.806000	4.479300	-0.848100
C	0.430800	0.602900	-0.003100
C	0.218900	2.870800	-1.063300
C	0.725300	2.044200	-0.087500
C	1.600900	2.728000	0.824200
H	2.099800	2.247900	1.656900
C	1.733300	4.053700	0.557900

C	-0.656000	2.546700	-2.237300
H	-0.689500	1.468200	-2.415700
H	-0.274500	3.017000	-3.148900
H	-1.682300	2.893600	-2.079600
C	2.541800	5.073000	1.299500
H	1.913600	5.877200	1.696600
H	3.301100	5.528600	0.655600
H	3.054100	4.595700	2.139100
C	2.715400	0.018700	0.001400
C	3.428200	-0.094400	1.203200
C	4.785900	0.214600	1.188700
H	5.356100	0.143200	2.110500
C	5.414000	0.606700	0.010300
H	6.473600	0.840400	0.012800
C	4.688600	0.686600	-1.170900
H	5.184500	0.978200	-2.092300
C	3.323900	0.390100	-1.202600
C	2.731100	-0.519900	2.469800
H	2.247600	-1.497500	2.349500
H	1.942100	0.185100	2.760700
H	3.437500	-0.591800	3.300400
C	2.550500	0.483800	-2.492700
H	2.051400	1.455800	-2.577800
H	1.778300	-0.290100	-2.569600
H	3.218700	0.377000	-3.351000
N	-1.071200	-1.204200	0.056400
S	-3.792400	2.827500	0.730900
C	-0.985500	0.084600	0.048800
C	-2.309300	1.990200	1.008500
C	-2.144900	0.991300	0.077100
C	-3.238400	0.907600	-0.852000
H	-3.293500	0.184400	-1.656300
C	-4.200000	1.844000	-0.642400
C	-1.453400	2.356700	2.183800
H	-0.721000	1.572600	2.395500
H	-2.062800	2.486500	3.083600
H	-0.907100	3.288600	2.006200
C	-5.461800	2.067800	-1.417100
H	-5.494500	3.069800	-1.857400
H	-6.347200	1.951600	-0.783600
H	-5.529400	1.337700	-2.227900
C	-2.354000	-1.846000	0.074100
C	-2.787700	-2.445300	-1.115900
C	-4.017000	-3.100000	-1.103900
H	-4.381100	-3.560800	-2.017900
C	-4.773000	-3.174800	0.061800
H	-5.725900	-3.693800	0.057700
C	-4.301300	-2.599100	1.234300
H	-4.884300	-2.675100	2.147700
C	-3.080400	-1.922400	1.266500
C	-1.949600	-2.368500	-2.365800
H	-1.746400	-1.332000	-2.663000
H	-2.447900	-2.864400	-3.202300
H	-0.973700	-2.850700	-2.220200
C	-2.571200	-1.310600	2.545800
H	-2.778700	-0.235000	2.577700
H	-1.488000	-1.439900	2.657800
H	-3.056400	-1.767400	3.412000
C	1.119100	-4.100900	0.810900
C	-0.257300	-3.863500	0.621000
H	1.576200	-3.853800	1.768200
H	1.586100	-4.947900	0.324200
H	-0.873900	-3.572100	1.468100
H	-0.786000	-4.401000	-0.164200
C	2.297100	-3.087600	-0.631800
H	2.065600	-3.857500	-1.372500
H	2.322000	-2.132600	-1.174500
C	3.653700	-3.319100	0.019400
H	3.704600	-4.326900	0.448000
H	3.794500	-2.616200	0.846300

C	4.793400	-3.141200	-0.986400
H	5.759200	-3.336000	-0.510500
H	4.688400	-3.832300	-1.830000
H	4.812100	-2.119500	-1.378400

Ni₂P₂

Ni	-0.873400	-1.832700	-0.409400
N	-1.223200	0.074500	-0.422400
S	0.077700	4.484800	1.341500
C	-0.195400	0.793300	-0.117600
C	0.399700	2.791900	1.287200
C	-0.242400	2.220500	0.210300
C	-1.005400	3.169300	-0.554100
H	-1.579900	2.909300	-1.435000
C	-0.917800	4.440300	-0.082900
C	1.217400	2.154200	2.370800
H	1.031900	1.077400	2.421800
H	0.962600	2.575200	3.347900
H	2.289000	2.305100	2.204900
C	-1.551300	5.681300	-0.631200
H	-0.800900	6.424300	-0.920500
H	-2.219300	6.147400	0.100400
H	-2.142000	5.431900	-1.516600
C	-2.572000	0.540800	-0.366600
C	-3.267800	0.647700	-1.578600
C	-4.614300	1.001600	-1.528900
H	-5.170500	1.103800	-2.456200
C	-5.249600	1.212700	-0.309100
H	-6.301200	1.478900	-0.284600
C	-4.543100	1.067500	0.878600
H	-5.048400	1.211500	1.829300
C	-3.189800	0.725600	0.878000
C	-2.564100	0.392200	-2.886000
H	-2.140800	-0.620300	-2.921400
H	-1.729300	1.086400	-3.043300
H	-3.251400	0.499400	-3.728500
C	-2.443300	0.535800	2.173300
H	-1.790500	1.390400	2.385000
H	-1.814100	-0.362600	2.152600
H	-3.141700	0.435500	3.007900
N	0.893600	-1.284000	-0.069000
S	4.351800	2.155600	-0.801200
C	1.090100	-0.004300	-0.103600
C	2.718600	1.652400	-1.024600
C	2.404800	0.642800	-0.139100
C	3.509600	0.279900	0.706600
H	3.464500	-0.494500	1.461600
C	4.626600	1.020500	0.485900
C	1.896100	2.266600	-2.118600
H	1.039100	1.635900	-2.371500
H	2.490900	2.387200	-3.028900
H	1.517100	3.251800	-1.827900
C	5.948200	0.937400	1.184900
H	6.205200	1.880800	1.677800
H	6.756000	0.692900	0.487600
H	5.911700	0.154200	1.946700
C	1.968400	-2.230200	-0.047000
C	2.249300	-2.859800	1.171500
C	3.263200	-3.816000	1.186900
H	3.509400	-4.312500	2.121200
C	3.952800	-4.141100	0.023400
H	4.736000	-4.891800	0.050000
C	3.633300	-3.514600	-1.175500
H	4.165500	-3.780800	-2.084300
C	2.631500	-2.545800	-1.237100
C	1.501900	-2.481200	2.423900
H	1.713500	-1.447000	2.726100
H	1.779900	-3.131300	3.256900
H	0.417100	-2.552200	2.281100
C	2.267800	-1.873900	-2.535300

H	2.572300	-0.820700	-2.538100
H	1.185400	-1.905600	-2.713100
H	2.760900	-2.365100	-3.377500
C	-3.306500	-3.394800	0.660300
H	-3.500200	-4.435300	0.946800
H	-2.843200	-2.911300	1.531800
C	-2.304500	-3.390900	-0.494600
C	-0.883700	-3.694400	-0.205700
H	-2.690000	-3.874900	-1.398600
H	-0.320600	-4.230900	-0.970900
H	-0.648000	-4.032700	0.804300
C	-4.616000	-2.682100	0.316300
H	-5.138300	-3.241300	-0.470600
H	-4.391400	-1.691100	-0.101600
C	-5.529000	-2.510000	1.526800
H	-6.457300	-2.003000	1.247800
H	-5.792500	-3.476100	1.971000
H	-5.037800	-1.906700	2.299600
H	-2.367800	-2.266300	-0.904000

Ni₂A₃

Ni	1.211300	-1.535000	0.374900
N	-0.724500	-1.549600	0.080300
S	-5.040200	0.790400	0.489900
C	-1.258300	-0.374900	0.064200
C	-3.350600	0.795000	0.835100
C	-2.699000	-0.111500	0.028100
C	-3.588200	-0.816100	-0.855500
H	-3.261700	-1.570600	-1.561600
C	-4.884500	-0.427200	-0.741900
C	-2.819500	1.654000	1.943400
H	-1.839600	1.302800	2.278300
H	-3.488400	1.627100	2.808800
H	-2.715200	2.697200	1.627800
C	-6.073400	-0.917100	-1.509300
H	-6.553300	-0.108800	-2.070700
H	-6.825400	-1.356400	-0.845900
H	-5.760200	-1.686000	-2.220400
C	-1.465100	-2.766100	0.153000
C	-1.378600	-3.622000	-0.957200
C	-2.053600	-4.837900	-0.898400
H	-2.016900	-5.507800	-1.752500
C	-2.763500	-5.201400	0.242000
H	-3.277600	-6.156300	0.278500
C	-2.803200	-4.351000	1.339300
H	-3.343000	-6.480000	2.233800
C	-2.157200	-3.113400	1.322000
C	-0.609100	-3.208300	-2.186400
H	0.453500	-3.039300	-1.964900
H	-0.995100	-2.274700	-2.613900
H	-0.664900	-3.979100	-2.958800
C	-2.211800	-2.210900	2.527700
H	-3.023200	-1.480100	2.434400
H	-1.279000	-1.654000	2.669900
H	-2.392700	-2.794800	3.433700
N	0.979700	0.313600	0.298700
S	-1.522700	4.235800	-1.291600
C	-0.224500	0.728200	0.057200
C	-1.338000	2.522000	-1.291700
C	-0.572000	2.126200	-0.216000
C	-0.130900	3.230000	0.592600
H	0.481500	3.123000	1.478900
C	-0.579500	4.434800	0.154700
C	-1.919100	1.712700	-2.412900
H	-1.462000	0.720600	-2.463200
H	-1.742800	2.202500	-3.375400
H	-2.999300	1.580500	-2.292600
C	-0.342400	5.787200	0.752200
H	-1.280600	6.271800	1.041600
H	0.174600	6.450100	0.050800

H	0.280100	5.690000	1.645500
C	2.112800	1.188600	0.279000
C	2.694500	1.528800	1.506600
C	3.836900	2.325800	1.480900
H	4.303800	2.612700	2.418700
C	4.384500	2.748400	0.273400
H	5.278400	3.363700	0.270300
C	3.796600	2.373900	-0.928400
H	4.237600	2.690400	-1.869100
C	2.648700	1.580900	-0.952400
C	2.094600	1.053000	2.803500
H	1.059400	1.395300	2.927500
H	2.670200	1.418300	3.657300
H	2.072500	-0.042200	2.851900
C	2.033700	1.142700	-2.255200
H	1.100800	1.681400	-2.457200
H	1.803500	0.070100	-2.250600
H	2.715000	1.335400	-3.087300
C	2.969000	-1.874900	0.709200
H	3.249800	-1.851600	1.769500
H	2.651300	-2.839600	0.484900
C	4.103100	-1.434100	-0.188500
H	4.363600	-0.401900	0.079000
H	3.778600	-1.415000	-1.238100
C	5.359700	-2.306800	-0.066000
H	5.682200	-2.328500	0.984100
H	5.115600	-3.343400	-0.337400
C	6.508300	-1.805900	-0.942900
H	6.741500	-0.767900	-0.670200
H	6.179400	-1.783700	-1.990700
C	7.764500	-2.666000	-0.818300
H	8.569600	-2.286800	-1.455200
H	8.131700	-2.679000	0.214100
H	7.563400	-3.701900	-1.113800

Ni₃R₃

Ni	0.756900	-1.939800	-0.566200
C	2.614900	-2.353100	-0.759600
H	2.773600	-3.273000	-1.333000
H	2.985500	-1.521900	-1.370400
C	3.370100	-2.423100	0.564000
H	3.240600	-3.410700	1.026800
H	2.967500	-1.702800	1.282800
C	4.864900	-2.131000	0.384500
H	5.321500	-2.912800	-0.237700
H	4.973600	-1.189000	-0.169500
C	5.619000	-2.014900	1.708400
H	5.124800	-1.256600	2.332600
H	5.549000	-2.961500	2.260100
C	7.084800	-1.632400	1.514700
H	7.168800	-0.668900	0.998000
H	7.607100	-1.548600	2.473000
H	7.610700	-2.380100	0.910800
N	1.086700	0.017900	-0.210000
S	-0.662800	4.490500	-1.335800
C	0.022700	0.750500	-0.189300
C	-0.873300	2.780700	-1.303000
C	-0.025500	2.209300	-0.377200
C	0.797200	3.179300	0.291500
H	1.532900	2.934600	1.045000
C	0.556000	4.458000	-0.099900
C	-1.835900	2.133800	-2.255200
H	-1.619200	1.068500	-2.377300
H	-1.770100	2.592100	-3.246400
H	-2.867900	2.233800	-1.902700
C	1.205400	5.714700	0.391400
H	0.476800	6.397500	0.840500
H	1.709900	6.249400	-0.419900
H	1.953900	5.469100	1.149500
C	2.372300	0.653100	-0.281900

C	3.074100	0.868300	0.909600
C	4.348900	1.429700	0.820000
H	4.914800	1.601200	1.731600
C	4.898500	1.762100	-0.411700
H	5.894000	2.191000	-0.463700
C	4.174600	1.542300	-1.579100
H	4.604800	1.804800	-2.541300
C	2.897800	0.985600	-1.537200
C	2.471400	0.573500	2.261900
H	1.710100	-0.210800	2.217700
H	1.995600	1.467100	2.686900
H	3.242600	0.254400	2.968500
C	2.097200	0.762700	-2.793500
H	1.231100	1.434000	-2.831600
H	1.718900	-0.265800	-2.856600
H	2.705300	0.950600	-3.681500
N	-1.166800	-1.268800	-0.313800
S	-3.997200	2.000100	2.057400
C	-1.262800	-0.022900	-0.006500
C	-2.419200	1.424800	1.669900
C	-2.458700	0.639500	0.538200
C	-3.785900	0.506100	0.003400
H	-4.029100	-0.073300	-0.877200
C	-4.724800	1.199600	0.699200
C	-1.265800	1.756900	2.569200
H	-0.425300	1.078000	2.401600
H	-1.552200	1.663200	3.621100
H	-0.914800	2.780600	2.402700
C	-6.192200	1.308400	0.421400
H	-6.491300	2.344100	0.229900
H	-6.788500	0.937300	1.261200
H	-6.444600	0.713100	-0.460100
C	-2.289800	-2.143200	-0.175400
C	-3.004500	-2.493400	-1.328500
C	-4.050100	-3.407400	-1.193300
H	-4.621500	-3.691200	-2.072700
C	-4.364400	-3.953900	0.045100
H	-5.177100	-4.667600	0.132400
C	-3.635000	-3.591200	1.172200
H	-3.881900	-4.021900	2.138400
C	-2.583700	-2.679200	1.086300
C	-2.701100	-1.858700	-2.664400
H	-3.217000	-0.895900	-2.774900
H	-3.035800	-2.498500	-3.485300
H	-1.632300	-1.659800	-2.798300
C	-1.800700	-2.272900	2.309000
H	-2.059500	-1.253300	2.617500
H	-0.718400	-2.294700	2.129900
H	-2.016400	-2.939500	3.147500
C	0.418700	-3.963100	-0.242000
C	0.225400	-3.679800	-1.568100
H	-0.431700	-4.000900	0.434900
H	1.349300	-4.383100	0.124600
H	-0.778600	-3.512600	-1.943500
H	0.996100	-3.858700	-2.311200

Ni₃TS₃

Ni	0.589500	-2.211500	0.067100
N	1.326400	-0.325100	0.030300
S	0.806000	4.479300	-0.848100
C	0.430800	0.602900	-0.003100
C	0.218900	2.870800	-1.063300
C	0.725300	2.044200	-0.087500
C	1.600900	2.728000	0.824200
H	2.099800	2.247900	1.656900
C	1.733300	4.053700	0.557900
C	-0.656000	2.546700	-2.237300
H	-0.689500	1.468200	-2.415700
H	-0.274500	3.017000	-3.148900
H	-1.682300	2.893600	-2.079600

C	2.541800	5.073000	1.299500
H	1.913600	5.877200	1.696600
H	3.301100	5.528600	0.655600
H	3.054100	4.595700	2.139100
C	2.715400	0.018700	0.001400
C	3.428200	-0.094400	1.203200
C	4.785900	0.214600	1.188700
H	5.356100	0.143200	2.110500
C	5.414000	0.606700	0.010300
H	6.473600	0.840400	0.012800
C	4.688600	0.686600	-1.170900
H	5.184500	0.978200	-2.092300
C	3.323900	0.390100	-1.202600
C	2.731100	-0.519900	2.469800
H	2.247600	-1.497500	2.349500
H	1.942100	0.185100	2.607700
H	3.437500	-0.591800	3.300400
C	2.550500	0.483800	-2.492700
H	2.051400	1.455800	-2.577800
H	1.778300	-0.290100	-2.569600
H	3.218700	0.377000	-3.351000
N	-1.071200	-1.204200	0.056400
S	-3.792400	2.827500	0.730900
C	-0.985500	0.084600	0.048800
C	-2.309300	1.990200	1.008500
C	-2.144900	0.991300	0.077100
C	-3.238400	0.907600	-0.852000
H	-3.293500	0.184400	-1.656300
C	-4.200000	1.844000	-0.642400
C	-1.453400	2.356700	2.183800
H	-0.721000	1.572600	2.395500
H	-2.062800	2.486500	3.083600
H	-0.907100	3.288600	2.006200
C	-5.461800	2.067800	-1.417100
H	-5.494500	3.069800	-1.857400
H	-6.347200	1.951600	-0.783600
H	-5.529400	1.337700	-2.227900
C	-2.354000	-1.846000	0.074100
C	-2.787700	-2.445300	-1.115900
C	-4.017000	-3.100000	-1.103900
H	-4.381100	-3.560800	-2.017900
C	-4.773000	-3.174800	0.061800
H	-5.725900	-3.693800	0.057700
C	-4.301300	-2.599100	1.234300
H	-4.884300	-2.675100	2.147700
C	-3.080400	-1.922400	1.266500
C	-1.949600	-2.368500	-2.365800
H	-1.746400	-1.332000	-2.663000
H	-2.447900	-2.864400	-3.202300
H	-0.973700	-2.850700	-2.220200
C	-2.571200	-1.310600	2.545800
H	-2.778700	-0.235000	2.577700
H	-1.488000	-1.439900	2.657800
H	-3.056400	-1.767400	3.412000
C	1.119100	-4.100900	0.810900
C	-0.257300	-3.863500	0.621000
H	1.576200	-3.853800	1.768200
H	1.586100	-4.947900	0.324200
H	-0.873900	-3.572100	1.468100
H	-0.786000	-4.401000	-0.164200
C	2.297100	-3.087600	-0.631800
H	2.065600	-3.857500	-1.372500
H	2.322000	-2.132600	-1.174500
C	3.653700	-3.319100	0.019400
H	3.704600	-4.326900	0.448000
H	3.794500	-2.616200	0.846300
C	4.793400	-3.141200	-0.986400
H	5.759200	-3.336000	-0.510500
H	4.688400	-3.832300	-1.830000
H	4.812100	-2.119500	-1.378400

Ni_P₃

Ni	-0.672400	-1.701100	-0.576800
N	-0.825400	0.232700	-0.579400
S	0.778500	4.452200	1.388700
C	0.244400	0.836900	-0.183600
C	0.926800	2.736100	1.313700
C	0.318500	2.255800	0.174600
C	-0.277500	3.293900	-0.621500
H	-0.802800	3.112700	-1.551600
C	-0.097100	4.539500	-0.110600
C	1.583500	1.994600	2.440000
H	1.281200	0.943300	2.447600
H	1.297400	2.422400	3.405400
H	2.674900	2.032600	2.361700
C	-0.552000	5.850400	-0.673500
H	0.292400	6.515000	-0.883500
H	-1.224700	6.371200	0.015700
H	-1.092200	5.681000	-1.608600
C	-2.116000	0.843400	-0.618100
C	-2.692300	1.051700	-1.878600
C	-3.984300	1.570500	-1.927300
H	-4.446100	1.755200	-2.892900
C	-4.685200	1.842900	-0.756700
H	-5.693800	2.240200	-0.808300
C	-4.103800	1.588000	0.479500
H	-4.666700	1.774700	1.389700
C	-2.807500	1.080700	0.577800
C	-1.919400	0.732800	-3.131800
H	-1.611600	-0.320800	-3.154900
H	-1.001700	1.329200	-3.208800
H	-2.520400	0.927800	-4.023200
C	-2.198100	0.782300	1.923300
H	-1.485500	1.561200	2.218300
H	-1.660900	-0.173900	1.924700
H	-2.972800	0.731200	2.692600
N	1.111500	-1.341100	-0.101100
S	4.942700	1.736900	-0.513000
C	1.438000	-0.088000	-0.093300
C	3.288300	1.404100	-0.862800
C	2.810400	0.422300	-0.020600
C	3.807600	-0.059200	0.896400
H	3.629800	-0.831900	1.633300
C	5.006500	0.566700	0.770200
C	2.613700	2.109400	-2.002100
H	1.721800	1.567700	-2.330200
H	3.284200	1.283300	-2.863400
H	2.309700	3.122900	-1.720500
C	6.257700	0.343300	1.561800
H	6.570000	1.250400	2.089600
H	7.086800	0.026800	0.920600
H	6.087400	-0.440900	2.304200
C	2.080900	-2.392200	-0.022100
C	2.211400	-3.061100	1.200900
C	3.120000	-4.115900	1.267300
H	3.249200	-4.645700	2.206800
C	3.852700	-4.496100	0.147700
H	4.552300	-5.323000	0.213700
C	3.682600	-3.826200	-1.058300
H	4.247500	-4.134400	-1.933400
C	2.790400	-2.759700	-1.169800
C	1.420900	-2.622900	2.406500
H	1.716400	-1.620500	2.743700
H	1.571300	-3.309400	3.243200
H	0.347300	-2.578400	2.188700
C	2.587600	-2.038700	-2.476700
H	2.991000	-1.020100	-2.436800
H	1.522700	-1.962800	-2.730900
H	3.090700	-2.564200	-3.291800
C	-3.301500	-2.985700	0.336900

H	-3.597000	-3.996900	0.640400
H	-2.839000	-2.519000	1.218000
C	-2.248500	-3.099500	-0.765500
C	-0.886400	-3.552800	-0.399700
H	-2.637000	-3.544900	-1.687900
H	-0.338700	-4.139500	-1.138900
H	-0.747300	-3.922500	0.617200
C	-4.527900	-2.175500	-0.087000
H	-5.105900	-2.746700	-0.826000
H	-4.204800	-1.252600	-0.591600
C	-5.422700	-1.791200	1.089800
H	-5.683800	-2.686700	1.670700
H	-4.850900	-1.139100	1.767000
C	-6.701000	-1.073100	0.657900
H	-6.434900	-0.237600	-0.002600
H	-7.314200	-1.757400	0.057400
C	-7.515400	-0.553800	1.840700
H	-6.936800	0.169200	2.428600
H	-8.431900	-0.057300	1.507300
H	-7.803000	-1.370800	2.512000
H	-2.166500	-1.978900	-1.181400

Mn_A₁

N	1.218200	-1.151100	0.041000
S	2.466800	3.508000	-0.905900
C	0.655500	0.084400	0.022900
C	1.316300	2.232700	-1.088100
C	1.486100	1.291000	-0.098200
C	2.567400	1.610800	0.793100
H	2.858200	0.993800	1.634600
C	3.189200	2.782300	0.497600
C	0.345600	2.258800	-2.229700
H	-0.065900	1.261600	-2.410100
H	0.831500	2.593900	-3.151100
H	-0.495000	2.931000	-2.025300
C	4.335300	3.430800	1.210500
H	4.067000	4.421800	1.591200
H	5.202300	3.549100	0.552300
H	4.638100	2.811700	2.059200
C	2.627300	-1.370600	0.016300
C	3.266100	-1.688800	1.224400
C	4.639400	-1.920400	1.195100
H	5.159000	-2.159000	2.118500
C	5.345200	-1.852700	-0.001800
H	6.414800	-2.036300	-0.009500
C	4.684300	-1.562600	-1.190200
H	5.239700	-1.524100	-2.122700
C	3.311000	-1.323800	-1.206700
C	2.483600	-1.783200	2.508100
H	1.797700	-2.642100	2.495900
H	1.872300	-0.890800	2.685500
H	3.149900	-1.913400	3.364300
C	2.585900	-1.025400	-2.491000
H	2.231600	0.011000	-2.513700
H	1.709600	-1.674600	-2.619700
H	3.240700	-1.176100	-3.352500
N	-1.294600	-1.144900	0.111800
S	-2.635100	3.592300	0.499500
C	-0.773600	0.089600	0.092900
C	-1.439100	2.400900	0.867900
C	-1.606000	1.296200	0.065800
C	-2.722700	1.421100	-0.831400
H	-3.012900	0.651100	-1.538100
C	-3.373600	2.609600	-0.729600
C	-0.463700	2.639400	1.979100
H	-0.037200	1.694000	2.325200
H	-0.952100	3.119900	2.832200
H	0.364900	3.279500	1.657400
C	-4.552800	3.095600	-1.514200
H	-4.313300	3.998000	-2.086300

H	-5.401200	3.329000	-0.862600
H	-4.870600	2.322000	-2.218400
C	-2.665100	-1.496800	0.228100
C	-3.159100	-2.352400	-0.778400
C	-4.479700	-2.781800	-0.711900
H	-4.874700	-3.428400	-1.490100
C	-5.292300	-2.388000	0.347300
H	-6.322000	-2.726400	0.395900
C	-4.778000	-1.582300	1.354000
H	-5.408100	-1.304500	2.194300
C	-3.457800	-1.125800	1.327500
C	-2.265600	-2.778300	-1.923000
H	-1.785300	-1.927400	-2.419200
H	-2.827900	-3.333000	-2.678700
H	-1.470600	-3.494400	-1.618200
C	-2.937900	-0.290000	2.466800
H	-3.146300	0.772200	2.300200
H	-1.856400	-0.396200	2.596200
H	-3.422100	-0.583600	3.402200
C	1.191800	-4.196700	-0.261200
H	0.554300	-5.094100	-0.294100
H	1.760400	-4.118700	-1.195500
H	1.900200	-4.280200	0.569500
Mn	0.004800	-2.596500	-0.063500

Mn_R₁

N	-1.215500	-1.107600	0.098400
S	-2.796800	3.515300	0.746800
C	-0.750000	0.162000	0.060200
C	-1.571700	2.328800	1.025600
C	-1.659100	1.320300	0.094500
C	-2.738200	1.518400	-0.834600
H	-2.971700	0.834800	-1.641700
C	-3.440300	2.662100	-0.622300
C	-0.631900	2.482900	2.182400
H	-0.165300	1.524600	2.429000
H	-1.159300	2.837900	3.073100
H	0.169400	3.194300	1.955700
C	-4.610200	3.189500	-1.394300
H	-4.399200	4.171700	-1.830200
H	-5.497800	3.289100	-0.760700
H	-4.853300	2.501800	-2.208800
C	-2.619000	-1.376900	0.125900
C	-3.227100	-1.813100	-1.060600
C	-4.590200	-2.097900	-1.037000
H	-5.082200	-2.427000	-1.947900
C	-5.321600	-1.966100	0.139300
H	-6.383000	-2.191700	0.145400
C	-4.692400	-1.557800	1.308500
H	-5.264200	-1.469900	2.227900
C	-3.328900	-1.260300	1.327200
C	-2.420400	-1.968100	-2.324700
H	-1.696800	-2.793200	-2.241500
H	-1.847500	-1.064000	-2.562200
H	-3.065600	-2.194300	-3.177400
C	-2.650900	-0.822500	2.598000
H	-2.489700	0.261200	2.601400
H	-1.669800	-1.297500	2.718300
H	-3.259500	-1.073700	3.470300
N	1.313200	-0.903400	0.033100
S	2.202800	3.864200	-0.838600
C	0.673200	0.274600	-0.002400
C	1.154600	2.508000	-1.060400
C	1.390800	1.557100	-0.096100
C	2.438800	1.937700	0.811300
H	2.769600	1.323600	1.640700
C	2.970400	3.161300	0.551700
C	0.195700	2.483300	-2.211300
H	-0.112800	1.457000	-2.431400
H	0.653200	2.897900	-3.114800

H	-0.708700	3.060300	-1.991200
C	4.055900	3.878900	1.293000
H	3.705600	4.833100	1.700300
H	4.914900	4.087100	0.646600
H	4.402700	3.261500	2.126100
C	2.734900	-0.993400	-0.025700
C	3.411000	-1.357900	1.152000
C	4.792800	-1.525900	1.101100
H	5.331200	-1.796600	2.005100
C	5.485000	-1.349300	-0.094000
H	6.561200	-1.485300	-0.122700
C	4.797400	-1.003300	-1.249500
H	5.340100	-0.870600	-2.181400
C	3.412400	-0.818100	-1.240700
C	2.647400	-1.564400	2.436700
H	2.010300	-0.706300	2.678100
H	3.327600	-1.730500	3.275800
H	1.985200	-2.443600	2.386900
C	2.691500	-0.419100	-2.502500
H	2.596000	0.670800	-2.561400
H	1.675600	-0.828400	-2.546800
H	3.238500	-0.754600	-3.387900
C	-1.170400	-3.964700	0.655300
H	-0.644500	-4.901900	0.866600
H	-1.694700	-3.614500	1.551200
H	-1.906100	-4.119700	-0.140700
Mn	0.113600	-2.500200	0.108900
C	1.437500	-3.960300	-1.310700
C	1.995600	-4.222300	-0.112400
H	1.857200	-3.193600	-1.960800
H	0.628700	-4.573000	-1.705000
H	2.863400	-3.664400	0.232900
H	1.645100	-5.043100	0.507400

Mn_TS_i

N	-1.269500	-1.013000	0.055900
S	-2.546100	3.691000	0.767100
C	-0.724500	0.216200	0.034900
C	-1.398900	2.425100	1.031100
C	-1.548600	1.437200	0.087200
C	-2.611600	1.715100	-0.839700
H	-2.885600	1.058600	-1.656900
C	-3.240100	2.898700	-0.613700
C	-0.453100	2.502500	2.190500
H	-0.051000	1.512300	2.424200
H	-0.956900	2.880200	3.085700
H	0.394200	3.161600	1.973000
C	-4.371400	3.510500	-1.380900
H	-4.095100	4.481400	-1.805400
H	-5.251800	3.661600	-0.747500
H	-4.657700	2.849700	-2.203700
C	-2.682900	-1.197400	0.107300
C	-3.329700	-1.615300	-1.067400
C	-4.702000	-1.850100	-1.021200
H	-5.220800	-2.161700	-1.923400
C	-5.408800	-1.689000	0.166600
H	-6.477600	-1.875500	0.191000
C	-4.745200	-1.300300	1.323100
H	-5.298300	-1.187700	2.251300
C	-3.371200	-1.051700	1.318800
C	-2.550400	-1.800400	-2.345600
H	-1.845400	-2.643800	-2.276800
H	-1.956800	-0.914300	-2.597800
H	-3.217400	-2.013100	-3.184900
C	-2.666100	-0.623100	2.578800
H	-2.540400	0.465100	2.601400
H	-1.665000	-1.063100	2.659100
H	-3.238500	-0.913100	3.463700
N	1.274600	-0.992100	-0.032600
S	2.455400	3.734400	-0.789700

C	0.703300	0.228700	-0.036000
C	1.335900	2.443100	-1.048700
C	1.504300	1.463800	-0.098900
C	2.558900	1.769900	0.829100
H	2.843900	1.123900	1.651100
C	3.163000	2.964800	0.597400
C	0.391200	2.493300	-2.210500
H	0.006500	1.494100	-2.435100
H	0.890400	2.870600	-3.108500
H	-0.467400	3.140200	-2.001300
C	4.279300	3.605100	1.363400
H	3.981500	4.572500	1.781300
H	5.157800	3.770800	0.731000
H	4.577500	2.955400	2.190800
C	2.695600	-1.139600	-0.078400
C	3.345800	-1.546400	1.097500
C	4.724600	-1.741200	1.060800
H	5.244900	-2.044600	1.965000
C	5.435700	-1.550400	-0.120000
H	6.509700	-1.704800	-0.137700
C	4.768600	-1.174900	-1.278700
H	5.324200	-1.041600	-2.202700
C	3.387500	-0.967000	-1.283900
C	2.560300	-1.771600	2.365100
H	1.934600	-0.909100	2.621500
H	3.224200	-1.973400	3.209500
H	1.885600	-2.639100	2.278400
C	2.679400	-0.564900	-2.550800
H	2.536300	0.520600	-2.588600
H	1.686300	-1.023000	-2.626400
H	3.259600	-0.856600	-3.430200
Mn	0.028800	-2.498500	0.032800
C	-1.360700	-3.988900	0.617400
H	-1.437700	-5.034800	0.899300
H	-1.476200	-3.397000	1.541600
H	-2.163300	-3.745700	-0.084800
C	0.485000	-4.827700	-0.290400
C	1.444400	-3.885100	-0.661700
H	-0.159400	-5.282900	-1.036300
H	0.650600	-5.414800	0.606400
H	1.533000	-3.577900	-1.704700
H	2.333000	-3.745300	-0.050400

Mn_P_i

N	1.306300	0.872500	0.128000
S	2.420300	-3.909800	0.568900
C	0.720900	-0.334000	0.078000
C	1.288400	-2.647900	0.904100
C	1.501900	-1.579000	0.065300
C	2.602000	-1.792100	-0.835800
H	2.925300	-1.065500	-1.572200
C	3.193600	-3.007500	-0.698700
C	0.300100	-2.807700	2.018600
H	-0.082400	-1.833200	2.335100
H	0.762600	-3.285200	2.887800
H	-0.556300	-3.417300	1.711400
C	4.343500	-3.574300	-1.472800
H	4.061700	-4.488900	-2.005100
H	5.188400	-3.815100	-0.819300
H	4.685600	-2.843800	-2.210900
C	2.713200	1.064600	0.269800
C	3.395000	1.642200	-0.815800
C	4.758100	1.895500	-0.686400
H	5.302300	2.326800	-1.521900
C	5.424300	1.597600	0.498300
H	6.486500	1.800200	0.589300
C	4.727800	1.049800	1.567400
H	5.248700	0.830900	2.495400
C	3.361500	0.774100	1.479700
C	2.666000	1.955200	-2.099200

H	1.934400	2.769500	-1.974100
H	2.113000	1.088600	-2.479400
H	3.362100	2.281400	-2.876100
C	2.632500	0.181200	2.657500
H	2.608000	-0.911900	2.589600
H	1.594000	0.525600	2.715300
H	3.131200	0.447000	3.593400
N	-1.240300	0.953900	0.124200
S	-2.589600	-3.632400	-1.067200
C	-0.711700	-0.287600	0.018900
C	-1.405400	-2.379900	-1.184700
C	-1.564300	-1.471700	-0.162800
C	-2.666500	-1.799000	0.700600
H	-2.953600	-1.207800	1.561600
C	-3.313200	-2.942200	0.353200
C	-0.424700	-2.384800	-2.317700
H	0.011800	-1.391000	-2.454200
H	-0.910100	-2.670200	-3.256100
H	0.397200	-3.085100	-2.133800
C	-4.484400	-3.587900	1.027000
H	-4.245700	-4.598900	1.373700
H	-5.345500	-3.660000	0.354500
H	-4.783100	-2.993300	1.894600
C	-2.648100	1.202600	0.076800
C	-3.303900	1.497900	1.280800
C	-4.669100	1.773900	1.234800
H	-5.199100	1.993000	2.157400
C	-5.353900	1.771300	0.024100
H	-6.417100	1.987800	0.002500
C	-4.676500	1.501600	-1.159100
H	-5.212700	1.512500	-2.103800
C	-3.310700	1.217100	-1.157400
C	-2.549400	1.508000	2.585500
H	-1.992500	0.577600	2.746700
H	-3.228900	1.646100	3.430200
H	-1.815200	2.325500	2.621500
C	-2.575400	0.936600	-2.441200
H	-2.312600	-0.123700	-2.522300
H	-1.640200	1.508200	-2.506600
H	-3.189200	1.197800	-3.306800
C	0.724900	5.417200	-1.250000
H	1.780600	5.697100	-1.293700
H	0.493700	4.799000	-2.124400
H	0.120900	6.325900	-1.314200
C	0.392500	4.682700	0.049700
C	-0.985300	4.079500	0.129500
H	0.629600	5.279200	0.936000
H	-1.602000	4.176300	-0.767100
H	-1.554000	4.270600	1.040400
Mn	0.024500	2.365300	0.153800
H	1.212500	3.862900	0.139900

Fe_A_i

N	1.258100	-1.154500	0.057800
S	2.431300	3.541600	-0.856600
C	0.745300	0.033800	-0.035500
C	1.288400	2.265400	-1.056600
C	1.527600	1.266600	-0.139200
C	2.654000	1.542800	0.710900
H	2.998100	0.873300	1.490800
C	3.238400	2.743200	0.461000
C	0.287000	2.327300	-2.170500
H	-0.136600	1.339900	-2.372300
H	0.756500	2.677300	-3.094700
H	-0.538500	3.005800	-1.931300
C	4.406600	3.372000	1.155300
H	4.134700	4.324700	1.621700
H	5.230900	3.562900	0.460600
H	4.772900	2.702500	1.938000
C	2.656900	-1.437000	0.024400

C	3.199500	-2.001600	1.191000
C	4.549800	-2.337400	1.191200
H	4.994400	-2.759200	2.087800
C	5.326600	-2.140600	0.053300
H	6.376700	-2.414000	0.061000
C	4.758400	-1.606100	-1.095300
H	5.366400	-1.470100	-1.985100
C	3.411500	-1.239400	-1.139400
C	2.344200	-2.195300	2.418800
H	1.530200	-2.918500	2.245800
H	1.876500	-1.258600	2.745000
H	2.935100	-2.584300	3.251400
C	2.828000	-0.660800	-2.401100
H	2.940800	0.429500	-2.415600
H	1.763200	-0.888300	-2.503500
H	3.343100	-1.061900	-3.277700
N	-1.246400	-1.185800	-0.043200
S	-2.516300	3.467500	0.915500
C	-0.758100	0.015400	0.011000
C	-1.351700	2.206700	1.081500
C	-1.568900	1.231600	0.132400
C	-2.692600	1.517800	-0.716900
H	-3.016000	0.875500	-1.526400
C	-3.298400	2.700300	-0.433100
C	-0.343700	2.267600	2.190500
H	0.098400	1.284900	2.377100
H	-0.810600	2.600100	3.122500
H	0.470500	2.960400	1.953200
C	-4.473700	3.329100	-1.115500
H	-4.220400	4.306400	-1.539200
H	-5.310400	3.470600	-0.423700
H	-4.814400	2.683700	-1.929500
C	-2.644300	-1.476200	0.092500
C	-3.389900	-1.794800	-1.049100
C	-4.731800	-2.132700	-0.867700
H	-5.337200	-2.368800	-1.738300
C	-5.296600	-2.172600	0.400700
H	-6.340700	-2.442600	0.520500
C	-4.526200	-1.869200	1.517900
H	-4.969700	-1.905200	2.508600
C	-3.185000	-1.515400	1.387100
C	-2.789100	-1.771800	-2.431800
H	-1.978600	-1.042400	-2.524000
H	-3.551600	-1.531900	-3.178000
H	-2.368300	-2.748600	-2.692900
C	-2.350900	-1.177800	2.597200
H	-2.110500	-0.110100	2.624700
H	-1.403700	-1.733900	2.616900
H	-2.888600	-1.419400	3.517000
C	0.223400	-3.338000	-1.690900
H	-0.571700	-4.092600	-1.822000
H	0.181000	-2.646800	-2.537900
H	1.198000	-3.853900	-1.711800
Fe	0.015700	-2.589500	0.052700

Fe_R_I

N	-1.256100	-0.975300	-0.027200
S	-2.296200	3.730700	0.889800
C	-0.699900	0.195400	0.000700
C	-1.217100	2.397600	1.077200
C	-1.444800	1.459800	0.096000
C	-2.507400	1.831100	-0.797200
H	-2.832000	1.226500	-1.634800
C	-3.056400	3.040600	-0.512000
C	-0.263900	2.365900	2.234200
H	0.126700	1.357300	2.395100
H	-0.762600	2.674100	3.158100
H	0.588200	3.033600	2.069500
C	-4.160000	3.752000	-1.232100
H	-3.830900	4.721200	-1.621100

H	-5.018400	3.928700	-0.575900
H	-4.499700	3.144900	-2.075400
C	-2.684300	-1.120900	0.043300
C	-3.390300	-1.409600	-1.132700
C	-4.762000	-1.639800	-1.029200
H	-5.329100	-1.854800	-1.930700
C	-5.407100	-1.587600	0.199900
H	-6.473300	-1.778900	0.263100
C	-4.688000	-1.268900	1.344200
H	-5.195700	-1.203700	2.302400
C	-3.316800	-1.018300	1.290100
C	-2.735800	-1.415500	-2.493700
H	-2.414600	-2.418000	-2.795900
H	-1.856700	-0.764900	-2.534700
H	-3.441900	-1.066500	-3.252600
C	-2.592100	-0.603000	2.545700
H	-2.705800	0.475200	2.708600
H	-1.520000	-0.815500	2.512400
H	-3.004500	-1.117700	3.417800
N	1.279600	-1.047500	-0.008600
S	2.644100	3.627400	-0.713800
C	0.806400	0.155800	-0.049700
C	1.463600	2.400300	-0.993100
C	1.631500	1.368300	-0.098800
C	2.734000	1.578400	0.799900
H	3.023500	0.874000	1.571300
C	3.370900	2.762800	0.608200
C	0.507800	2.530900	-2.140200
H	0.044300	1.568900	-2.374900
H	1.026500	2.873200	-3.040800
H	-0.292600	3.243900	-1.917300
C	4.533900	3.326900	1.364100
H	4.279200	4.274800	1.849400
H	5.390500	3.507300	0.706700
H	4.845700	2.621400	2.138900
C	2.673400	-1.350000	-0.080800
C	3.238600	-1.971300	1.046300
C	4.583100	-2.326400	0.998300
H	5.042500	-2.788500	1.867200
C	5.336300	-2.099700	-0.149700
H	6.381400	-2.390000	-0.179000
C	4.747700	-1.511100	-1.259800
H	5.334600	-1.347800	-2.159300
C	3.406800	-1.118600	-1.252700
C	2.419500	-2.216400	2.291500
H	1.866400	-1.323200	2.606500
H	3.058800	-2.519800	3.124300
H	1.688500	-3.028000	2.155700
C	2.816100	-0.476800	-2.481600
H	3.012900	0.601100	-2.487900
H	1.733400	-0.615100	-2.546000
H	3.262900	-0.901600	-3.384600
C	-1.153200	-3.658300	1.338900
H	-0.697900	-4.633200	1.560200
H	-1.054600	-3.030700	2.254500
H	-2.220800	-3.797600	1.152000
Fe	-0.062900	-2.493800	0.241500
C	-0.625000	-3.905200	-1.160400
C	0.277900	-3.013600	-1.718500
H	-1.693700	-3.820000	-1.325300
H	-0.291600	-4.885100	-0.829800
H	-0.055600	-2.203900	-2.359300
H	1.329600	-3.281000	-1.811400

Fe_TS_I

N	-1.267700	-0.907000	-0.018200
S	-2.164800	3.828900	0.941400
C	-0.682600	0.252800	0.016900
C	-1.124900	2.462100	1.109500
C	-1.394300	1.535200	0.128800

C	-2.454600	1.944100	-0.749800
H	-2.803200	1.355800	-1.589200
C	-2.963500	3.168700	-0.452600
C	-0.147500	2.400400	2.245100
H	0.191200	1.374300	2.414900
H	-0.605100	2.753100	3.174400
H	0.735500	3.016500	2.046200
C	-4.053100	3.916800	-1.156700
H	-3.699400	4.878200	-1.543600
H	-4.899300	4.115000	-0.490800
H	-4.419200	3.325500	-2.000200
C	-2.694000	-1.034500	0.076600
C	-3.438300	-1.261000	-1.088400
C	-4.807700	-1.495200	-0.952500
H	-5.403600	-1.663100	-1.845600
C	-5.412500	-1.506100	0.297100
H	-6.477100	-1.696900	0.384500
C	-4.655400	-1.251800	1.435000
H	-5.133300	-1.235900	2.410400
C	-3.286700	-1.002600	1.348400
C	-2.825500	-1.206300	-2.468100
H	-2.699600	-2.205200	-2.900800
H	-1.844900	-0.723600	-2.468500
H	-3.476000	-0.647200	-3.148200
C	-2.503800	-0.652400	2.589000
H	-2.422000	0.436200	2.691800
H	-1.483000	-1.049700	2.578300
H	-3.001800	-1.034600	3.483800
N	1.228500	-1.061400	0.046400
S	2.768800	3.529200	-0.866200
C	0.808300	0.163600	-0.032000
C	1.541500	2.332900	-1.073000
C	1.683600	1.338400	-0.133900
C	2.803400	1.551300	0.741500
H	3.078700	0.874400	1.542100
C	3.482000	2.700300	0.484900
C	0.564400	2.447400	-2.203900
H	0.083000	1.485200	-2.400700
H	1.068000	2.756900	-3.124800
H	-0.221300	3.177600	-1.983900
C	4.678100	3.252400	1.197000
H	4.471100	4.234700	1.634200
H	5.533000	3.360500	0.521500
H	4.969900	2.575700	2.004600
C	2.610900	-1.422200	-0.003700
C	3.169500	-1.958800	1.167800
C	4.499200	-2.370900	1.132000
H	4.956000	-2.771300	2.032500
C	5.240500	-2.275500	-0.041200
H	6.273400	-2.607500	-0.058400
C	4.657600	-1.760700	-1.191400
H	5.237000	-1.695600	-2.108000
C	3.332900	-1.319300	-1.200300
C	2.364900	-2.049500	2.442300
H	1.877300	-1.098800	2.688800
H	3.002300	-2.327400	3.285300
H	1.574600	-2.811300	2.378300
C	2.735800	-0.750600	-2.460900
H	2.892700	0.333100	-2.508200
H	1.659500	-0.933500	-2.524100
H	3.207000	-1.194500	-3.341900
C	-1.217700	-3.868300	0.932300
H	-0.624500	-4.739800	1.229300
H	-1.133600	-3.091200	1.742000
H	-2.274100	-4.137200	0.901800
C	-1.031800	-3.883000	-1.073800
C	0.026900	-3.106800	-1.675400
H	-2.056900	-3.621100	-1.319100
H	-0.889200	-4.958100	-0.989300
H	-0.234700	-2.385700	-2.445900

H	0.978800	-3.611800	-1.859800
Fe	-0.092700	-2.442500	0.145600

Fe_P₁

N	-1.292700	-0.775800	0.049200
S	-2.001400	4.016900	0.895100
C	-0.671300	0.364900	0.050000
C	-1.005500	2.620600	1.079800
C	-1.334000	1.673100	0.136000
C	-2.403000	2.092600	-0.727400
H	-2.792800	1.493300	-1.540100
C	-2.859800	3.343500	-0.456200
C	0.002500	2.565500	2.189100
H	0.316800	1.536400	2.385600
H	-0.416600	2.964500	3.117700
H	0.898000	3.145900	1.943100
C	-3.940700	4.108400	-1.155500
H	-3.564500	5.045200	-1.579400
H	-4.762300	4.355100	-0.475000
H	-4.348400	3.505900	-1.971500
C	-2.719100	-0.877700	0.147900
C	-3.482300	-1.061900	-1.008900
C	-4.859300	-1.238000	-0.853100
H	-5.475700	-1.370400	-1.738200
C	-5.443800	-1.245400	0.405900
H	-6.515100	-1.385300	0.505900
C	-4.656600	-1.074400	1.540800
H	-5.114900	-1.082700	2.525400
C	-3.280700	-0.891400	1.433000
C	-2.872800	-1.070800	-2.389600
H	-2.822500	-2.090000	-2.789900
H	-1.857200	-0.667100	-2.401800
H	-3.482500	-0.484600	-3.084600
C	-2.415200	-0.711300	2.653800
H	-1.955600	0.283500	2.674900
H	-1.601900	-1.450900	2.689800
H	-3.001200	-0.828900	3.568400
N	1.192900	-1.021300	0.117300
S	2.892200	3.470900	-0.985200
C	0.820100	0.215400	-0.007000
C	1.611100	2.324000	-1.128400
C	1.739500	1.345900	-0.168700
C	2.893400	1.531200	0.668500
H	3.164000	0.862400	1.477400
C	3.609800	2.645100	0.365600
C	0.610400	2.454500	-2.237000
H	0.095500	1.505600	-2.411600
H	1.101300	2.737800	-3.172900
H	-0.146600	3.211600	-2.007500
C	4.846900	3.164600	1.030600
H	4.691400	4.163900	1.450100
H	5.685300	3.223100	0.328900
H	5.135100	2.495000	1.845400
C	2.549300	-1.461200	0.059200
C	3.088500	-1.988400	1.242900
C	4.392400	-2.475900	1.208700
H	4.837300	-2.872500	2.116800
C	5.121100	-2.461600	0.023600
H	6.134100	-2.850200	0.006500
C	4.549900	-1.964900	-1.141600
H	5.117200	-1.975500	-2.067800
C	3.250800	-1.454400	-1.153000
C	2.281800	-1.988900	2.518100
H	1.950700	-0.980800	2.795500
H	2.862400	-2.393800	3.350500
H	1.374800	-2.610200	2.433300
C	2.638200	-0.935100	-2.426800
H	2.736600	0.154400	-2.494200
H	1.572700	-1.180500	-2.489300
H	3.137500	-1.369200	-3.296700

C	-1.200800	-5.454800	-0.371100
H	-1.202300	-6.005300	-1.316200
H	-0.242700	-5.649200	0.124300
H	-1.999900	-5.852800	0.261300
C	-1.383300	-3.963500	-0.647600
C	-0.251700	-3.267100	-1.367000
H	-2.360900	-3.749000	-1.088600
H	-0.510900	-2.766300	-2.299600
H	0.640200	-3.894500	-1.503300
Fe	-0.179100	-2.311200	0.265900
H	-1.527800	-3.482200	0.402200

Co_A₁

N	1.299300	-1.120300	0.123900
S	2.386000	3.530000	-1.043300
C	0.758100	0.047300	-0.023600
C	1.244300	2.244000	-1.148800
C	1.519100	1.285200	-0.196600
C	2.673100	1.602900	0.601600
H	3.046900	0.971000	1.398600
C	3.239400	2.794900	0.282500
C	0.211000	2.256200	-2.235300
H	-0.204700	1.257900	-2.397000
H	0.650000	2.583100	-3.182600
H	-0.615600	2.932100	-1.993600
C	4.424300	3.460100	0.911200
H	4.160400	4.430200	1.344800
H	5.224200	3.625500	0.182200
H	4.820600	2.826800	1.709100
C	2.705100	-1.368700	0.039000
C	3.328100	-1.842100	1.205100
C	4.688000	-2.132400	1.145300
H	5.195900	-2.482400	2.039100
C	5.393400	-1.988300	-0.045600
H	6.451100	-2.228100	-0.080700
C	4.743000	-1.555100	-1.193200
H	5.293400	-1.465600	-2.125300
C	3.384400	-1.233500	-1.180200
C	2.547800	-1.998300	2.485400
H	1.753700	-2.750700	2.384700
H	2.066600	-1.060600	2.789300
H	3.199800	-2.319700	3.301000
C	2.707200	-0.774000	-2.445700
H	2.731300	0.318400	-2.530000
H	1.658500	-1.087300	-2.495800
H	3.217000	-1.185800	-3.320400
N	-1.295800	-1.125300	-0.131300
S	-2.399300	3.515100	1.060600
C	-0.759400	0.043800	0.021000
C	-1.253700	2.232000	1.158500
C	-1.525100	1.278300	0.200100
C	-2.679600	1.597700	-0.596700
H	-3.051200	0.970100	-1.397900
C	-3.249600	2.785900	-0.270300
C	-0.220500	2.241000	2.245200
H	0.197000	1.242900	2.402600
H	-0.660300	2.562900	3.193900
H	0.604900	2.919700	2.006800
C	-4.436400	3.451200	-0.895200
H	-4.175700	4.425300	-1.321900
H	-5.237400	3.608700	-0.165700
H	-4.829800	2.822000	-1.697800
C	-2.701400	-1.377100	-0.050200
C	-3.324600	-1.833900	-1.222500
C	-4.684400	-2.125900	-1.165600
H	-5.192800	-2.463700	-2.063900
C	-5.389000	-1.999000	0.027600
H	-6.446500	-2.240000	0.060100
C	-4.738100	-1.581400	1.180800
H	-5.288000	-1.505000	2.114400

C	-3.379700	-1.259200	1.171100
C	-2.545100	-1.970000	-2.505400
H	-2.073200	-1.024500	-2.800400
H	-3.195300	-2.288700	-3.323400
H	-1.743700	-2.715300	-2.412900
C	-2.699700	-0.816400	2.441100
H	-2.704600	0.275900	2.530000
H	-1.656800	-1.148600	2.493300
H	-3.219500	-1.222700	3.312400
Co	0.005200	-2.650000	0.000900
C	0.015400	-4.633800	0.015600
H	-0.610000	-5.022900	0.825500
H	-0.337700	-5.036800	-0.939300
H	1.049100	-4.965800	0.173900

Co_R₁

N	-1.287000	-1.013500	-0.074400
S	-2.539600	3.645600	0.843100
C	-0.777800	0.169300	0.011700
C	-1.383700	2.381900	1.052800
C	-1.573900	1.401600	0.106500
C	-2.675000	1.680400	-0.775100
H	-2.983500	1.022100	-1.578900
C	-3.287000	2.865600	-0.519600
C	-0.423400	2.431900	2.202800
H	0.021500	1.449900	2.385300
H	-0.934500	2.733600	3.122100
H	0.389100	3.141800	2.016600
C	-4.443000	3.489400	-1.238500
H	-4.174900	4.458200	-1.672600
H	-5.294100	3.647300	-0.568100
H	-4.769600	2.832100	-2.048600
C	-2.694100	-1.254300	-0.016600
C	-3.283600	-1.787100	-1.173700
C	-4.646100	-2.069400	-1.150100
H	-5.123400	-2.463100	-2.042900
C	-5.393400	-1.859700	0.004900
H	-6.453000	-2.093400	0.015900
C	-4.779700	-1.363400	1.146200
H	-5.361400	-1.216500	2.051900
C	-3.419600	-1.044900	1.163700
C	-2.463200	-2.019300	-2.417300
H	-1.709300	-2.800700	-2.257000
H	-1.927500	-1.116200	-2.734200
H	-3.095900	-2.343200	-3.247400
C	-2.800000	-0.505300	2.426400
H	-2.955900	0.576900	2.502900
H	-1.724800	-0.696100	2.476700
H	-3.259500	-0.971400	3.302300
N	1.313400	-0.943100	0.108800
S	2.310200	3.758700	-0.912700
C	0.737700	0.207900	-0.015100
C	1.223500	2.432100	-1.100600
C	1.468600	1.476400	-0.141100
C	2.553400	1.829000	0.734900
H	2.893000	1.204400	1.552900
C	3.099600	3.041600	0.460900
C	0.258800	2.418300	-2.247800
H	-0.148200	1.416400	-2.407700
H	0.753800	2.723200	-3.175000
H	-0.581600	3.097500	-2.072200
C	4.216100	3.741200	1.172500
H	3.890400	4.697900	1.593800
H	5.057600	3.940400	0.501000
H	4.579100	3.114900	1.991700
C	2.732800	-1.104000	0.032900
C	3.380100	-1.582900	1.184800
C	4.754300	-1.798600	1.124600
H	5.274300	-2.149000	2.011500
C	5.461100	-1.575900	-0.052800

H	6.530200	-1.758000	-0.087500
C	4.795600	-1.126800	-1.184500
H	5.346400	-0.962300	-2.106500
C	3.421600	-0.873900	-1.168000
C	2.616900	-1.822800	2.463900
H	1.989600	-0.965900	2.735800
H	3.303200	-2.013700	3.292600
H	1.949900	-2.691600	2.389500
C	2.751000	-0.381100	-2.425700
H	2.869100	0.703300	-2.526900
H	1.677900	-0.594500	-2.443300
H	3.202400	-0.847000	-3.306500
C	-0.788600	-3.405000	1.949200
H	-0.358700	-4.398400	2.142200
H	-0.602200	-2.796500	2.843800
H	-1.874300	-3.516800	1.848400
Co	0.041400	-2.581900	0.333500
C	0.579300	-4.447200	-1.170400
C	1.182700	-3.462300	-1.856500
H	-0.446300	-4.748800	-1.375800
H	1.123200	-5.048200	-0.444000
H	0.661000	-2.908700	-2.633500
H	2.228900	-3.218600	-1.694900

Co_TS₁

N	-1.282900	-0.906700	-0.184600
S	-2.401300	3.699900	1.152400
C	-0.759500	0.259600	0.010700
C	-1.253300	2.414600	1.204400
C	-1.529300	1.488800	0.222100
C	-2.687900	1.830900	-0.558100
H	-3.063800	1.226000	-1.374800
C	-3.259300	3.007400	-0.192700
C	-0.205500	2.396200	2.276800
H	0.207700	1.391900	2.406200
H	-0.628800	2.700800	3.238600
H	0.621100	3.073800	2.039400
C	-4.452000	3.687400	-0.790300
H	-4.196800	4.674400	-1.189700
H	-5.249300	3.821000	-0.052000
H	-4.848500	3.081000	-1.608900
C	-2.684700	-1.166200	-0.118100
C	-3.301800	-1.600900	-1.302600
C	-4.652700	-1.933400	-1.254800
H	-5.152800	-2.254400	-2.163900
C	-5.360300	-1.863100	-0.058500
H	-6.410400	-2.135600	-0.032500
C	-4.721500	-1.451800	1.103100
H	-5.274400	-1.407200	2.037200
C	-3.372500	-1.089100	1.101600
C	-2.528200	-1.651700	-2.595400
H	-1.645400	-2.296900	-2.515400
H	-2.167200	-0.657700	-2.888600
H	-3.151800	-2.032400	-3.407900
C	-2.723100	-0.629300	2.381900
H	-2.849900	0.451500	2.513500
H	-1.648500	-0.836300	2.408100
H	-3.179600	-1.126200	3.242100
N	1.294600	-0.885900	0.213000
S	2.338600	3.714200	-1.217800
C	0.757000	0.269900	-0.005400
C	1.215300	2.406900	-1.244600
C	1.508100	1.506000	-0.243500
C	2.659300	1.886200	0.530100
H	3.046900	1.304900	1.358200
C	3.207900	3.066200	0.141500
C	0.167800	2.347600	-2.316200
H	-0.227400	1.333600	-2.425000
H	0.585900	2.639700	-3.284100
H	-0.670200	3.016000	-2.092800

C	4.387800	3.779900	0.725000
H	4.114600	4.770200	1.104100
H	5.182900	3.912700	-0.015900
H	4.794900	3.197800	1.556000
C	2.701500	-1.125600	0.154700
C	3.337900	-1.470400	1.355900
C	4.698600	-1.765200	1.314500
H	5.215800	-2.015900	2.236200
C	5.392800	-1.749300	0.108900
H	6.450800	-1.989600	0.089100
C	4.729500	-1.439600	-1.071700
H	5.271300	-1.445400	-2.013300
C	3.370700	-1.119500	-1.077500
C	2.569000	-1.488600	2.652300
H	2.115700	-0.514000	2.872300
H	3.221400	-1.749300	3.489200
H	1.753500	-2.221600	2.623900
C	2.667300	-0.795000	-2.370100
H	2.546900	0.287100	-2.494700
H	1.670300	-1.249100	-2.418100
H	3.242900	-1.165100	-3.222300
C	-0.762500	-3.761100	1.421500
H	-0.504200	-4.638100	2.010800
H	-0.529900	-2.882800	2.052800
H	-1.830100	-3.767100	1.181500
C	0.302000	-4.674400	-0.178100
C	0.718400	-3.907300	-1.306700
H	-0.562200	-5.325000	-0.273800
H	1.068500	-5.054100	0.491100
H	0.122700	-3.971100	-2.215000
H	1.784800	-3.744200	-1.452500
Co	0.032400	-2.462100	-0.040200

Co_P₁

N	-1.138300	-1.200800	-0.225800
S	-3.370600	2.896700	1.363600
C	-0.944800	0.054500	0.012900
C	-1.914800	1.979500	1.298700
C	-1.999700	1.020500	0.309400
C	-3.263400	1.037400	-0.378600
H	-3.519600	0.361400	-1.185600
C	-4.103800	2.009900	0.058600
C	-0.829800	2.240100	2.300800
H	-0.164500	1.377700	2.398200
H	-1.255300	2.434300	3.289700
H	-0.224600	3.106800	2.015900
C	-5.476400	2.345300	-0.436500
H	-5.526800	3.367600	-0.825200
H	-6.223200	2.252000	0.358600
H	-5.753700	1.660500	-1.242100
C	-2.408800	-1.849200	-0.134600
C	-2.917400	-2.403400	-1.320700
C	-4.131300	-3.081600	-1.256900
H	-4.552900	-3.502700	-2.164900
C	-4.798400	-3.231200	-0.044800
H	-5.738900	-3.771200	-0.007300
C	-4.254700	-2.705200	1.119400
H	-4.769300	-2.842400	2.066100
C	-3.049000	-2.000900	1.104200
C	-2.182800	-2.232000	-2.626500
H	-1.188800	-2.699000	-2.600700
H	-2.034000	-1.174100	-2.875100
H	-2.736400	-2.693700	-3.447400
C	-2.487100	-1.444300	2.387600
H	-2.819800	-0.412200	2.546800
H	-1.391300	-1.442000	2.400000
H	-2.825800	-2.038000	3.240300
N	1.348500	-0.486900	0.186600
S	1.029800	4.169800	-1.412400
C	0.518600	0.476500	-0.039400

C	0.304400	2.610600	-1.333400
C	0.890900	1.861300	-0.332300
C	1.939500	2.569700	0.351900
H	2.521500	2.151900	1.163400
C	2.119100	3.838000	-0.098800
C	-0.750500	2.235700	-2.332100
H	-0.847000	1.149900	-2.420900
H	-0.497600	2.620100	-3.324500
H	-1.727600	2.641200	-2.049800
C	3.091400	4.867800	0.387000
H	2.580700	5.761500	0.760400
H	3.774800	5.180400	-0.409100
H	3.690100	4.451900	1.201500
C	2.769500	-0.334000	0.166400
C	3.433300	-0.380200	1.398400
C	4.825800	-0.324300	1.388600
H	5.363900	-0.353800	2.331600
C	5.525700	-0.238800	0.190400
H	6.610100	-0.204000	0.197600
C	4.839300	-0.208100	-1.018300
H	5.390900	-0.154500	-1.952300
C	3.446300	-0.259600	-1.057900
C	2.659100	-0.437700	2.689900
H	2.172700	0.522300	2.909900
H	3.317400	-0.672500	3.529600
H	1.868900	-1.196500	2.658900
C	2.706100	-0.275500	-2.369600
H	2.063700	0.604700	-2.485100
H	2.073500	-1.168600	-2.460000
H	3.407000	-0.287300	-3.207500
C	3.187100	-3.999200	1.362200
H	4.208800	-3.999600	1.755200
H	2.651300	-3.165400	1.834800
H	2.700400	-4.927900	1.682500
C	3.171500	-3.868600	-0.158300
C	1.752100	-3.854900	-0.742900
H	3.737300	-4.706200	-0.588500
H	3.707400	-2.957300	-0.449400
H	1.235900	-4.794900	-0.486900
H	1.798100	-3.836900	-1.844100
Co	0.551900	-2.370500	-0.234400

Cu_A₁

N	1.313300	-1.046100	0.160000
S	2.175100	3.597300	-1.209900
C	0.728900	0.088900	-0.020500
C	1.097700	2.253000	-1.237400
C	1.433200	1.354300	-0.246500
C	2.579600	1.766300	0.517600
H	2.997600	1.192600	1.335600
C	3.081000	2.968800	0.134500
C	0.042700	2.168700	-2.300400
H	-0.319400	1.143500	-2.418300
H	0.442300	2.485500	-3.268300
H	-0.815500	2.805500	-2.062400
C	4.241600	3.718500	0.711600
H	3.938000	4.695100	1.102600
H	5.022800	3.885300	-0.036900
H	4.678200	3.143700	1.532500
C	2.723500	-1.242800	0.120300
C	3.360000	-1.534000	1.334200
C	4.731200	-1.777400	1.305700
H	5.251700	-1.991100	2.234800
C	5.431000	-1.760600	0.103600
H	6.497600	-1.960300	0.095300
C	4.764900	-1.505400	-1.089400
H	5.312600	-1.513600	-2.027300
C	3.395000	-1.243800	-1.108800
C	2.578100	-1.555100	2.621400
H	1.752400	-2.276400	2.574100

H	2.135100	-0.576400	2.846600
H	3.217600	-1.831500	3.463000
C	2.668900	-0.992000	-2.404300
H	2.381700	0.061000	-2.504300
H	1.754100	-1.593800	-2.478700
H	3.302400	-1.246300	-3.257200
N	-1.270100	-1.167600	-0.125000
S	-2.560200	3.426200	1.078400
C	-0.792200	0.021600	0.027100
C	-1.358200	2.194200	1.160800
C	-1.607100	1.223100	0.214200
C	-2.789800	1.487100	-0.561100
H	-3.150000	0.837500	-1.350100
C	-3.404500	2.651700	-0.230300
C	-0.303800	2.256100	2.225300
H	0.152700	1.275700	2.387100
H	-0.735200	2.574700	3.178800
H	0.491200	2.960700	1.960300
C	-4.631300	3.260800	-0.835200
H	-4.420900	4.240900	-1.275600
H	-5.422900	3.391300	-0.090300
H	-5.014500	2.608200	-1.624100
C	-2.658400	-1.490400	-0.035300
C	-3.263800	-1.984800	-1.202300
C	-4.605800	-2.348300	-1.138600
H	-5.099900	-2.715500	-2.033300
C	-5.310900	-2.253600	0.057500
H	-6.354100	-2.549800	0.096100
C	-4.677700	-1.796300	1.205400
H	-5.227200	-1.743200	2.140900
C	-3.338200	-1.402100	1.188100
C	-2.485200	-2.078700	-2.490200
H	-2.085400	-1.104700	-2.797900
H	-3.115800	-2.452800	-3.300100
H	-1.629300	-2.761600	-2.400400
C	-2.679400	-0.911700	2.451800
H	-2.754500	0.178600	2.535200
H	-1.616500	-1.173500	2.497300
H	-3.166100	-1.346300	3.328600
C	1.202100	-4.171600	-0.003200
H	0.560800	-5.060200	-0.057700
H	1.873700	-4.129300	-0.867100
H	1.793200	-4.183500	0.916700
Cu	0.079700	-2.632400	-0.047200

Cu_R_i

N	-1.267300	-1.008200	-0.076300
S	-2.630300	3.594700	0.999800
C	-0.800500	0.186000	0.050300
C	-1.436800	2.357900	1.147100
C	-1.631100	1.391300	0.186700
C	-2.764900	1.660300	-0.655600
H	-3.081500	1.011800	-1.463900
C	-3.398000	2.824200	-0.356800
C	-0.439100	2.413400	2.265100
H	0.026300	1.436600	2.424900
H	-0.922900	2.700400	3.203600
H	0.355700	3.137000	2.057000
C	-4.590600	3.432400	-1.027600
H	-4.360400	4.416700	-1.448400
H	-5.425000	3.553800	-0.329300
H	-4.924300	2.783700	-1.841800
C	-2.661700	-1.300200	-0.042300
C	-3.228700	-1.784900	-1.230000
C	-4.579900	-2.119600	-1.223400
H	-5.042800	-2.480200	-2.137600
C	-5.333000	-2.007000	-0.058700
H	-6.383200	-2.280300	-0.063200
C	-4.736700	-1.563000	1.114100
H	-5.321900	-1.498700	2.027100

C	-3.389200	-1.199600	1.150400
C	-2.392000	-1.911000	-2.476400
H	-1.533100	-2.574000	-2.310500
H	-1.988400	-0.942800	-2.798600
H	-2.978600	-2.320200	-3.302500
C	-2.761900	-0.736500	2.439800
H	-2.771400	0.356800	2.513400
H	-1.720400	-1.065400	2.531300
H	-3.313100	-1.132000	3.296800
N	1.327700	-0.843100	0.185000
S	2.129100	3.838100	-1.083100
C	0.715100	0.278700	0.015700
C	1.087100	2.466300	-1.175300
C	1.393800	1.567100	-0.179500
C	2.489600	1.999400	0.645500
H	2.876000	1.427000	1.480700
C	2.982900	3.216100	0.298300
C	0.089800	2.362700	-2.289800
H	-0.267800	1.335600	-2.403900
H	0.539100	2.660000	-3.242200
H	-0.779400	3.003200	-2.109000
C	4.092900	3.988000	0.942100
H	3.744100	4.951200	1.328900
H	4.906400	4.185700	0.236500
H	4.502800	3.414400	1.777600
C	2.745500	-0.966100	0.111800
C	3.396500	-1.383400	1.285900
C	4.771300	-1.593900	1.238500
H	5.293500	-1.900700	2.140100
C	5.475200	-1.425100	0.048900
H	6.545200	-1.602900	0.021500
C	4.805800	-1.039400	-1.103600
H	5.355600	-0.920000	-2.033000
C	3.429400	-0.796000	-1.100200
C	2.615400	-1.585600	2.558800
H	2.073800	-0.679500	2.855100
H	3.275900	-1.867400	3.382400
H	1.864600	-2.381000	2.449000
C	2.751100	-0.365900	-2.376600
H	2.838900	0.717600	-2.514100
H	1.683300	-0.607500	-2.391200
H	3.219500	-0.847500	-3.239900
C	-1.125000	-3.901700	0.848100
H	-0.583600	-4.780300	1.208800
H	-1.715800	-3.452100	1.651900
H	-1.779700	-4.165800	0.011500
Cu	0.111900	-2.523800	0.213500
C	1.834700	-4.121300	-0.348700
C	1.239700	-3.759500	-1.501500
H	1.502400	-4.993100	0.206000
H	2.726100	-3.612200	0.009700
H	0.403700	-4.323000	-1.907500
H	1.632200	-2.944900	-2.104900

Cu_TS_i

N	-1.306000	-0.884700	-0.166600
S	-2.340400	3.754100	1.121700
C	-0.759900	0.268400	0.014700
C	-1.223500	2.441300	1.196900
C	-1.504300	1.519400	0.214400
C	-2.640700	1.885800	-0.586600
H	-3.017100	1.284800	-1.406200
C	-3.191500	3.076400	-0.234800
C	-0.191600	2.401600	2.283900
H	0.207500	1.391000	2.409000
H	-0.624300	2.702700	3.242700
H	0.646600	3.070600	2.063500
C	-4.359100	3.780300	-0.854200
H	-4.075800	4.760100	-1.252600
H	-5.165500	3.934100	-0.129800

H	-4.755200	3.179900	-1.677400
C	-2.709700	-1.103100	-0.091400
C	-3.335900	-1.560100	-1.262900
C	-4.695500	-1.853800	-1.212400
H	-5.200800	-2.188800	-2.113800
C	-5.404800	-1.731000	-0.021000
H	-6.462500	-1.971900	0.008400
C	-4.755500	-1.316000	1.133200
H	-5.306600	-1.240700	2.066200
C	-3.396100	-0.991900	1.126400
C	-2.548100	-1.699900	-2.539800
H	-1.709200	-2.397600	-2.416800
H	-2.117200	-0.743400	-2.859800
H	-3.179400	-2.071500	-3.350700
C	-2.725700	-0.551700	2.402800
H	-2.792900	0.535200	2.525100
H	-1.662800	-0.815900	2.430000
H	-3.209200	-1.014400	3.267600
N	1.286800	-0.898800	0.206000
S	2.379000	3.688700	-1.216900
C	0.757400	0.257100	-0.010300
C	1.249300	2.385600	-1.253200
C	1.519100	1.491800	-0.241400
C	2.657600	1.872200	0.550200
H	3.027100	1.294200	1.389000
C	3.220600	3.045700	0.162000
C	0.218900	2.322200	-2.340700
H	-0.192200	1.312900	-2.433800
H	0.657500	2.586100	-3.307800
H	-0.611100	3.008900	-2.145100
C	4.394200	3.756900	0.761400
H	4.119900	4.750700	1.130300
H	5.202600	3.881600	0.033500
H	4.784300	3.177400	1.602300
C	2.692800	-1.130000	0.172500
C	3.292000	-1.521600	1.379700
C	4.654400	-1.809500	1.375000
H	5.140200	-2.095100	2.303700
C	5.390000	-1.744200	0.195700
H	6.449200	-1.979900	0.202800
C	4.764700	-1.393700	-0.993800
H	5.337200	-1.363900	-1.916800
C	3.405000	-1.077500	-1.033900
C	2.476000	-1.597400	2.644500
H	2.038800	-0.626100	2.906600
H	3.089400	-1.926400	3.486900
H	1.641100	-2.302700	2.539500
C	2.750000	-0.712900	-2.341000
H	2.736600	0.373400	-2.485100
H	1.713300	-1.064100	-2.392700
H	3.297000	-1.152600	-3.179300
C	-1.228100	-3.875400	0.985000
H	-1.233700	-4.874800	1.410700
H	-1.048000	-3.153000	1.795500
H	-2.154100	-3.669500	0.445800
C	0.242700	-4.609200	-0.326400
C	1.072700	-3.803700	-1.152400
H	-0.558700	-5.161700	-0.809600
H	0.740400	-5.143500	0.477800
H	0.786400	-3.598200	-2.181300
H	2.115000	-3.643100	-0.890500
Cu	0.011500	-2.488900	-0.005300

Cu_P_i

N	-1.323000	-0.733700	-0.329400
S	-2.144600	3.806500	1.390500
C	-0.731600	0.376900	-0.047700
C	-1.073100	2.458500	1.319400
C	-1.422400	1.627500	0.276500
C	-2.574100	2.093300	-0.448100

H	-3.001300	1.574200	-1.297700
C	-3.066900	3.270100	0.017400
C	-0.008200	2.299500	2.363500
H	0.343700	1.265200	2.414100
H	-0.394400	2.559800	3.353500
H	0.853600	2.942000	2.156000
C	-4.228500	4.061400	-0.499000
H	-3.922400	5.058800	-0.831200
H	-5.001100	4.185800	0.266700
H	-4.677400	3.542100	-1.349800
C	-2.734600	-0.932400	-0.255300
C	-3.402800	-1.197700	-1.460000
C	-4.769500	-1.458400	-1.405400
H	-5.311100	-1.648500	-2.327500
C	-5.439000	-1.487400	-0.185900
H	-6.502400	-1.701300	-0.156500
C	-4.744800	-1.259600	0.995600
H	-5.267800	-1.303600	1.946700
C	-3.377900	-0.976500	0.990100
C	-2.656700	-1.168400	-2.769200
H	-1.831500	-1.892500	-2.779400
H	-2.216300	-0.182900	-2.965700
H	-3.320500	-1.409700	-3.602700
C	-2.640800	-0.742700	2.284200
H	-2.511500	0.328200	2.477800
H	-1.643900	-1.199400	2.280900
H	-3.197000	-1.167800	3.123400
N	1.259500	-0.892500	0.073400
S	2.555100	3.711600	-1.103600
C	0.789800	0.298400	-0.076100
C	1.354400	2.478100	-1.185700
C	1.609500	1.502000	-0.245900
C	2.794700	1.764700	0.525100
H	3.162100	1.111700	1.307400
C	3.406300	2.932100	0.196700
C	0.285400	2.551200	-2.235400
H	-0.162700	1.569400	-2.413000
H	0.700200	2.895300	-3.187400
H	-0.513000	3.241400	-1.944000
C	4.637400	3.537400	0.796800
H	4.431400	4.517100	1.240200
H	5.425700	3.667500	0.048300
H	5.022900	2.882200	1.582300
C	2.642500	-1.226800	0.043200
C	3.219300	-1.647100	1.249900
C	4.557200	-2.034700	1.231900
H	5.031200	-2.349200	2.157300
C	5.281900	-2.030900	0.044500
H	6.321200	-2.343100	0.043200
C	4.673300	-1.643100	-1.143400
H	5.238400	-1.659700	-2.070900
C	3.339800	-1.234300	-1.171900
C	2.413600	-1.639900	2.522900
H	2.114800	-0.623000	2.808400
H	2.987400	-2.061500	3.351600
H	1.490900	-2.224200	2.416100
C	2.679400	-0.831600	-2.464700
H	2.543100	0.254500	-2.521900
H	1.690800	-1.294300	-2.577500
H	3.287700	-1.136400	-3.319700
C	-1.313800	-4.783700	1.179900
H	-2.042300	-5.589200	1.309900
H	-0.747800	-4.684700	2.113300
H	-1.888600	-3.855600	1.034900
C	-0.377500	-5.067300	-0.001100
C	0.745700	-4.050700	-0.145000
H	-0.959600	-5.132300	-0.929600
H	0.073900	-6.062500	1.034400
H	1.339400	-4.158600	-1.060200
H	1.413800	-4.012400	0.722500

Cu	-0.127300	-2.339200	-0.260000
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Zn_A1

N	1.293100	-1.076200	0.170500
S	2.373500	3.546400	-1.133700
C	0.762400	0.084700	-0.019500
C	1.228000	2.260800	-1.192700
C	1.520900	1.318000	-0.229500
C	2.691600	1.648300	0.539000
H	3.080700	1.030600	1.339600
C	3.252700	2.833500	0.187600
C	0.172000	2.258800	-2.257400
H	-0.238000	1.256300	-2.407300
H	0.587800	2.586100	-3.214900
H	-0.655500	2.928100	-2.000300
C	4.450700	3.508100	0.780400
H	4.196400	4.485600	1.203000
H	5.235600	3.660500	0.032500
H	4.862900	2.887700	1.580500
C	2.694300	-1.341000	0.092000
C	3.306200	-1.807700	1.266700
C	4.663500	-2.111400	1.220900
H	5.161600	-2.455400	2.122600
C	5.378700	-1.989100	0.033400
H	6.434300	-2.239400	0.008400
C	4.739700	-1.565200	-1.123800
H	5.296900	-1.493600	-2.053500
C	3.384300	-1.229200	-1.123700
C	2.513700	-1.942000	2.541700
H	1.704200	-2.676800	2.436500
H	2.052000	-0.992600	2.839200
H	3.151800	-2.275200	3.363500
C	2.722600	-0.779600	-2.401300
H	2.768400	0.310400	-2.505500
H	1.667400	-1.070800	-2.452100
H	3.228000	-1.217700	-3.265700
N	-1.296200	-1.073000	-0.162500
S	-2.364300	3.559800	1.116500
C	-0.762400	0.087100	0.022600
C	-1.221900	2.271800	1.183400
C	-1.517300	1.323600	0.226400
C	-2.687700	1.651600	-0.543700
H	-3.078700	1.028700	-1.339500
C	-3.245900	2.840200	-0.199700
C	-0.165700	2.273700	2.248000
H	0.242200	1.271200	2.403200
H	-0.580800	2.607100	3.203700
H	0.663100	2.939900	1.987200
C	-4.442700	3.513700	-0.796200
H	-4.186400	4.487900	-1.225200
H	-5.226800	3.672800	-0.048900
H	-4.856700	2.889200	-1.592100
C	-2.697200	-1.335700	-0.079700
C	-3.310100	-1.816000	-1.248600
C	-4.667700	-2.117600	-1.198900
H	-5.166400	-2.471600	-2.096400
C	-5.382500	-1.980800	-0.012700
H	-6.438300	-2.229400	0.015500
C	-4.742400	-1.544900	1.139500
H	-5.299000	-1.462600	2.068700
C	-3.386600	-1.210200	1.135100
C	-2.517900	-1.969500	-2.521700
H	-2.043200	-1.028700	-2.825600
H	-3.159500	-2.300500	-3.341700
H	-1.719200	-2.715200	-2.409700
C	-2.724700	-0.749200	2.408500
H	-2.775900	0.341200	2.506200
H	-1.668100	-1.034800	2.459100
H	-3.226400	-1.184600	3.276400
C	-0.016200	-4.591300	-0.024600

H	0.326300	-4.962100	-0.996500
H	0.649400	-4.998200	0.742800
H	-1.025800	-4.974800	0.151000
Zn	-0.001500	-2.667200	-0.001800

Zn_R1

N	1.265200	-0.987000	0.231400
S	2.596000	3.515100	-1.265300
C	0.807000	0.196800	0.008400
C	1.392000	2.281900	-1.261600
C	1.631800	1.384000	-0.243700
C	2.809000	1.704800	0.517000
H	3.166500	1.115300	1.352300
C	3.428800	2.840300	0.103400
C	0.338900	2.269000	-2.329500
H	-0.114500	1.278300	-2.425900
H	0.770100	2.523100	-3.302300
H	-0.457800	2.988100	-2.113200
C	4.655400	3.487700	0.667500
H	4.448300	4.500100	1.029700
H	5.452500	3.556000	-0.079900
H	5.030100	2.895800	1.506700
C	2.659600	-1.300700	0.163000
C	3.300900	-1.634600	1.364300
C	4.644000	-1.998800	1.312000
H	5.162800	-2.246200	2.233700
C	5.318500	-2.053800	0.096900
H	6.362000	-2.350000	0.068100
C	4.654000	-1.738300	-1.080800
H	5.181000	-1.791400	-2.029200
C	3.312900	-1.350500	-1.076800
C	2.567200	-1.540600	2.676800
H	1.625400	-2.097000	2.650900
H	2.314800	-0.501400	2.926000
H	3.174100	-1.937500	3.494100
C	2.627500	-0.991800	-2.370800
H	2.631100	0.093000	-2.527900
H	1.585700	-1.328900	-2.400900
H	3.144500	-1.451700	-3.216600
N	-1.318200	-0.815700	-0.236400
S	-2.073200	3.819500	1.253400
C	-0.710600	0.295000	0.012600
C	-1.029800	2.447800	1.264700
C	-1.380400	1.574200	0.258000
C	-2.509500	2.028600	-0.508600
H	-2.932800	1.478600	-1.340900
C	-2.985000	3.235800	-0.108200
C	0.017100	2.318400	2.330300
H	0.342700	1.280000	2.440500
H	-0.373100	2.642000	3.299800
H	0.897800	2.925900	2.097800
C	-4.119200	4.026400	-0.683200
H	-3.784000	4.998100	-1.060200
H	-4.900400	4.207900	0.062100
H	-4.567100	3.475000	-1.514100
C	-2.737600	-0.966000	-0.209600
C	-3.349800	-1.355300	-1.413200
C	-4.724500	-1.575700	-1.408100
H	-5.218800	-1.860500	-2.332300
C	-5.463700	-1.441400	-0.236900
H	-6.532600	-1.627700	-0.245300
C	-4.832300	-1.075200	0.943700
H	-5.410000	-0.979300	1.858900
C	-3.459000	-0.822300	0.985200
C	-2.546000	-1.483100	-2.682800
H	-2.014400	-0.553300	-2.919600
H	-3.194800	-1.720400	-3.529200
H	-1.791900	-2.276300	-2.611200
C	-2.821200	-0.422300	2.291200
H	-2.918200	0.656900	2.455300

H	-1.754200	-0.660900	2.327500
H	-3.310200	-0.930600	3.127200
C	0.292700	-4.014000	-1.466600
H	0.852200	-3.719000	-2.360200
H	0.902100	-4.744600	-0.922600
H	-0.621700	-4.520700	-1.794900
Zn	-0.108200	-2.494400	-0.326400
C	-1.687600	-3.884900	1.398000
C	-0.636700	-3.504000	2.133400
H	-1.643100	-4.766800	0.764800
H	-2.632300	-3.348400	1.428400
H	0.290500	-4.073500	2.134100
H	-0.693900	-2.654500	2.808800

Zn_TS_i

N	-1.287700	-0.898400	-0.178600
S	-2.396300	3.702100	1.167400
C	-0.758800	0.262600	0.023500
C	-1.251600	2.414400	1.219200
C	-1.525600	1.493700	0.231500
C	-2.679600	1.841400	-0.553000
H	-3.053300	1.240900	-1.373900
C	-3.249500	3.017800	-0.185100
C	-0.209100	2.387900	2.296500
H	0.202400	1.382400	2.422000
H	-0.636600	2.687100	3.258000
H	0.619200	3.066000	2.066500
C	-4.437200	3.703900	-0.785700
H	-4.176400	4.690700	-1.181900
H	-5.236800	3.839100	-0.050100
H	-4.833000	3.100900	-1.607100
C	-2.692800	-1.153900	-0.133700
C	-3.288600	-1.589000	-1.329200
C	-4.644200	-1.904300	-1.307300
H	-5.128900	-2.225700	-2.224600
C	-5.376000	-1.816700	-0.126800
H	-6.429700	-2.076300	-0.121400
C	-4.757300	-1.405100	1.045300
H	-5.329200	-1.347100	1.967100
C	-3.404200	-1.058600	1.070800
C	-2.490600	-1.655300	-2.606700
H	-1.617700	-2.311100	-2.509800
H	-2.113100	-0.666500	-2.896800
H	-3.104400	-2.030900	-3.428900
C	-2.778500	-0.597300	2.362000
H	-2.915400	0.482200	2.493300
H	-1.704800	-0.801800	2.405100
H	-3.246500	-1.099300	3.213000
N	1.307500	-0.873900	0.217600
S	2.323600	3.721400	-1.224500
C	0.760200	0.275900	0.008200
C	1.208200	2.407500	-1.244400
C	1.502400	1.517700	-0.234000
C	2.647900	1.911000	0.540700
H	3.036400	1.339100	1.374700
C	3.190900	3.091100	0.144000
C	0.164800	2.332700	-2.319100
H	-0.224500	1.315600	-2.420700
H	0.584900	2.618000	-3.288200
H	-0.677400	2.998600	-2.104600
C	4.365100	3.816200	0.725100
H	4.085900	4.809200	1.092400
H	5.162800	3.944500	-0.013800
H	4.771100	3.244800	1.563900
C	2.716900	-1.102400	0.129100
C	3.392300	-1.415800	1.316600
C	4.756300	-1.688100	1.239600
H	5.303900	-1.914300	2.150000
C	5.414900	-1.681300	0.014500
H	6.476000	-1.903700	-0.032000

C	4.712500	-1.403400	-1.151200
H	5.226500	-1.416200	-2.108000
C	3.348800	-1.106500	-1.122500
C	2.663100	-1.429800	2.635700
H	2.166800	-0.473100	2.840900
H	3.352000	-1.630700	3.459700
H	1.887500	-2.204000	2.653400
C	2.600300	-0.817500	-2.398100
H	2.416400	0.256400	-2.515600
H	1.631600	-1.330200	-2.425200
H	3.177400	-1.151300	-3.264000
C	0.282500	-4.609600	0.044400
C	0.608900	-3.974800	-1.213900
H	-0.589600	-5.254600	0.093400
H	1.101200	-4.922800	0.685500
H	-0.043300	-2.002000	-2.053900
H	1.667200	-3.899600	-1.455100
Zn	0.025400	-2.437800	-0.070400
C	-0.640300	-3.531100	1.669700
H	-0.295700	-2.702600	2.304800
H	-1.723100	-3.449800	1.520100
H	-0.437300	-4.442700	2.228600

Zn_P_i

N	-1.118100	-1.173400	-0.045300
S	-3.442200	3.061100	0.897400
C	-0.921700	0.097700	0.070400
C	-1.998900	2.137000	1.074400
C	-1.990700	1.090700	0.175700
C	-3.174700	1.045000	-0.640700
H	-3.352100	0.295500	-1.402800
C	-4.045100	2.055900	-0.388400
C	-1.025200	2.484900	2.160500
H	-0.366600	1.642100	2.386900
H	-1.552200	2.743200	3.083800
H	-0.399000	3.337300	1.877400
C	-5.354200	2.345100	-1.055100
H	-5.352700	3.326800	-1.539900
H	-6.181600	2.326800	-0.338300
H	-5.552300	1.588400	-1.818600
C	-2.401000	-1.798900	0.019400
C	-2.813200	-2.489600	-1.132200
C	-4.041500	-3.143000	-1.097900
H	-4.389300	-3.667100	-1.983300
C	-4.815900	-3.138700	0.058400
H	-5.767000	-3.660800	0.075300
C	-4.365200	-2.483300	1.196100
H	-4.962400	-2.502500	2.103200
C	-3.149200	-1.796700	1.205300
C	-1.957100	-2.491800	-2.373000
H	-0.991500	-2.985600	-2.196700
H	-1.740500	-1.475400	-2.723600
H	-2.452200	-3.027800	-3.186200
C	-2.687600	-1.102900	2.461200
H	-3.020800	-0.059000	2.478700
H	-1.596400	-1.101500	2.561100
H	-3.100000	-1.599100	3.343400
N	1.364400	-0.451800	0.310200
S	1.207900	4.232200	-1.195400
C	0.547100	0.510400	0.050300
C	0.448000	2.685200	-1.219600
C	0.950700	1.892900	-0.209800
C	1.968100	2.551700	0.565300
H	2.483000	2.087500	1.398400
C	2.205600	3.829200	0.172200
C	-0.531900	2.358000	-2.306300
H	-0.667700	1.277600	-2.404300
H	-0.176300	2.729900	-3.271800
H	-1.511700	2.805700	-2.110500
C	3.162700	4.820900	0.757400

H	2.644500	5.708900	1.133800
H	3.899500	5.151400	0.018200
C	3.702300	4.362800	1.590400
C	2.785100	-0.356900	0.523300
C	3.473600	-0.676300	1.435300
C	4.864400	-0.665200	1.409400
H	5.414600	-0.890700	2.318100
C	5.550000	-0.384700	0.231000
H	6.635000	-0.392900	0.219900
C	4.847000	-0.112100	-0.934000
H	5.385700	0.082600	-1.857000
C	3.450800	-0.087000	-0.952900
C	2.717600	-1.012400	2.694900
H	2.000500	-0.229200	2.967100
H	3.402400	-1.147500	3.535500
H	2.152100	-1.947500	2.580900
C	2.731700	0.193500	-2.247200
H	2.575600	1.269400	-2.385000
H	1.749900	-0.290000	-2.295800
H	3.320800	-0.170300	-3.093300
C	2.908800	-3.700300	-1.616900
H	2.325200	-4.356600	-2.273100
H	2.547400	-2.672000	-1.767000
H	3.950800	-3.727200	-1.950400
C	2.772600	-4.123800	-0.155700
C	1.316400	-4.123200	0.336700
H	3.385600	-3.461300	0.469000
H	3.194500	-5.130900	-0.038700
H	1.260800	-4.457700	1.380200
H	0.718800	-4.835500	-0.245600
Zn	0.528200	-2.357700	0.209800

Ru_A_i

N	1.233500	-1.029300	-0.069300
S	2.510100	3.677900	-0.779800
C	0.729200	0.183400	-0.115000
C	1.357500	2.421400	-1.049600
C	1.547500	1.400500	-0.147400
C	2.641700	1.644400	0.752100
H	2.947000	0.955700	1.531500
C	3.256300	2.838900	0.546800
C	0.377900	2.529300	-2.178600
H	-0.012900	1.543900	-2.448700
H	0.852000	2.952500	-3.069200
H	-0.472800	3.165200	-1.911300
C	4.410500	3.430700	1.295100
H	4.141000	4.380300	1.769200
H	5.264000	3.617200	0.635200
H	4.734100	2.739900	2.078300
C	2.633800	-1.315500	-0.002800
C	3.100300	-1.852500	1.210000
C	4.447200	-2.189600	1.300500
H	4.834100	-2.594100	2.231200
C	5.295700	-2.011400	0.211300
H	6.342800	-2.284600	0.291100
C	4.805200	-1.488300	-0.977700
H	5.472000	-1.355300	-1.824800
C	3.463600	-1.124500	-1.114100
C	2.172800	-2.013700	2.389600
H	1.387500	-2.764900	2.198500
H	1.665300	-1.074800	2.641500
H	2.718100	-2.350500	3.274600
C	2.966200	-0.528400	-2.403900
H	3.061700	0.563400	-2.382100
H	1.915300	-0.764600	-2.588300
H	3.551200	-0.899500	-3.249500
N	-1.246800	-1.030700	-0.077600
S	-2.524600	3.607700	0.905900
C	-0.739100	0.181400	-0.063900
C	-1.367500	2.336000	1.064100

C	-1.560200	1.392800	0.081100
C	-2.656800	1.711100	-0.790400
H	-2.955100	1.098000	-1.631800
C	-3.273100	2.883100	-0.483200
C	-0.370300	2.373000	2.183100
H	0.079200	1.388500	2.340800
H	-0.845300	2.675600	3.121400
H	0.441600	3.076800	1.971300
C	-4.432400	3.531800	-1.174500
H	-4.173800	4.526800	-1.551300
H	-5.290200	3.640900	-0.503000
H	-4.744600	2.918300	-2.023900
C	-2.636700	-1.303900	0.151500
C	-3.485000	-1.573500	-0.929200
C	-4.810700	-1.904100	-0.641400
H	-5.492600	-2.102800	-1.463400
C	-5.264100	-1.977900	0.668400
H	-6.297600	-2.240000	0.870200
C	-4.396500	-1.713600	1.723800
H	-4.754900	-1.769900	2.747400
C	-3.068200	-1.371500	1.487700
C	-3.023600	-1.504500	-2.362600
H	-2.112500	-0.913100	-2.481000
H	-3.801700	-1.063600	-2.993000
H	-2.815500	-2.504900	-2.757600
C	-2.134100	-1.064300	2.630100
H	-1.905400	0.006400	2.671800
H	-1.180100	-1.601200	2.542900
H	-2.583700	-1.347300	3.584700
C	0.082900	-2.857200	-2.078900
H	-0.722200	-3.570100	-2.325300
H	-0.030300	-1.978800	-2.722400
H	1.060600	-3.321200	-2.289100
Ru	-0.008400	-2.529000	-0.099200

Ru_R_i

N	-1.287400	-0.756100	-0.067500
S	-1.989500	3.960900	1.036500
C	-0.636400	0.374700	-0.035900
C	-1.013500	2.542900	1.154800
C	-1.298500	1.680500	0.121100
C	-2.315300	2.182700	-0.759400
H	-2.659700	1.658100	-1.641100
C	-2.780200	3.410300	-0.408300
C	-0.059600	2.386700	2.301400
H	0.254000	1.344800	2.413000
H	-0.525800	2.691400	3.243500
H	0.840000	2.993600	2.155800
C	-3.819500	4.240700	-1.096200
H	-3.418600	5.207900	-1.416500
H	-4.676200	4.433400	-0.442200
H	-4.183900	3.714000	-1.982300
C	-2.722500	-0.781500	0.091400
C	-3.550200	-0.892200	-1.030500
C	-4.923800	-1.016400	-0.813500
H	-5.584400	-1.100000	-1.672200
C	-5.450300	-1.025800	0.470000
H	-6.520000	-1.130800	0.618600
C	-4.605500	-0.889000	1.565900
H	-5.018500	-0.880700	2.570500
C	-3.229100	-0.759600	1.400200
C	-3.038300	-0.822000	-2.448700
H	-3.285100	-1.729000	-3.009700
H	-1.957100	-0.678200	-2.499600
H	-3.511600	0.010800	-2.981400
C	-2.345000	-0.558300	2.605000
H	-2.196700	0.511000	2.795200
H	-1.353500	-1.009500	2.489800
H	-2.802100	-0.994600	3.496800
N	1.264500	-0.978100	0.015200

S	2.871800	3.593400	-0.835400
C	0.854600	0.245900	-0.073700
C	1.626700	2.422200	-1.070500
C	1.740400	1.414700	-0.141100
C	2.854400	1.595800	0.749400
H	3.108800	0.903700	1.544000
C	3.554200	2.736300	0.515100
C	0.674900	2.561400	-2.219700
H	0.153300	1.619600	-2.412300
H	1.208100	2.833800	-3.135600
H	-0.080400	3.329200	-2.023600
C	4.748400	3.262000	1.249700
H	4.547200	4.238600	1.702100
H	5.611700	3.372600	0.585500
H	5.023800	2.567700	2.048000
C	2.638700	-1.356600	0.029800
C	3.094500	-1.967700	1.211800
C	4.414200	-2.404000	1.263600
H	4.788200	-2.862600	2.174400
C	5.251200	-2.260600	0.160600
H	6.276000	-2.614000	0.207500
C	4.772700	-1.671200	-1.000800
H	5.426400	-1.568000	-1.862400
C	3.460500	-1.199300	-1.094200
C	2.184100	-2.099000	2.407400
H	1.778700	-1.130400	2.724300
H	2.713000	-2.535400	3.258300
H	1.325000	-2.758000	2.199200
C	2.997800	-0.544700	-2.370000
H	3.280100	0.514300	-2.382900
H	1.914000	-0.598000	-2.498800
H	3.463600	-1.023900	-3.235700
C	-1.687500	-3.717700	0.884100
H	-1.374800	-4.771700	0.895700
H	-1.602500	-3.323000	1.920900
H	-2.738100	-3.663800	0.587300
Ru	-0.291100	-2.472100	0.047500
C	-1.069000	-3.486600	-1.634200
C	0.048800	-2.691400	-2.011500
H	-2.079400	-3.190100	-1.893700
H	-0.943200	-4.564800	-1.545700
H	-0.100700	-1.770300	-2.572500
H	1.017900	-3.159700	-2.192700

Ru_TS_i

N	1.279600	-0.676600	0.028400
S	1.875100	4.083900	-1.017200
C	0.609700	0.454700	0.016200
C	0.933600	2.642600	-1.144200
C	1.250800	1.773100	-0.126200
C	2.265100	2.289300	0.749200
H	2.636500	1.763400	1.619200
C	2.697300	3.532500	0.408500
C	-0.041800	2.482100	-2.271600
H	-0.292400	1.427800	-2.423700
H	0.374300	2.862200	-3.209600
H	-0.974300	3.019500	-2.069700
C	3.726200	4.377100	1.094800
H	3.307300	5.330200	1.433800
H	4.570100	4.599100	0.433300
H	4.113800	3.847200	1.969100
C	2.710900	-0.705800	-0.095200
C	3.506300	-0.792900	1.053200
C	4.885500	-0.928900	0.879200
H	5.522700	-0.990000	1.757300
C	5.447000	-0.975500	-0.389200
H	6.520300	-1.085600	-0.504300
C	4.634900	-0.863200	-1.513500
H	5.078000	-0.877600	-2.505100
C	3.255300	-0.721000	-1.389100

C	2.938600	-0.705400	2.449900
H	2.984900	-1.669500	2.968700
H	1.897100	-0.375100	2.455700
H	3.519200	0.002000	3.051100
C	2.389700	-0.536200	-2.609100
H	2.091400	0.513800	-2.711000
H	1.467500	-1.129000	-2.569500
H	2.928500	-0.820500	-3.516300
N	-1.185000	-0.988500	-0.028700
S	-3.029300	3.482700	0.953700
C	-0.845600	0.273300	0.061600
C	-1.731100	2.359200	1.138600
C	-1.804000	1.382200	0.174000
C	-2.928700	1.549600	-0.704700
H	-3.157600	0.880300	-1.525700
C	-3.681400	2.645500	-0.421800
C	-0.758500	2.512900	2.268500
H	-0.227000	1.574100	2.451400
H	-1.272800	2.787300	3.194500
H	-0.011500	3.283900	2.052400
C	-4.907700	3.137200	-1.127100
H	-4.764000	4.143100	-1.535300
H	-5.771800	3.169400	-0.455400
H	-5.149400	2.465900	-1.955400
C	-2.544500	-1.430900	-0.026000
C	-3.068500	-1.907700	-1.238400
C	-4.373500	-2.394500	-1.239500
H	-4.805400	-2.754400	-2.168900
C	-5.122500	-2.422800	-0.067300
H	-6.135800	-2.810600	-0.081400
C	-4.574000	-1.958000	1.121200
H	-5.161000	-1.985400	2.034800
C	-3.275100	-1.449000	1.169000
C	-2.255300	-1.858400	-2.508900
H	-1.845800	-0.858300	-2.694900
H	-2.863900	-2.138100	-3.372500
H	-1.403400	-2.553100	-2.475600
C	-2.703500	-0.925600	2.460200
H	-2.831800	0.160900	2.527700
H	-1.633400	-1.137000	2.545400
H	-3.210400	-1.375800	3.317700
C	1.497100	-3.665500	1.263900
C	0.345900	-2.974700	1.832100
H	2.478200	-3.250800	1.474300
H	1.488200	-4.752300	1.320200
H	0.538200	-2.193700	2.566300
H	-0.527700	-3.582600	2.090000
Ru	0.269500	-2.368200	-0.105900
C	1.680300	-3.929100	-0.719300
H	1.151100	-4.870900	-0.894100
H	1.628000	-3.298100	-1.634000
H	2.742100	-4.131100	-0.576900

Ru_P_i

N	-1.308400	-0.533300	0.055900
S	-1.601400	4.304200	0.884800
C	-0.571800	0.555900	0.031700
C	-0.744100	2.818300	1.078900
C	-1.129400	1.915100	0.115000
C	-2.126500	2.442200	-0.774000
H	-2.542200	1.891800	-1.608100
C	-2.479200	3.725400	-0.496800
C	0.236600	2.662900	2.202400
H	0.457000	1.607200	2.387100
H	-0.159400	3.085800	3.130700
H	1.183600	3.164700	1.976800
C	-3.468100	4.591400	-1.214400
H	-2.999600	5.497900	-1.611400
H	-4.285800	4.899000	-0.554400
H	-3.901300	4.038600	-2.052400

C	-2.739200	-0.483100	0.163400
C	-3.528800	-0.569300	-0.987200
C	-4.915500	-0.599400	-0.819100
H	-5.550500	-0.655400	-1.699200
C	-5.485600	-0.553200	0.445100
H	-6.564900	-0.578300	0.554800
C	-4.674300	-0.470300	1.573500
H	-5.122600	-0.429800	2.561900
C	-3.288300	-0.436200	1.454500
C	-2.943800	-0.615300	-2.377600
H	-3.077000	-1.605900	-2.827400
H	-1.875400	-0.386000	-2.389500
H	-3.452500	0.099800	-3.032600
C	-2.400800	-0.346000	2.668400
H	-1.831400	0.590200	2.675700
H	-1.678500	-1.174500	2.702600
H	-2.990600	-0.387300	3.587100
N	1.139000	-0.998100	0.094800
S	3.252900	3.306000	-1.036100
C	0.872100	0.279800	-0.020200
C	1.876700	2.272800	-1.172000
C	1.900000	1.315800	-0.184100
C	3.050000	1.424500	0.670700
H	3.246700	0.760500	1.504200
C	3.870700	2.458900	0.349100
C	0.898900	2.468500	-2.291100
H	0.313900	1.559300	-2.458600
H	1.416200	2.705000	-3.225800
H	0.199000	3.282100	-2.074000
C	5.139900	2.881900	1.022100
H	5.071500	3.904000	1.408900
H	5.991700	2.840600	0.335400
H	5.351100	2.214500	1.861900
C	2.458300	-1.542100	0.038900
C	3.000100	-2.035100	1.236100
C	4.262500	-2.621000	1.186900
H	4.711100	-2.996900	2.102000
C	4.947000	-2.728800	-0.019800
H	5.927900	-3.192300	-0.045400
C	4.374500	-2.254400	-1.194100
H	4.908700	-2.354300	-2.134600
C	3.116500	-1.650700	-1.192500
C	2.244800	-1.900300	2.535200
H	1.984900	-0.857400	2.753200
H	2.832900	-2.282800	3.373000
H	1.299600	-2.467000	2.520800
C	2.495100	-1.141700	-2.466000
H	2.616600	-0.055800	-2.553100
H	1.422300	-1.360700	-2.503300
H	2.968200	-1.601800	-3.337100
C	-1.967500	-5.261400	-0.538500
H	-2.097200	-5.735800	-1.515600
H	-1.027300	-5.627100	-0.110900
H	-2.786700	-5.582100	0.111200
C	-1.941800	-3.743200	-0.702600
C	-0.757700	-3.168700	-1.440600
H	-2.893000	-3.352400	-1.075100
H	-0.980200	-2.577000	-2.327900
H	0.039400	-3.895600	-1.655300
Ru	-0.383800	-2.246900	0.293900
H	-1.965700	-3.319000	0.388400

Rh_A₁

N	1.299200	-0.924500	0.050400
S	2.062200	3.774500	-1.106100
C	0.670200	0.210100	-0.029300
C	1.044700	2.386200	-1.197100
C	1.357300	1.499200	-0.189800
C	2.435000	1.957800	0.643300
H	2.826200	1.405200	1.487800

C	2.910200	3.180100	0.288800
C	0.050300	2.264700	-2.313400
H	-0.294700	1.232800	-2.425800
H	0.497300	2.565000	-3.265900
H	-0.826900	2.895100	-2.135700
C	4.003900	3.973000	0.934900
H	3.640400	4.937700	1.303800
H	4.823400	4.169000	0.236000
H	4.410100	3.415700	1.783100
C	2.732700	-1.005100	0.025600
C	3.392200	-1.207800	1.243500
C	4.780200	-1.321800	1.211800
H	5.321400	-1.469700	2.141800
C	5.472600	-1.257700	0.006900
H	6.553400	-1.354000	-0.001300
C	4.783700	-1.086100	-1.187900
H	5.327700	-1.053800	-2.127400
C	3.394700	-0.960500	-1.204800
C	2.623200	-1.293300	2.536200
H	1.927300	-2.142400	2.529000
H	2.025400	-0.392300	2.722900
H	3.298600	-1.425800	3.384600
C	2.636900	-0.797500	-2.495700
H	2.212200	0.208900	-2.585100
H	1.809300	-1.515100	-2.569800
H	3.293300	-0.959500	-3.353800
N	-1.285300	-1.086400	-0.060100
S	-2.717500	3.501600	0.972800
C	-0.835200	0.119500	0.028100
C	-1.501600	2.287000	1.123000
C	-1.680600	1.314100	0.166400
C	-2.820500	1.558700	-0.674300
H	-3.126200	0.902900	-1.481000
C	-3.475000	2.711800	-0.377500
C	-0.499800	2.365900	2.235900
H	-0.024300	1.395300	2.404700
H	-0.981800	2.659500	3.173300
H	0.287600	3.093900	2.015800
C	-4.680300	3.295500	-1.047600
H	-4.469300	4.282800	-1.471300
H	-5.515300	3.403200	-0.347800
H	-5.003400	2.638900	-1.859700
C	-2.670200	-1.415700	0.025500
C	-3.281900	-1.901000	-1.141200
C	-4.619500	-2.279800	-1.067800
H	-5.118900	-2.640700	-1.962300
C	-5.313900	-2.207400	0.136000
H	-6.353500	-2.514900	0.181100
C	-4.674100	-1.755600	1.282800
H	-5.215200	-1.716800	2.224000
C	-3.339200	-1.347900	1.255300
C	-2.516000	-1.970700	-2.438200
H	-2.136500	-0.987800	-2.744000
H	-3.147200	-2.351000	-3.244900
H	-1.645100	-2.636300	-2.360600
C	-2.662400	-0.862100	2.511300
H	-2.676000	0.232400	2.566700
H	-1.615300	-1.182100	2.565900
H	-3.174800	-1.246700	3.396600
C	1.734100	-3.987000	0.065600
H	1.246600	-4.976000	-0.012700
H	2.430400	-3.868100	-0.774300
H	2.313800	-3.957600	0.995800
Rh	0.239000	-2.626400	-0.007200

Rh_R₁

N	-1.205300	-0.960500	-0.098500
S	-2.797300	3.488200	1.283600
C	-0.828200	0.269400	0.029100
C	-1.548200	2.300000	1.286900

C	-1.730400	1.411100	0.250300
C	-2.898200	1.703400	-0.534500
H	-3.216500	1.119000	-1.388000
C	-3.570000	2.807400	-0.115500
C	-0.511400	2.311900	2.371100
H	0.005000	1.349200	2.434300
H	-0.970800	2.497600	3.346700
H	0.239500	3.089000	2.195400
C	-4.808200	3.415500	-0.697900
H	-4.634900	4.443100	-1.034100
H	-5.626100	3.434700	0.029700
H	-5.136600	2.826700	-1.558500
C	-2.602600	-1.278700	-0.086300
C	-3.220900	-1.531600	-1.316300
C	-4.570200	-1.881600	-1.302600
H	-5.076900	-2.074900	-2.243900
C	-5.265100	-1.992900	-0.103100
H	-6.313900	-2.271300	-0.108500
C	-4.614600	-1.763800	1.103800
H	-5.155900	-1.868700	2.039700
C	-3.267000	-1.405200	1.317700
C	-2.452000	-1.403700	-2.606200
H	-1.517500	-1.977200	-2.576300
H	-2.175200	-0.361700	-2.814000
H	-3.045600	-1.760500	-3.451500
C	-2.546000	-1.179000	2.440300
H	-2.304500	-0.119300	2.583200
H	-1.602900	-1.739900	2.478600
H	-3.161400	-1.496900	3.285400
N	1.333300	-0.616300	0.112700
S	1.823700	4.074400	-1.251800
C	0.662700	0.474400	-0.021800
C	0.874200	2.635200	-1.266200
C	1.260500	1.798900	-0.242600
C	2.340300	2.335500	0.538800
H	2.786100	1.827200	1.384600
C	2.743700	3.567700	0.131500
C	-0.148400	2.425000	-2.342900
H	-0.401000	1.365100	-2.443500
H	0.230900	2.761900	-3.312200
H	-1.070800	2.974200	-2.128300
C	3.816200	4.433600	0.716700
H	3.415400	5.388400	1.072500
H	4.600100	4.651800	-0.015700
H	4.279700	3.922500	1.564700
C	2.759800	-0.662700	0.080900
C	3.429600	-0.831700	1.301800
C	4.817800	-0.948700	1.267200
H	5.363200	-1.070200	2.198600
C	5.505400	-0.915000	0.058000
H	6.585900	-1.014500	0.047400
C	4.812100	-0.761900	-1.137400
H	5.353900	-0.743000	-2.078700
C	3.423200	-0.633100	-1.153300
C	2.669200	-0.848100	2.603600
H	2.246700	0.137900	2.836000
H	3.322300	-1.129400	3.433300
H	1.827900	-1.551100	2.574600
C	2.667100	-0.470700	-2.446100
H	2.330900	0.564700	-2.575100
H	1.778300	-1.112600	-2.478600
H	3.300600	-0.723500	-3.299800
C	-1.148300	-3.873200	-0.119800
H	-0.686800	-4.867100	-0.069600
H	-1.829100	-3.745800	0.728200
H	-1.691000	-3.767700	-1.062600
Rh	0.351000	-2.517100	0.029900
C	1.883900	-3.854900	-0.723800
C	1.870400	-3.929500	0.664600
H	2.631400	-3.250700	-1.233200

H	1.386900	-4.602400	-1.337300
H	2.617300	-3.394300	1.245800
H	1.367400	-4.743000	1.182300

Rh_TS1

N	-1.306200	-0.780300	-0.117300
S	-2.359700	3.811800	1.272600
C	-0.765600	0.386400	0.020200
C	-1.248900	2.492300	1.284400
C	-1.519900	1.630600	0.245600
C	-2.643900	2.048200	-0.545800
H	-3.017200	1.500900	-1.402300
C	-3.194600	3.219100	-0.130400
C	-0.223400	2.388400	2.373700
H	0.165900	1.368700	2.451300
H	-0.658400	2.644200	3.344600
H	0.621200	3.060900	2.191800
C	-4.354600	3.959800	-0.720700
H	-4.065800	4.960600	-1.058400
H	-5.168800	4.072500	0.002500
H	-4.742400	3.409100	-1.581800
C	-2.721100	-0.968800	-0.092600
C	-3.360600	-1.214400	-1.315100
C	-4.728800	-1.480500	-1.291600
H	-5.249900	-1.660200	-2.227700
C	-5.425200	-1.524000	-0.088700
H	-6.488900	-1.738100	-0.085600
C	-4.757800	-1.306300	1.111000
H	-5.302200	-1.354600	2.049700
C	-3.390800	-1.027400	1.135700
C	-2.593500	-1.153600	-2.611700
H	-1.698900	-1.788500	-2.588400
H	-2.245300	-0.135900	-2.831000
H	-3.216500	-1.476300	-3.449500
C	-2.663300	-0.801500	2.435600
H	-2.406600	0.256100	2.565900
H	-1.728100	-1.373800	2.481500
H	-3.283700	-1.100600	3.284000
N	1.294600	-0.772800	0.087400
S	2.299600	3.845700	-1.238600
C	0.737800	0.391900	-0.031700
C	1.203400	2.514900	-1.267400
C	1.484300	1.642200	-0.239800
C	2.603300	2.062500	0.557800
H	2.981700	1.509900	1.408400
C	3.140400	3.244700	0.157500
C	0.179100	2.414700	-2.358400
H	-0.208100	1.394800	-2.442900
H	0.614900	2.677800	-3.327100
H	-0.667000	3.084300	-2.173000
C	4.291500	3.991100	0.757900
H	3.991800	4.985200	1.105600
H	5.105800	4.119700	0.037500
H	4.683400	3.435300	1.613800
C	2.718900	-0.938300	0.052000
C	3.375200	-1.172700	1.266900
C	4.750500	-1.396100	1.228000
H	5.285600	-1.568300	2.157600
C	5.436900	-1.406100	0.018400
H	6.506800	-1.586400	0.003900
C	4.752000	-1.198200	-1.172900
H	5.288700	-1.221000	-2.117100
C	3.376900	-0.962300	-1.182700
C	2.617800	-1.157800	2.569500
H	2.187200	-0.170800	2.781600
H	3.272300	-1.419300	3.404600
H	1.780400	-1.866900	2.558300
C	2.628600	-0.755300	-2.473300
H	2.316200	0.288900	-2.588200
H	1.725000	-1.376500	-2.517800

H	3.256600	-1.010700	-3.330300
C	-1.516900	-3.991500	-0.128700
H	-1.802500	-5.039600	-0.134600
H	-2.041700	-3.528700	0.717000
H	-1.868700	-3.566600	-1.076500
C	0.314000	-4.784200	0.054900
C	1.459500	-3.931900	0.188400
H	0.218200	-5.339800	-0.874300
H	0.026300	-5.355400	0.933500
H	2.153600	-3.851900	-0.650500
H	1.951900	-3.877600	1.160800
Rh	0.066700	-2.451200	0.022900

Rh_P1

N	1.313200	-0.728800	0.175000
S	2.428400	3.866700	-1.169300
C	0.777000	0.437400	0.000200
C	1.295300	2.568200	-1.230500
C	1.545300	1.669800	-0.217400
C	2.671600	2.042500	0.594800
H	3.024900	1.461000	1.438000
C	3.244300	3.216000	0.221200
C	0.285600	2.510800	-2.337400
H	-0.126300	1.502800	-2.441300
H	0.743600	2.775700	-3.295200
H	-0.546100	3.199300	-2.156100
C	4.409900	3.920900	0.843100
H	4.133400	4.915500	1.208100
H	5.231900	4.042400	0.130200
H	4.781700	3.338600	1.690400
C	2.723100	-0.951900	0.103000
C	3.371600	-1.305800	1.295500
C	4.736100	-1.577700	1.241200
H	5.262800	-1.835900	2.155500
C	5.422900	-1.528500	0.032000
H	6.484900	-1.749500	0.002300
C	4.747200	-1.211900	-1.139600
H	5.282800	-1.194000	-2.084500
C	3.382900	-0.916200	-1.132500
C	2.607800	-1.364200	2.593100
H	1.792400	-2.099900	2.546500
H	2.146500	-0.400500	2.842500
H	3.263100	-1.646300	3.420700
C	2.663300	-0.589300	-2.415600
H	2.557500	0.493900	-2.544100
H	1.658500	-1.026700	-2.443200
H	3.219400	-0.972400	-3.275000
N	-1.280300	-0.724600	-0.012400
S	-2.336700	3.961900	0.995100
C	-0.729900	0.447000	0.045300
C	-1.229300	2.647100	1.133100
C	-1.488300	1.701500	0.166100
C	-2.600100	2.053300	-0.673900
H	-2.960700	1.438600	-1.488900
C	-3.153800	3.255000	-0.365300
C	-0.220800	2.635700	2.243100
H	0.175000	1.628900	2.406300
H	-0.673900	2.963800	3.183500
H	0.622700	3.298100	2.023000
C	-4.303600	3.945300	-1.031500
H	-4.009400	4.916500	-1.442800
H	-5.129500	4.113900	-0.332800
H	-4.677500	3.327400	-1.852200
C	-2.701900	-0.906800	0.032500
C	-3.350500	-1.233300	-1.165600
C	-4.723700	-1.465400	-1.115800
H	-5.253500	-1.707400	-2.032700
C	-5.415100	-1.395200	0.089100
H	-6.483500	-1.583500	0.112400
C	-4.737800	-1.095300	1.265000

H	-5.278700	-1.054600	2.206100
C	-3.365100	-0.846000	1.263400
C	-2.587400	-1.304400	-2.462800
H	-2.139700	-0.338300	-2.728700
H	-3.242200	-1.603800	-3.284700
H	-1.762100	-2.024800	-2.404100
C	-2.626900	-0.536700	2.539400
H	-2.333400	0.518400	2.582300
H	-1.714000	-1.138300	2.631900
H	-3.255300	-0.742700	3.409300
C	0.638900	-5.507400	-1.026200
H	1.675100	-5.797900	-0.834400
H	0.047000	-6.415900	-1.169600
H	0.607700	-4.927200	-1.953300
C	0.053400	-4.706800	0.134500
C	-1.236000	-4.016100	-0.086600
H	0.103600	-5.243500	1.085900
H	-1.995100	-4.090200	0.694900
H	-1.670900	-4.093700	-1.085800
Rh	-0.062400	-2.378000	0.172600
H	0.913600	-3.869300	0.349800

Pd_A1

N	-1.312000	-0.930000	-0.078900
S	-2.070700	3.733100	1.207900
C	-0.683700	0.198900	0.032700
C	-1.047700	2.346900	1.251300
C	-1.369400	1.484800	0.225000
C	-2.459000	1.960200	-0.582700
H	-2.859700	1.426900	-1.434900
C	-2.933100	3.171800	-0.191900
C	-0.040200	2.200300	2.352800
H	0.300200	1.164800	2.444100
H	-0.473800	2.485900	3.315900
H	0.837500	2.830100	2.174800
C	-4.036800	3.977400	-0.804400
H	-3.680200	4.951600	-1.154500
H	-4.847600	4.154300	-0.090300
H	-4.452800	3.439600	-1.660400
C	-2.741100	-1.016900	-0.066000
C	-3.390600	-1.195300	-1.293900
C	-4.778200	-1.322400	-1.274900
H	-5.311200	-1.451300	-2.212400
C	-5.479900	-1.294300	-0.074100
H	-6.559800	-1.399500	-0.076300
C	-4.800900	-1.146900	1.129900
H	-5.351900	-1.142300	2.065800
C	-3.413300	-1.010000	1.160900
C	-2.612100	-1.233300	-2.582900
H	-1.850500	-2.023100	-2.567200
H	-2.083100	-0.290400	-2.771700
H	-3.273600	-1.417700	-3.432600
C	-2.664800	-0.874900	2.459800
H	-2.238000	0.128400	2.571200
H	-1.837800	-1.594300	2.521000
H	-3.328000	-1.051200	3.309900
N	1.303800	-1.067600	0.103000
S	2.637000	3.508000	-1.085000
C	0.827900	0.123700	-0.019500
C	1.439800	2.270100	-1.180500
C	1.649200	1.329200	-0.198000
C	2.797200	1.617200	0.617500
H	3.125600	0.990900	1.438500
C	3.427000	2.771900	0.277000
C	0.421300	2.297800	-2.280700
H	-0.034900	1.312900	-2.417900
H	0.883900	2.576000	-3.232300
H	-0.378100	3.015000	-2.068300
C	4.631200	3.395800	0.911900
H	4.408200	4.390800	1.310800

H	5.453700	3.498500	0.196600
H	4.978300	2.768400	1.737000
C	2.693300	-1.377400	0.020000
C	3.317800	-1.817300	1.197700
C	4.660600	-2.178400	1.127400
H	5.170300	-2.505000	2.029200
C	5.347000	-2.131600	-0.082300
H	6.390800	-2.424800	-0.124300
C	4.694300	-1.724300	-1.238700
H	5.229700	-1.706100	-2.183700
C	3.353400	-1.336900	-1.216100
C	2.560200	-1.853400	2.500900
H	2.221500	-0.854300	2.802900
H	3.185100	-2.250200	3.304500
H	1.662900	-2.482400	2.433400
C	2.661000	-0.900700	-2.481700
H	2.648500	0.192000	-2.565500
H	1.622500	-1.248400	-2.523400
H	3.180700	-1.295500	-3.358400
C	-1.667300	-3.933900	-0.122200
H	-2.357200	-3.817400	0.719900
H	-2.216400	-3.841900	-1.063300
H	-1.152600	-4.908000	-0.072500
Pd	-0.178200	-2.614900	0.022900

Pd_R_i

N	1.287100	-0.887600	0.113900
S	2.396800	3.650800	-1.391300
C	0.770400	0.288400	-0.024900
C	1.289200	2.329700	-1.356700
C	1.547800	1.515900	-0.276900
C	2.658200	1.973600	0.510900
H	3.023900	1.469000	1.395600
C	3.211300	3.126000	0.049500
C	0.274500	2.176400	-2.450800
H	-0.151400	1.168500	-2.455700
H	0.730600	2.339200	-3.432200
H	-0.545600	2.892100	-2.334100
C	4.361700	3.895200	0.621600
H	4.066500	4.909300	0.910200
H	5.185500	3.977200	-0.094900
H	4.739000	3.384400	1.511500
C	2.711600	-1.041600	0.100000
C	3.364300	-1.180200	1.330700
C	4.745200	-1.371000	1.312600
H	5.277900	-1.473800	2.253700
C	5.439400	-1.438700	0.109800
H	6.513600	-1.592100	0.112400
C	4.757900	-1.326500	-1.096500
H	5.301300	-1.396300	-2.034400
C	3.377400	-1.130700	-1.126900
C	2.600300	-1.099600	2.627900
H	1.715900	-1.748000	2.619900
H	2.242400	-0.081300	2.827600
H	3.231100	-1.395400	3.469700
C	2.628400	-1.024800	-2.429000
H	2.279600	-0.000400	-2.603000
H	1.747300	-1.679200	-2.440000
H	3.268300	-1.305700	-3.268900
N	-1.342400	-0.770700	-0.117700
S	-2.094700	3.852500	1.360300
C	-0.735700	0.356300	0.030500
C	-1.088700	2.451900	1.344700
C	-1.407100	1.646000	0.275600
C	-2.480900	2.173800	-0.519100
H	-2.882100	1.684600	-1.397500
C	-2.947000	3.370400	-0.073800
C	-0.087100	2.235700	2.439800
H	0.236700	1.191000	2.475400
H	-0.517700	2.474000	3.417100

H	0.799000	2.862600	2.296500
C	-4.037000	4.215800	-0.656700
H	-3.666900	5.201100	-0.958500
H	-4.852100	4.368700	0.058100
H	-4.451700	3.723100	-1.540100
C	-2.772100	-0.831000	-0.097400
C	-3.432800	-0.970900	-1.324300
C	-4.821200	-1.096100	-1.304400
H	-5.357700	-1.196500	-2.243700
C	-5.518900	-1.100200	-0.101400
H	-6.599000	-1.203900	-0.101400
C	-4.832600	-0.985900	1.102100
H	-5.379100	-1.004200	2.040700
C	-3.444100	-0.851400	1.130300
C	-2.663200	-0.959000	-2.620700
H	-2.277200	0.041700	-2.854300
H	-3.298300	-1.266800	-3.455200
H	-1.794000	-1.627100	-2.585400
C	-2.695100	-0.746600	2.433200
H	-2.336500	0.275400	2.601200
H	-1.820000	-1.408500	2.451400
H	-3.339500	-1.015000	3.273900
C	1.567200	-3.797400	0.221000
H	2.175300	-3.567100	-0.659400
H	2.069300	-3.450100	1.126600
H	1.420200	-4.873200	0.286700
Pd	-0.050700	-2.535700	0.016100
C	-0.912900	-4.644600	-0.038500
C	-1.907600	-3.722200	-0.203500
H	-0.718400	-5.083100	0.935200
H	-0.472000	-5.145400	-0.894700
H	-2.524000	-3.403600	0.633100
H	-2.279400	-3.470700	-1.193000

Pd_TS_i

N	-1.311400	-0.769700	-0.139800
S	-2.354200	3.807400	1.310500
C	-0.773600	0.389900	0.019200
C	-1.243500	2.487700	1.303500
C	-1.524800	1.632500	0.262400
C	-2.656500	2.054500	-0.515600
H	-3.038000	1.511200	-1.371100
C	-3.202900	3.223000	-0.087900
C	-0.207700	2.376100	2.382600
H	0.184200	1.356500	2.447500
H	-0.634700	2.621700	3.359700
H	0.633500	3.052400	2.199300
C	-4.368500	3.967400	-0.662200
H	-4.082900	4.970000	-0.997000
H	-5.175400	4.076100	0.069800
H	-4.765200	3.421800	-1.522500
C	-2.721500	-0.971900	-0.109700
C	-3.364000	-1.215800	-1.330900
C	-4.729500	-1.494900	-1.303900
H	-5.252800	-1.673200	-2.239100
C	-5.420100	-1.553700	-0.098300
H	-6.481800	-1.777900	-0.092100
C	-4.749400	-1.339300	1.100300
H	-5.289100	-1.400700	2.041000
C	-3.385200	-1.047500	1.121200
C	-2.600500	-1.138400	-2.628500
H	-1.684400	-1.741100	-2.598000
H	-2.289300	-0.110300	-2.855100
H	-3.212100	-1.488500	-3.463700
C	-2.652500	-0.827700	2.419200
H	-2.405500	0.230900	2.559400
H	-1.711400	-1.391200	2.452700
H	-3.264700	-1.142200	3.268000
N	1.299600	-0.755500	0.105200
S	2.267800	3.852800	-1.283800

C	0.739500	0.399300	-0.032400
C	1.180900	2.513800	-1.291600
C	1.475900	1.653300	-0.258100
C	2.597800	2.088700	0.526800
H	2.987100	1.546000	1.379000
C	3.123500	3.270900	0.111300
C	0.148300	2.395800	-2.373200
H	-0.231500	1.372200	-2.445700
H	0.574100	2.653200	-3.347800
H	-0.701100	3.060900	-2.187000
C	4.273900	4.031000	0.695700
H	3.969300	5.025400	1.038300
H	5.080900	4.160400	-0.032800
H	4.677600	3.485000	1.552500
C	2.720900	-0.922700	0.071400
C	3.376900	-1.143700	1.289000
C	4.751500	-1.372300	1.253000
H	5.286100	-1.534400	2.184700
C	5.437500	-1.400300	0.043500
H	6.506900	-1.584400	0.031100
C	4.753000	-1.206000	-1.150600
H	5.289400	-1.243100	-2.094500
C	3.378700	-0.965800	-1.163000
C	2.618000	-1.107300	2.590400
H	2.236100	-0.102200	2.811500
H	3.257500	-1.407200	3.424200
H	1.747200	-1.773900	2.567800
C	2.629200	-0.774000	-2.455300
H	2.323300	0.270400	-2.585300
H	1.721200	-1.389500	-2.487800
H	3.253600	-1.046600	-3.309700
C	0.379300	-4.747300	0.069700
C	1.493300	-3.870800	0.226300
H	0.300600	-5.295000	-0.865000
H	0.063700	-5.308100	0.944700
H	2.191800	-3.756000	-0.602800
H	1.947900	-3.778700	1.212100
Pd	0.068900	-2.439400	0.017400
C	-1.497700	-3.961200	-0.161400
H	-2.034100	-3.521400	0.685600
H	-1.827800	-3.543200	-1.116300
H	-1.735800	-5.020600	-0.177000

Pd_P_i

N	1.291000	-0.776400	0.170600
S	2.593700	3.762200	-1.194100
C	0.808600	0.406700	-0.001100
C	1.410800	2.507600	-1.244800
C	1.625700	1.608900	-0.225200
C	2.765800	1.943200	0.583500
H	3.097800	1.353400	1.429500
C	3.384900	3.090100	0.199900
C	0.393900	2.482900	-2.346700
H	-0.047900	1.487400	-2.450300
H	0.854100	2.735400	-3.306800
H	-0.416200	3.195100	-2.159700
C	4.579800	3.751100	0.814300
H	4.345900	4.759600	1.170800
H	5.405400	3.831700	0.099700
H	4.928000	3.161400	1.666500
C	2.687500	-1.064600	0.103700
C	3.323200	-1.425900	1.300500
C	4.673500	-1.762400	1.246000
H	5.191300	-2.028200	2.163300
C	5.357100	-1.767500	0.034100
H	6.407500	-2.038500	0.005200
C	4.692400	-1.440100	-1.140900
H	5.224600	-1.462900	-2.087700
C	3.343400	-1.081400	-1.134100
C	2.563700	-1.420200	2.601900

H	1.693900	-2.088800	2.560300
H	2.179900	-0.421900	2.847300
H	3.200900	-1.744900	3.428100
C	2.631400	-0.741500	-2.418100
H	2.548600	0.343500	-2.548800
H	1.617000	-1.156900	-2.443400
H	3.178200	-1.138500	-3.277100
N	-1.313000	-0.654900	-0.040600
S	-2.137000	4.060300	1.034300
C	-0.705000	0.482500	0.043700
C	-1.091600	2.694200	1.155300
C	-1.401100	1.769700	0.182700
C	-2.500600	2.179300	-0.647500
H	-2.893500	1.588000	-1.465200
C	-2.994700	3.403400	-0.326700
C	-0.081600	2.624000	2.261700
H	0.278800	1.601000	2.402900
H	-0.521400	2.947900	3.209900
H	0.783600	3.261500	2.053200
C	-4.113300	4.153600	-0.981100
H	-3.774200	5.111800	-1.388200
H	-4.925600	4.357900	-0.276100
H	-4.521900	3.560100	-1.803300
C	-2.738000	-0.781300	0.006000
C	-3.398000	-1.084600	-1.191900
C	-4.779000	-1.264500	-1.143500
H	-5.316900	-1.486200	-2.060900
C	-5.467700	-1.169300	0.061300
H	-6.542600	-1.316800	0.084000
C	-4.779600	-0.899000	1.238200
H	-5.318700	-0.841700	2.179500
C	-3.398400	-0.701500	1.237500
C	-2.633300	-1.190300	-2.485500
H	-2.148400	-0.242900	-2.753400
H	-3.295000	-1.469000	-3.309200
H	-1.835700	-1.940900	-2.417600
C	-2.648400	-0.429600	2.515000
H	-2.326200	0.616400	2.571500
H	-1.751300	-1.056100	2.595700
H	-3.279500	-0.630500	3.384100
C	0.253700	-5.549000	-0.939000
H	-0.404300	-6.419000	-1.017500
H	0.214900	-5.001600	-1.885300
H	1.276000	-5.903600	-0.785300
C	-0.215500	-4.669500	0.217100
C	-1.455200	-3.890200	0.031900
H	-0.156300	-5.169700	1.187700
H	-2.161400	-3.849500	0.862100
H	-1.945000	-3.961400	-0.940800
Pd	-0.158000	-2.356300	0.132700
H	0.705800	-3.884200	0.372100

Ag_A₁

N	-1.337700	-0.802600	-0.627000
S	-2.203700	3.277600	2.064200
C	-0.789600	0.215000	-0.082400
C	-1.144100	1.958900	1.701900
C	-1.493200	1.376300	0.509600
C	-2.634700	2.000200	-0.099300
H	-3.073400	1.662200	-1.031200
C	-3.125700	3.051100	0.608600
C	-0.059700	1.570900	2.661600
H	0.199400	0.515200	2.538600
H	-0.380500	1.710700	3.698100
H	0.845100	2.168800	2.502900
C	-4.292300	3.928900	0.274900
H	-3.993600	4.976900	0.161700
H	-5.066400	3.882900	1.048500
H	-4.739300	3.599300	-0.667300
C	-2.735300	-1.006400	-0.649400

C	-3.350700	-1.024800	-1.912400
C	-4.720200	-1.266500	-1.986300
H	-5.205200	-1.267100	-2.959200
C	-5.459900	-1.523200	-0.837800
H	-6.524800	-1.723500	-0.906900
C	-4.824800	-1.546200	0.397600
H	-5.396400	-1.773000	1.293800
C	-3.458800	-1.290300	0.523000
C	-2.539500	-0.751800	-3.151600
H	-1.589400	-1.296200	-3.122700
H	-2.299300	0.315200	-3.248900
H	-3.086900	-1.048300	-4.050900
C	-2.799800	-1.352900	1.876500
H	-2.544800	-0.354000	2.248200
H	-1.879100	-1.948100	1.842000
H	-3.469900	-1.819600	2.603800
N	1.311000	-0.898000	0.097900
S	2.092500	3.751300	-1.394300
C	0.721100	0.222900	-0.115400
C	1.054500	2.368900	-1.385100
C	1.418500	1.500900	-0.384600
C	2.549900	1.968800	0.367500
H	2.995400	1.417700	1.186500
C	3.020500	3.174900	-0.043900
C	-0.037800	2.244000	-2.404000
H	-0.295700	1.194000	-2.564100
H	0.270600	2.661200	-3.367200
H	-0.941700	2.770800	-2.077600
C	4.171000	3.957600	0.509500
H	3.853100	4.936100	0.885900
H	4.945900	4.124800	-0.246400
H	4.623600	3.405700	1.338000
C	2.723800	-1.033500	-0.046300
C	3.498400	-1.237100	1.105100
C	4.871000	-1.418800	0.949000
H	5.487500	-1.564300	1.832100
C	5.451900	-1.429700	-0.314500
H	6.521700	-1.581800	-0.420100
C	4.657000	-1.266400	-1.442000
H	5.106000	-1.298400	-2.431200
C	3.280600	-1.068100	-1.332900
C	2.860200	-1.239000	2.469200
H	2.414000	-0.266400	2.712400
H	3.596800	-1.471500	3.243200
H	2.055500	-1.982900	2.525300
C	2.422100	-0.917100	-2.562600
H	2.144500	0.130800	-2.727200
H	1.495400	-1.495300	-2.476300
H	2.959200	-1.262900	-3.450100
Ag	0.271200	-2.874300	0.383900
C	-0.527400	-4.748000	0.839700
H	-0.006600	-5.546200	0.296600
H	-0.452700	-4.969200	1.911900
H	-1.588400	-4.784400	0.559900

Ag_R₁

N	-1.200400	-1.028400	-0.570400
S	-3.328500	2.726400	1.878600
C	-0.996400	0.129900	-0.070300
C	-1.915800	1.764600	1.610500
C	-2.031900	1.057200	0.440800
C	-3.280800	1.291500	-0.228200
H	-3.563700	0.800400	-1.152400
C	-4.085900	2.178800	0.413100
C	-0.803400	1.750000	2.615500
H	-0.250200	0.807700	2.558700
H	-1.190000	1.841900	3.634800
H	-0.100900	2.573400	2.442900
C	-5.444600	2.659500	0.006000
H	-5.461500	3.743100	-0.154700

H	-6.200500	2.421300	0.762100
H	-5.739100	2.172900	-0.928100
C	-2.474900	-1.635300	-0.620900
C	-2.988600	-1.907100	-1.900600
C	-4.223400	-2.542100	-2.006100
H	-4.633300	-2.740900	-2.993100
C	-4.919000	-2.936600	-0.869000
H	-5.874900	-3.443300	-0.961400
C	-4.372800	-2.701600	0.386300
H	-4.902400	-3.033600	1.275500
C	-3.148500	-2.050100	0.542500
C	-2.224000	-1.483000	-3.127000
H	-1.159300	-1.718200	-3.022600
H	-2.302000	-0.401000	-3.296400
H	-2.609100	-1.983300	-4.020300
C	-2.579200	-1.838700	1.921400
H	-2.677600	-0.795500	2.242500
H	-1.516800	-2.108300	1.957900
H	-3.105200	-2.464100	2.648200
N	1.333700	-0.301900	0.202200
S	0.749000	4.310600	-1.484200
C	0.444600	0.583600	-0.073100
C	0.170400	2.682000	-1.435100
C	0.739500	2.000600	-0.387200
C	1.651600	2.813500	0.369200
H	2.210200	2.451600	1.223700
C	1.756100	4.088900	-0.086300
C	-0.796900	2.198100	-2.472900
H	-0.760300	1.108800	-2.553200
H	-0.559800	2.612200	-3.457600
H	-1.823200	2.486300	-2.219400
C	2.599600	5.200200	0.457800
H	1.990700	6.051700	0.780600
H	3.316900	5.563800	-0.285900
H	3.165100	4.840200	1.321900
C	2.724600	-0.010000	0.088900
C	3.491500	0.066000	1.259800
C	4.859400	0.302900	1.135200
H	5.465500	0.379000	2.034200
C	5.452100	0.431200	-0.116400
H	6.519900	0.610300	-0.197400
C	4.676900	0.306800	-1.263200
H	5.142600	0.376300	-2.242700
C	3.303800	0.078000	-1.184600
C	2.846300	-0.089700	2.611600
H	2.104100	0.695700	2.002300
H	3.594200	-0.043900	3.408000
H	2.319900	-1.049600	2.687000
C	2.479500	-0.116000	-2.429900
H	1.854300	0.759500	-2.639800
H	1.817600	-0.983500	-2.329000
H	3.126600	-0.278600	-3.296500
C	0.559100	-4.441500	1.267100
H	0.731300	-4.552600	2.345400
H	-0.468800	-4.765500	1.057500
H	1.238800	-5.132400	0.750300
Ag	0.859200	-2.472900	0.619400
C	4.100600	-3.166700	-0.288000
C	3.584300	-3.441700	-1.482400
H	3.692800	-3.614200	0.615100
H	4.925800	-2.469200	-0.167300
H	2.743600	-4.122500	-1.590500
H	3.974300	-2.988100	-2.390900

Ag_TS₁

N	-1.300900	-0.681700	-0.255600
S	-2.241700	3.882600	1.381900
C	-0.721600	0.450300	0.003800
C	-1.168800	2.523900	1.358600
C	-1.452100	1.704000	0.295000

C	-2.555300	2.183700	-0.491200
H	-2.935900	1.666300	-1.364100
C	-3.082700	3.352800	-0.043800
C	-0.139400	2.360800	2.435400
H	0.195900	1.320800	2.486300
H	-0.547500	2.627300	3.415600
H	0.737800	2.989200	2.246600
C	-4.223400	4.135000	-0.618100
H	-3.914400	5.140600	-0.924000
H	-5.043000	4.241100	0.101000
H	-4.614500	3.617500	-1.498700
C	-2.707900	-0.845300	-0.164800
C	-3.417600	-1.071700	-1.355100
C	-4.789400	-1.297200	-1.274200
H	-5.353700	-1.458300	-2.189200
C	-5.435900	-1.332300	-0.042600
H	-6.504100	-1.520600	0.006500
C	-4.707400	-1.144100	1.124800
H	-5.207000	-1.191900	2.089100
C	-3.334200	-0.896800	1.090100
C	-2.701300	-1.050400	-2.680100
H	-1.879300	-1.775700	-2.692800
H	-2.255100	-0.068800	-2.885300
H	-3.387400	-1.285500	-3.498900
C	-2.556700	-0.703200	2.366300
H	-2.404900	0.362000	2.577000
H	-1.570100	-1.174800	2.309000
H	-3.093000	-1.141100	3.212800
N	1.303400	-0.710800	0.268400
S	2.361300	3.819800	-1.409400
C	0.763100	0.432700	-0.005000
C	1.256500	2.486800	-1.376500
C	1.520500	1.668700	-0.307200
C	2.636400	2.125200	0.474400
H	3.007100	1.600400	1.347500
C	3.191400	3.278500	0.018600
C	0.221900	2.338000	-2.450800
H	-0.135800	1.304900	-2.493700
H	0.634400	2.587400	-3.433500
H	-0.641000	2.987400	-2.265900
C	4.353500	4.035000	0.584400
H	4.071900	5.051000	0.882700
H	5.174100	4.113600	-0.137000
H	4.732600	3.514300	1.468400
C	2.702100	-0.921200	0.244000
C	3.321700	-1.182800	1.476800
C	4.690100	-1.440600	1.493000
H	5.182900	-1.628000	2.443800
C	5.420900	-1.474900	0.309900
H	6.485700	-1.686700	0.332600
C	4.779300	-1.258800	-0.903600
H	5.344800	-1.311000	-1.830600
C	3.413500	-0.979200	-0.965100
C	2.506700	-1.159900	2.743300
H	2.129100	-0.153000	2.964900
H	3.102500	-1.489200	3.599500
H	1.630500	-1.812700	2.653800
C	2.724200	-0.786000	-2.289500
H	2.466200	0.265900	-2.457400
H	1.797200	-1.371900	-2.331300
H	3.371900	-1.107900	-3.110100
C	-1.024000	-3.988800	1.483100
H	-0.514000	-3.458300	2.296900
H	-2.009000	-3.542400	1.291700
H	-1.176700	-5.023100	1.793800
C	0.188300	-4.881100	-0.075100
C	0.849400	-4.268700	-1.194100
H	-0.664200	-5.517600	-0.296500
H	0.814900	-5.259200	0.728900
H	0.434500	-4.426900	-2.186300

H	1.927400	-4.131400	-1.147800
Ag	-0.094700	-2.546800	-0.228600

Ag P₁

N	-0.967500	-1.234200	-0.110600
S	-3.937200	2.443000	1.351100
C	-1.005800	0.031700	0.107400
C	-2.353700	1.748900	1.353200
C	-2.241100	0.805900	0.360200
C	-3.454100	0.650900	-0.394700
H	-3.567900	-0.055000	-1.208300
C	-4.457700	1.473700	0.006400
C	-1.346200	2.183800	2.374900
H	-0.588100	1.410000	2.521400
H	-1.821700	2.371200	3.342300
H	-0.838300	3.102300	2.060300
C	-5.842200	1.586500	-0.553100
H	-6.042600	2.590900	-0.941800
H	-6.602400	1.361800	0.202700
H	-5.963600	0.874100	-1.373800
C	-2.133500	-2.046600	-0.002200
C	-2.667400	-2.602300	-1.174100
C	-3.777800	-3.435700	-1.059400
H	-4.212200	-3.863300	-1.959200
C	-4.321500	-3.734200	0.185400
H	-5.181500	-4.392700	0.259800
C	-3.748400	-3.204900	1.335000
H	-4.157300	-3.457000	2.310000
C	-2.644300	-2.355100	2.669000
C	-2.062300	-2.282800	-2.515600
H	-0.989600	-2.513100	-2.526800
H	-2.164200	-1.218800	-2.765000
H	-2.546200	-2.859300	-3.308800
C	-2.011600	-1.807400	2.520500
H	-2.284200	-0.757200	2.678500
H	-0.918300	-1.861600	2.471800
H	-2.342700	-2.373100	3.395700
N	1.282300	0.118400	0.643600
S	0.121900	4.157100	-1.998000
C	0.319500	0.756000	0.095800
C	-0.197500	2.490300	-1.661800
C	0.389600	2.118200	-0.478800
C	1.109800	3.192900	0.145000
H	1.656800	3.083500	1.074600
C	1.050700	4.363100	-0.543100
C	-0.978700	1.657200	-2.632700
H	-0.700600	0.603200	-2.540700
H	-0.778200	1.960300	-3.664700
H	-2.056600	1.745300	-2.455400
C	1.672300	5.679000	-0.189900
H	0.918300	6.463100	-0.059900
H	2.374100	6.014000	-0.961300
H	2.225900	5.581200	0.748100
C	2.617100	0.573100	0.661700
C	3.198500	0.752700	1.928700
C	4.535800	1.130900	2.003900
H	4.988600	1.285000	2.980000
C	5.295300	1.288400	0.849500
H	6.342600	1.566100	0.918800
C	4.715200	1.062900	-0.391800
H	5.316100	1.154800	-1.292800
C	3.372300	0.705000	-0.517200
C	2.367800	0.554700	3.168800
H	1.631600	1.359300	3.295600
H	2.996800	0.538200	4.063500
H	1.809700	-0.386600	3.113200
C	2.793800	0.430400	-1.881100
H	2.215600	1.283700	-2.253800
H	2.134200	-0.445700	-1.865900
H	3.594900	0.227700	-2.597500

C	5.217400	-3.733000	-0.489500
H	6.144000	-3.145400	-0.452300
H	5.237400	-4.448000	0.342400
H	5.220800	-4.313200	-1.421000
C	3.971300	-2.844200	-0.409200
C	2.655500	-3.633100	-0.467700
H	4.009100	-2.114900	-1.230400
H	4.020100	-2.248800	0.513100
H	2.652400	-4.386200	0.335200
H	2.613600	-4.198400	-1.410200
Ag	0.941800	-2.439800	-0.249500

Cd A₁

N	1.312700	-0.869800	0.240100
S	2.283600	3.686000	-1.364400
C	0.761300	0.265200	-0.018100
C	1.163700	2.377000	-1.318300
C	1.494200	1.502200	-0.305500
C	2.670700	1.904000	0.417900
H	3.088800	1.344900	1.246500
C	3.201400	3.075000	-0.019400
C	0.079700	2.290100	-2.350700
H	-0.319000	1.274000	-2.420400
H	0.463100	2.557200	-3.339900
H	-0.749800	2.964500	-2.114100
C	4.397200	3.807700	0.505300
H	4.131300	4.804400	0.872400
H	5.164000	3.928800	-0.266700
H	4.837800	3.246100	1.333300
C	2.719300	-1.103200	0.176600
C	3.346900	-1.473400	1.377300
C	4.709000	-1.757800	1.344900
H	5.217500	-2.026900	2.266100
C	5.416100	-1.710600	0.147300
H	6.475600	-1.944900	0.133600
C	4.763700	-1.380700	-1.033000
H	5.315200	-1.364800	-1.968700
C	3.403000	-1.067300	-1.047900
C	2.564900	-1.524500	2.664600
H	1.745400	-2.253800	2.611200
H	2.114400	-0.554500	2.907800
H	3.207200	-1.813400	3.499800
C	2.728300	-0.714100	-2.349100
H	2.734600	0.369300	-2.513800
H	1.682900	-1.042200	-2.383700
H	3.249600	-1.181900	-3.188200
N	-1.312400	-0.870300	-0.241200
S	-2.284900	3.684300	1.365600
C	-0.761300	0.264900	0.017200
C	-1.164600	2.375700	1.318700
C	-1.494700	1.501400	0.305300
C	-2.671300	1.903300	-0.417900
H	-3.089100	1.344700	-1.246900
C	-3.202500	3.073800	0.020200
C	-0.080400	2.288600	2.351000
H	0.318100	1.272500	2.420500
H	-0.463700	2.555700	3.340300
H	0.749000	2.963000	2.114300
C	-4.398600	3.806300	-0.504000
H	-4.133300	4.803500	-0.870100
H	-5.165600	3.926200	0.267900
H	-4.838700	3.245300	-1.332600
C	-2.719000	-1.103900	-0.176900
C	-3.347700	-1.472500	-1.377400
C	-4.709800	-1.757100	-1.343900
H	-5.219200	-2.025100	-2.265000
C	-5.415800	-1.711500	-0.145600
H	-6.475100	-1.945700	-0.131100
C	-4.762100	-1.383000	1.034400
H	-5.312700	-1.368200	1.970800

C	-3.401400	-1.069500	1.048400
C	-2.567000	-1.521900	-2.665500
H	-2.118100	-0.551100	-2.908500
H	-3.209900	-1.811100	-3.500200
H	-1.746700	-2.250200	-2.613200
C	-2.725500	-0.717700	2.349300
H	-2.730900	0.365600	2.514700
H	-1.680200	-1.046400	2.382800
H	-3.246300	-1.185700	3.188500
C	0.001500	-4.844200	-0.000700
H	-0.936600	-5.216900	0.418100
H	0.103200	-5.213700	-1.024600
H	0.837000	-5.219100	0.595400
Cd	0.000500	-2.738100	-0.000700

Cd_R₁

N	-1.308100	-0.752000	-0.241300
S	-2.413800	3.782000	1.327700
C	-0.784600	0.396600	0.007200
C	-1.274600	2.487900	1.310800
C	-1.549500	1.623500	0.274400
C	-2.699900	2.019100	-0.491500
H	-3.077500	1.464200	-1.342000
C	-3.265800	3.176600	-0.061200
C	-0.229800	2.400400	2.383100
H	0.188100	1.391400	2.444900
H	-0.656900	2.635200	3.362700
H	0.593400	3.097300	2.195000
C	-4.452200	3.896300	-0.624000
H	-4.190400	4.903700	-0.963900
H	-5.252800	3.990600	0.116900
H	-4.847500	3.340600	-1.478400
C	-2.714900	-0.994800	-0.210700
C	-3.327700	-1.381800	-1.433100
C	-4.687700	-1.607700	-1.429900
H	-5.183800	-1.834400	-2.369200
C	-5.407300	-1.627100	-0.239700
H	-6.464400	-1.871800	-0.248200
C	-4.769300	-1.347500	0.961900
H	-5.330600	-1.380200	1.891300
C	-3.412000	-1.023700	1.006100
C	-2.533900	-1.276000	-2.713600
H	-1.649000	-1.919800	-2.649800
H	-2.174100	-0.265000	-2.944300
H	-3.138800	-1.613700	-3.558700
C	-2.745300	-0.726000	2.324900
H	-2.606100	0.351800	2.464900
H	-1.760000	-1.200500	2.409400
H	-3.355800	-1.093700	3.153200
N	1.328800	-0.684500	0.221100
S	2.192700	3.934800	-1.240400
C	0.738300	0.436300	-0.011100
C	1.117700	2.586400	-1.261800
C	1.438500	1.704400	-0.254700
C	2.571800	2.130600	0.521200
H	2.975300	1.568500	1.355400
C	3.080100	3.326500	0.126300
C	0.080200	2.477900	-2.338400
H	-0.309500	1.458300	-2.408600
H	0.504400	2.732700	-3.314300
H	-0.763700	3.149000	-2.148100
C	4.228400	4.088400	0.712000
H	3.913200	5.066400	1.090400
H	5.018900	4.254600	-0.027000
H	4.657600	3.523900	1.544000
C	2.742400	-0.866100	0.158200
C	3.370000	-1.301700	1.340300
C	4.736300	-1.563200	1.303900
H	5.239100	-1.881500	2.212500
C	5.457300	-1.426100	0.121700

H	6.519900	-1.645200	0.104600
C	4.815100	-1.009800	-1.035100
H	5.378800	-0.904000	-1.958000
C	3.450100	-0.710000	-1.044700
C	2.592900	-1.436700	2.626200
H	2.034700	-0.523400	2.863100
H	3.264600	-1.644300	3.462700
H	1.865000	-2.257200	2.582300
C	2.822100	-0.229700	-2.328800
H	3.026700	0.836300	-2.478600
H	1.736600	-0.355800	-2.345700
H	3.239200	-0.770500	-3.183800
C	-0.365300	-4.222000	1.673000
H	0.525300	-4.851900	1.758100
H	-0.639500	-3.870500	2.671700
H	-1.187100	-4.828800	1.282200
Cd	0.012000	-2.578200	0.376800
C	0.276100	-4.214200	-1.892800
C	1.046300	-3.175000	-2.237600
H	-0.768000	-4.275600	-2.192300
H	0.672400	-5.059800	-1.336800
H	0.656400	-2.356800	-2.837100
H	2.101300	-3.131400	-1.975700

Cd_TS₁

N	-1.341200	-0.598700	-0.263400
S	-2.051600	4.004200	1.312900
C	-0.711900	0.496700	-0.009800
C	-1.017200	2.624800	1.292500
C	-1.370300	1.779700	0.264000
C	-2.494400	2.260000	-0.493300
H	-2.920600	1.731900	-1.338200
C	-2.963700	3.460000	-0.064000
C	0.026100	2.460400	2.356500
H	0.354200	1.419500	2.429000
H	-0.369300	2.744900	3.336200
H	0.905000	3.080200	2.151500
C	-4.093500	4.269900	-0.620600
H	-3.753800	5.249700	-0.971800
H	-4.875500	4.435100	0.127600
H	-4.542100	3.742000	-1.466300
C	-2.759600	-0.737000	-0.195800
C	-3.414100	-1.080400	-1.390600
C	-4.789600	-1.289100	-1.348000
H	-5.317800	-1.535400	-2.264600
C	-5.486500	-1.192900	-0.147200
H	-6.557100	-1.368600	-0.125800
C	-4.810700	-0.884300	1.025300
H	-5.355200	-0.825200	1.963500
C	-3.434400	-0.645100	1.030700
C	-2.646900	-1.179200	-2.684600
H	-1.865200	-1.948500	-2.637300
H	-2.147200	-0.235200	-2.934100
H	-3.312600	-1.433600	-3.512900
C	-2.740300	-0.307900	2.325500
H	-2.762400	0.772300	2.508700
H	-1.692100	-0.623000	2.332900
H	-3.239800	-0.799900	3.164300
N	1.291300	-0.767400	0.211300
S	2.550300	3.737000	-1.323200
C	0.805800	0.401900	-0.027700
C	1.364500	2.486000	-1.312400
C	1.615500	1.599600	-0.287900
C	2.785200	1.944000	0.473900
H	3.147600	1.366900	1.316000
C	3.389700	3.085000	0.052300
C	0.307300	2.452200	-2.375600
H	-0.140800	1.457500	-2.455100
H	0.731700	2.696100	-3.354100
H	-0.492700	3.169000	-2.163800

C	4.605000	3.755100	0.614500
H	4.381400	4.766600	0.969400
H	5.402800	3.830700	-0.131500
H	4.986800	3.174800	1.458700
C	2.688500	-1.064400	0.169300
C	3.302900	-1.397400	1.385200
C	4.652300	-1.742200	1.363100
H	5.153000	-1.985300	2.295900
C	5.355300	-1.785200	0.163600
H	6.404200	-2.063400	0.159300
C	4.711800	-1.487300	-1.031000
H	5.259400	-1.540200	-1.967600
C	3.365300	-1.120100	-1.057300
C	2.525000	-1.345100	2.675000
H	2.160900	-0.332500	2.890300
H	3.144500	-1.661200	3.517700
H	1.645400	-1.999400	2.641300
C	2.680100	-0.813100	-2.363900
H	2.543000	0.265800	-2.497400
H	1.691200	-1.283900	-2.428400
H	3.275300	-1.179500	-2.203900
C	-1.092100	-3.570500	1.765000
H	-1.115000	-4.527200	2.284600
H	-0.580900	-2.868000	2.439500
H	-2.125900	-3.240300	1.604700
C	-0.344500	-4.880900	0.108100
C	0.165900	-4.411800	-1.156900
H	-1.347900	-5.292600	0.147600
H	0.352100	-5.324900	0.811800
H	-0.486600	-4.520600	-2.019900
H	1.223000	-4.579400	-1.350400
Cd	-0.134300	-2.497500	-0.128800

Cd_P₁

N	-1.344600	-0.017300	-0.257800
S	-0.249400	4.536300	1.270300
C	-0.355600	0.763700	0.001300
C	0.196000	2.870800	1.265200
C	-0.476500	2.200800	0.266800
C	-1.363900	3.052700	-0.478500
H	-1.979200	2.706800	-1.301000
C	-1.339800	4.348200	-0.072000
C	1.128700	2.348700	2.316600
H	1.053400	1.261400	2.406500
H	0.886100	2.772900	3.295500
H	2.169500	2.598800	2.086900
C	-2.100800	5.512200	-0.627000
H	-1.429700	6.286800	-1.012500
H	-2.741200	5.971900	0.132700
H	-2.739400	5.175700	-1.448000
C	-2.716700	0.352300	-0.185600
C	-3.470800	0.163800	-1.357000
C	-4.837500	0.419600	-1.309600
H	-5.432700	0.296100	-2.209700
C	-5.444600	0.817500	-0.122400
H	-6.513500	1.002400	-0.094800
C	-4.686300	0.959400	1.031300
H	-5.168100	1.245100	1.962100
C	-3.308300	0.731500	1.030200
C	-2.804700	-0.290500	-2.630100
H	-2.378100	-1.297700	-2.523200
H	-1.985100	0.374900	-2.925200
H	-3.521800	-0.326600	-3.453700
C	-2.533500	0.859400	2.316500
H	-2.139600	1.874100	2.441900
H	-1.682000	0.171000	2.362700
H	-3.180400	0.644400	3.171000
N	1.005500	-1.172700	0.235000
S	3.910400	2.488900	-1.316400
C	1.011300	0.091300	-0.019400

C	2.327200	1.808300	-1.297700
C	2.220400	0.877000	-0.286800
C	3.440900	0.719300	0.458000
H	3.555300	0.033300	1.288700
C	4.441200	1.536000	0.038200
C	1.334200	2.211200	-2.346800
H	0.542200	1.464000	-2.449800
H	1.818400	2.308200	-3.322900
H	0.865900	3.170400	-2.102900
C	5.828200	1.665800	0.587200
H	6.022700	2.677000	0.959200
H	6.583100	1.437500	-0.172200
H	5.961700	0.966200	1.416500
C	2.171500	-1.996200	0.184800
C	2.570300	-2.592900	1.391700
C	3.672700	-3.442700	1.369800
H	4.009700	-3.899200	2.295900
C	4.334500	-3.717100	0.176900
H	5.186500	-4.389100	0.171800
C	3.895600	-3.144900	-1.009600
H	4.403000	-3.377400	-1.941600
C	2.806800	-2.271000	-1.035300
C	1.839500	-2.287500	2.673900
H	1.855100	-1.215900	2.907600
H	2.289500	-2.819700	3.515300
H	0.784400	-2.587200	2.620100
C	2.355900	-1.667400	-2.341100
H	2.811800	-0.683300	-2.498000
H	1.268700	-1.533400	-2.388300
H	2.646800	-2.307000	-3.178100
C	-4.244200	-3.019000	0.781400
H	-5.323000	-2.900300	0.642100
H	-4.082300	-3.534300	1.735600
H	-3.817700	-2.009700	0.865400
C	-3.615800	-3.795800	-0.373100
C	-2.119700	-4.075800	-0.193600
H	-3.792200	-3.255200	-1.312000
H	-4.135500	-4.758300	-0.475600
H	-1.720000	-4.650800	-1.035900
H	-1.943500	-4.670300	0.710200
Cd	-0.961400	-2.298900	-0.030700