

SUPPORTING INFORMATION

A Computational mechanistic study on the Ni-Catalyzed
Asymmetric Alkynyl Propyl Hydroxyaminations: Origin of
Enantioselectivity and Further Rational Design

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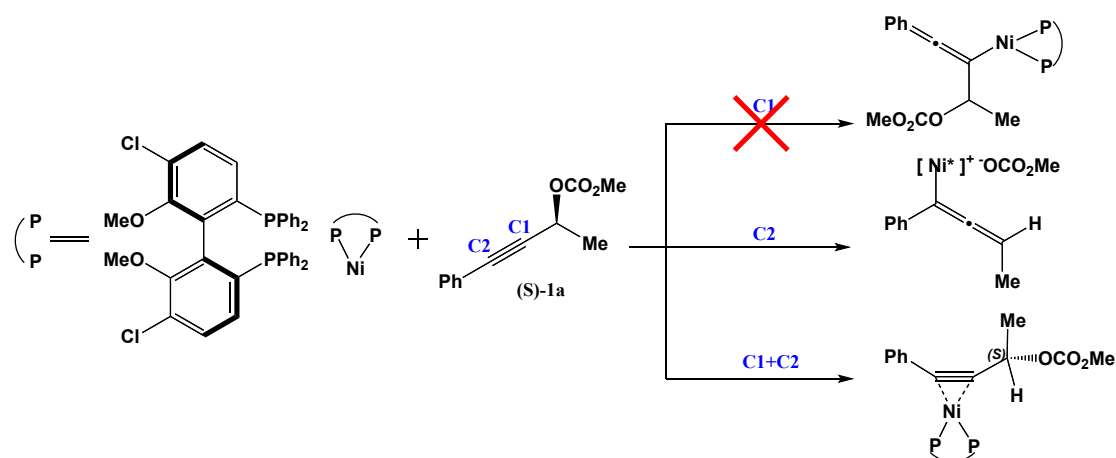


Figure S1. Three possible scenarios for the combination of nickel-phosphine- catalyst and substrate (S)-1a.

Table S1. Calculated Gibbs free energy barriers (in kcal mol⁻¹) on the rate-determining-step using different functionals.

Different computational levels	$\Delta G^\ddagger(\text{TS3A})$	$\Delta G^\ddagger(\text{TS3B})$	$\Delta\Delta G^\ddagger$
BP86+D3(BJ)/def2-TZVPP(IEFPCM, solvent=1,4-Dioxane) //BP86+ D3(BJ)/def2-SVP(IEFPCM, solvent = 1,4-Dioxane)	21.4	22.9	1.5
M06-L/def2-TZVPP(IEFPCM, solvent=1,4-Dioxane) //BP86+ D3(BJ)/def2-SVP(IEFPCM, solvent = 1,4-Dioxane)	21.5	22.9	1.4
B97D+D3(BJ)/def2-TZVPP(IEFPCM, solvent=1,4-Dioxane) //BP86+ D3(BJ)/def2-SVP(IEFPCM, solvent = 1,4-Dioxane)	20.5	22.1	1.6
B3PW91+D3(BJ)/def2-TZVPP(IEFPCM, solvent=1,4-Dioxane) //B3PW91+D3(BJ)/def2-SVP(IEFPCM, solvent = 1,4-Dioxane)	27.4	28.5	1.1
B3LYP+D3(BJ)/def2-TZVPP(IEFPCM, solvent=1,4-Dioxane) //BP86+ D3(BJ)/def2-SVP(IEFPCM, solvent = 1,4-Dioxane)	27.8	28.8	1.0

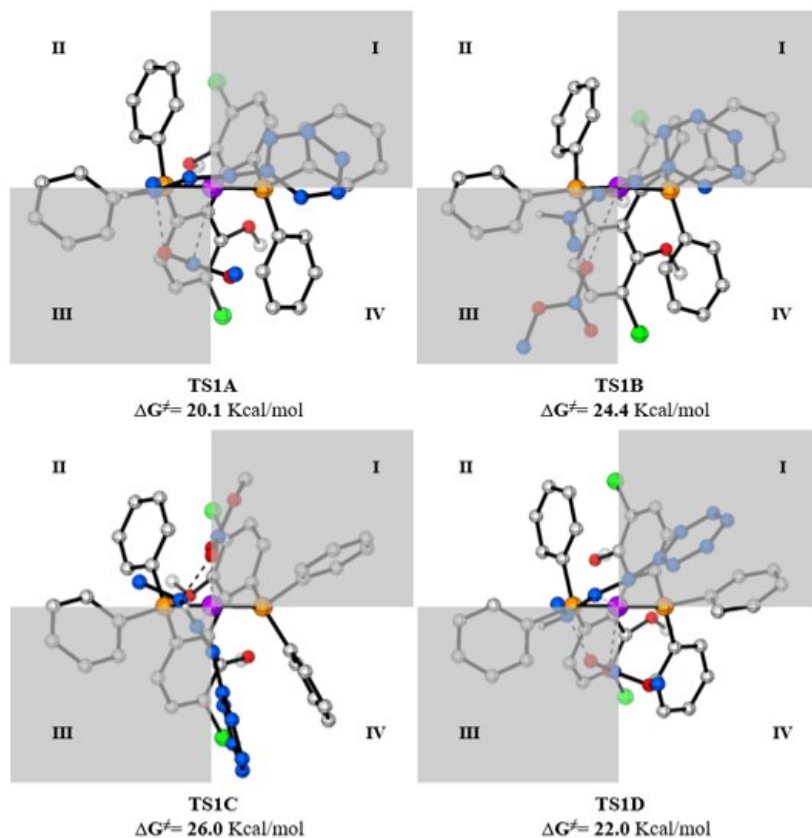


Figure S2. The geometry of the four optimized TS1 transition states is shown in the quadrant plot, with some hydrogen atoms omitted for clarity and selected bond distances given in Å (color code, C: gray, O: red, P: yellow, Ni: Purple, Cl: green). To highlight the differences in spatial configurations, the (S)-1a section has been highlighted in blue.

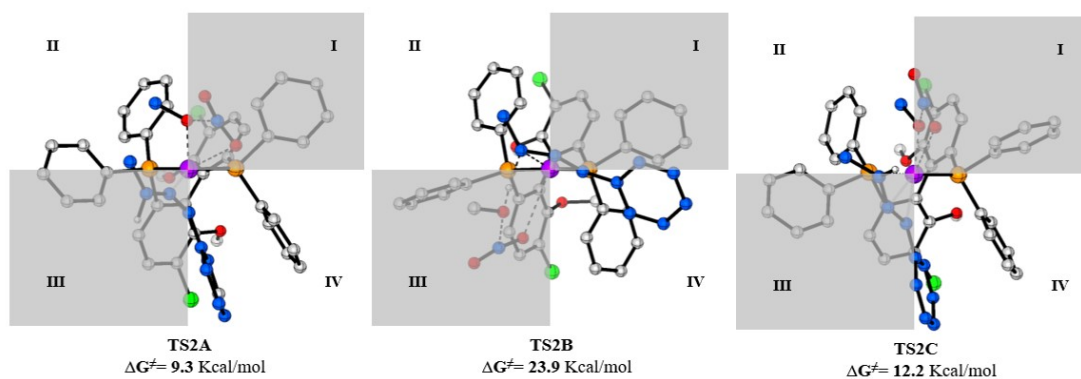


Figure S3. The geometry of the four optimized TS2 transition states is shown in the quadrant plot, with some hydrogen atoms omitted for clarity and selected bond distances given in Å (color code, C: gray, O: red, P: yellow, Ni: Purple, Cl: green). To highlight the differences in spatial configurations, the (S)-1a section has been highlighted in blue.

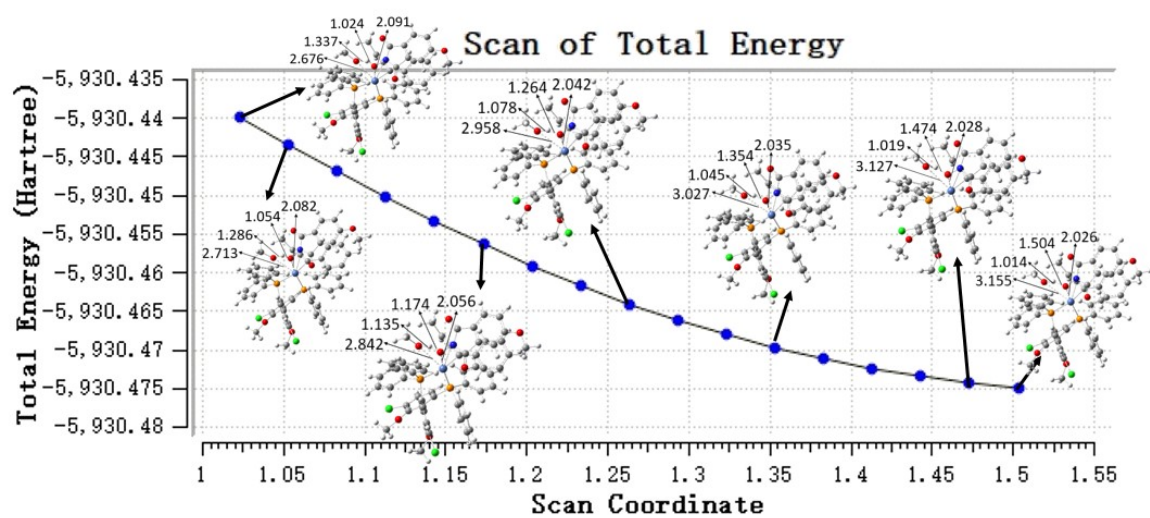


Figure S4. Scan of potential energy surface of the asymmetric Propargylic substitution from **IM5A** to **IM6A**.

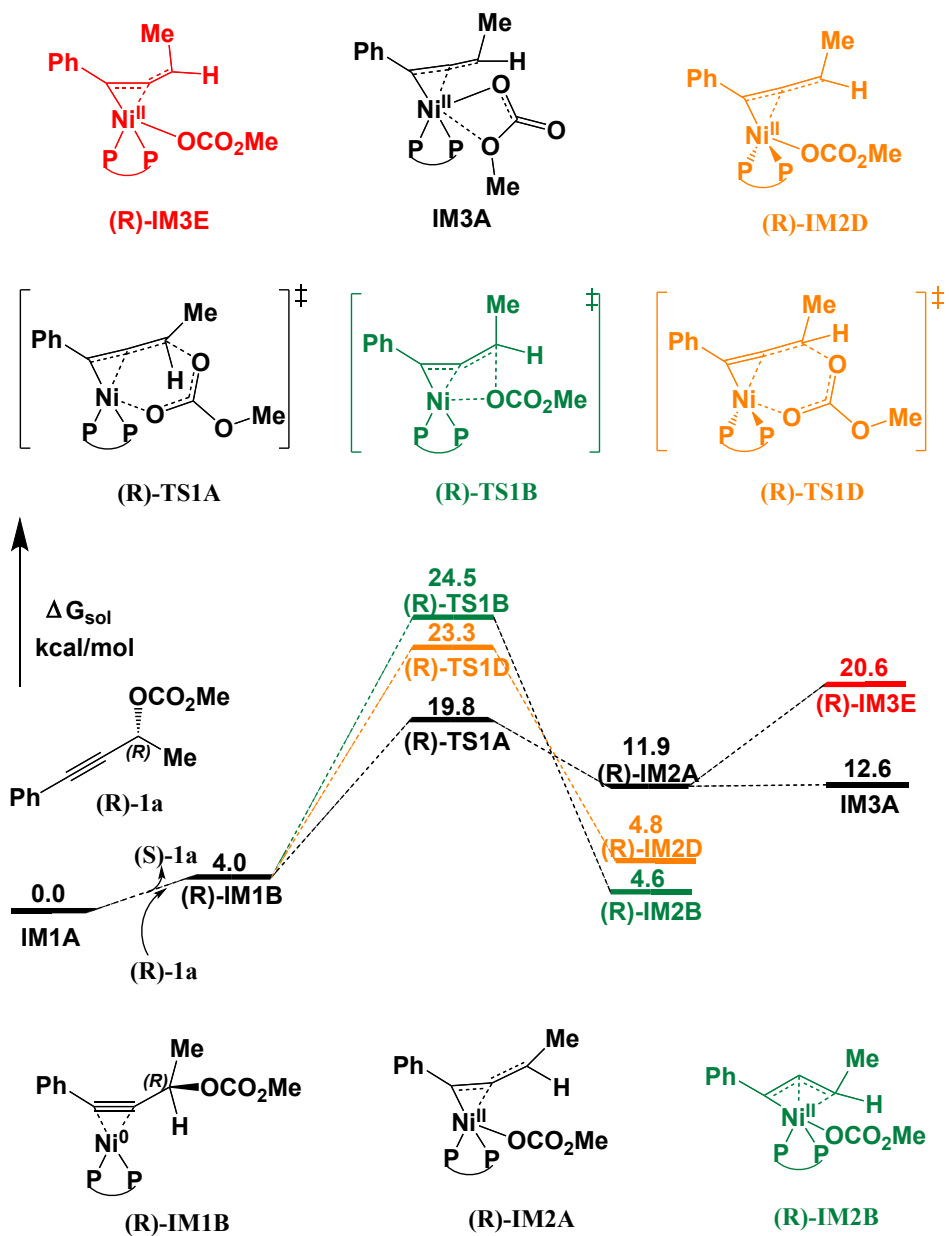


Figure S5 Gibbs free energy (in kcal/mol) profiles by using the reactant propyl carbonate ((R)-1a).

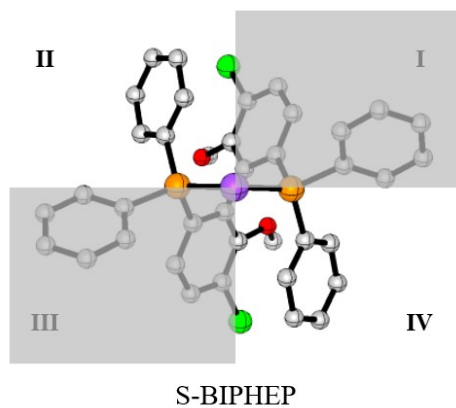


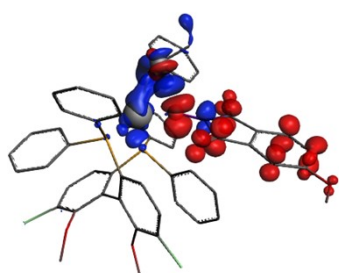
Figure S6 Quadrant diagram of (S)-Cl-MeO-BIPHEP ligand, with some hydrogen atoms omitted for clarity and selected bond distances given in Å (color code, C: gray, O: red, P: yellow, Ni: Purple, Cl: green).

Table S2. EDA-NOCV results of (S)-TS3A at the BP86+(D3BJ)/TZ2P level of theory. Fragments are given in singlet (S) or triplet (T) electronic states. Energy values are given in kcal/mol.

Fragment	(S)-L1/Ni-1a ⁺ (S)	(S)-L1/Ni-1a (D)
	+2a ⁺ (S)	+2a(D)
ΔE_{int}	-99.5	-46.3
ΔE_{Pauli}	83.3	80.8
$\Delta E_{\text{disp}}^{[a]}$	-21.2 (11.6%)	-21.2 (16.7%)
$\Delta E_{\text{elstat}}^{[a]}$	-99.2 (54.2%)	-34.8 (27.4%)
$\Delta E_{\text{orb}}^{[a]}$	-62.5 (34.2%)	-71.1 (55.9%)
$\Delta E_{\text{orb1}}^{[b]}$	-30.1 (48.2%)	
$\Delta E_{\text{orb2}}^{[b]}$	-6.2 (9.9%)	
$\Delta E_{\text{orb3}}^{[b]}$	-3.6(5.7%)	
ΔE_{rest}	-22.6 (36.3%)	

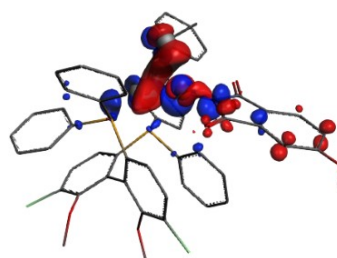
^aThe values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$.

^bThe values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb} .



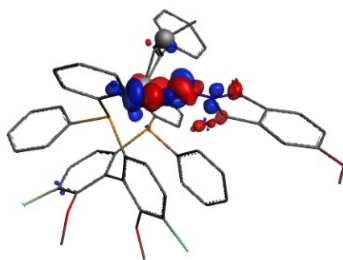
$$\Delta E_{\text{orb1}} = -30.1 \text{ kcal/mol}$$

$$v_1 = \pm 0.902$$



$$\Delta E_{\text{orb2}} = -6.2 \text{ kcal/mol}$$

$$v_2 = \pm 0.252$$



$$\Delta E_{\text{orb}3} = -3.6 \text{ kcal/mol}$$

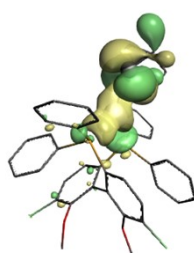
$$v_3 = \pm 0.172$$

Figure S7. Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions between the two fragments of **(S)-L1/Ni-1a⁺ (S) + 2a⁻(S)** in **(S)-TS3A** together with the associated interaction energies ΔE_{orb} (in kcal/mol). The eigenvalues v are a measure for the relative amount of charge transfer. The direction of the charge flow is from red to blue.



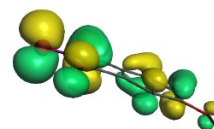
$$\Delta E_{\text{orb}1} = -30.1 \text{ kcal/mol}$$

$$v_1 = \pm 0.902$$



Frag1-LUMO

(0.407)



Frag2-HOMO

(-0.425)

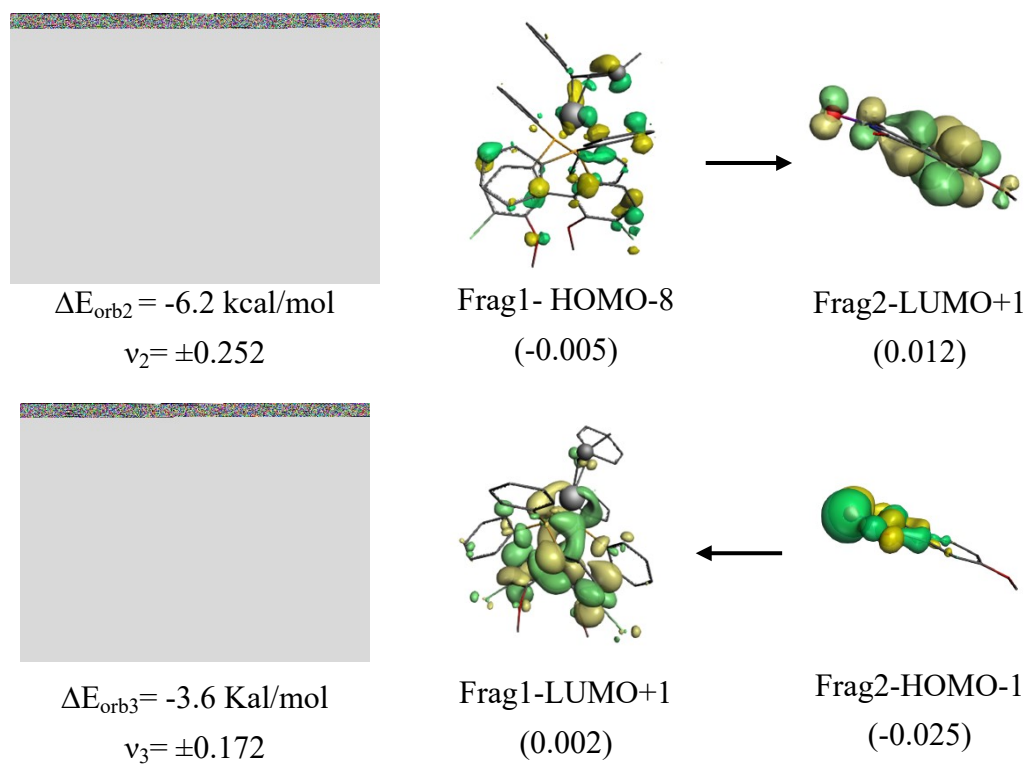


Figure S8 Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments, as well as the shape of the most important interacting MOs of the two fragments (S)-L1/Ni-1a⁺ (S) +2a⁻(S) in (S)-TS3A, The direction of the charge flow is red to blue.

Table S3. EDA-NOCV results of **(R)-TS3B** at the BP86+(D3BJ)/TZ2P level of theory. Fragments are given in singlet (S) or triplet (T) electronic states. Energy values are given in kcal/mol.

Fragment	(S)-L1/Ni-1a ⁺ (S)	(S)-L1/Ni-1a (D)
	+2a ⁺ (S)	+2a(D)
ΔE_{int}	-98.1	-47.1
ΔE_{Pauli}	84.6	83.5
$\Delta E_{\text{disp}}^{\text{[a]}}$	-20.3 (11.1%)	-20.3 (15.5%)
$\Delta E_{\text{elstat}}^{\text{[a]}}$	-99.3 (54.4%)	-36.4 (27.9%)
$\Delta E_{\text{orb}}^{\text{[a]}}$	-63.1 (34.5%)	-73.9 (56.6%)
$\Delta E_{\text{orb1}}^{\text{[b]}}$	-31.4 (49.7%)	
$\Delta E_{\text{orb2}}^{\text{[b]}}$	-6.2 (9.7%)	
$\Delta E_{\text{orb3}}^{\text{[b]}}$	-4.2 (6.6%)	
ΔE_{rest}	-21.4 (33.9%)	

^aThe values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$.

^bThe values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb} .

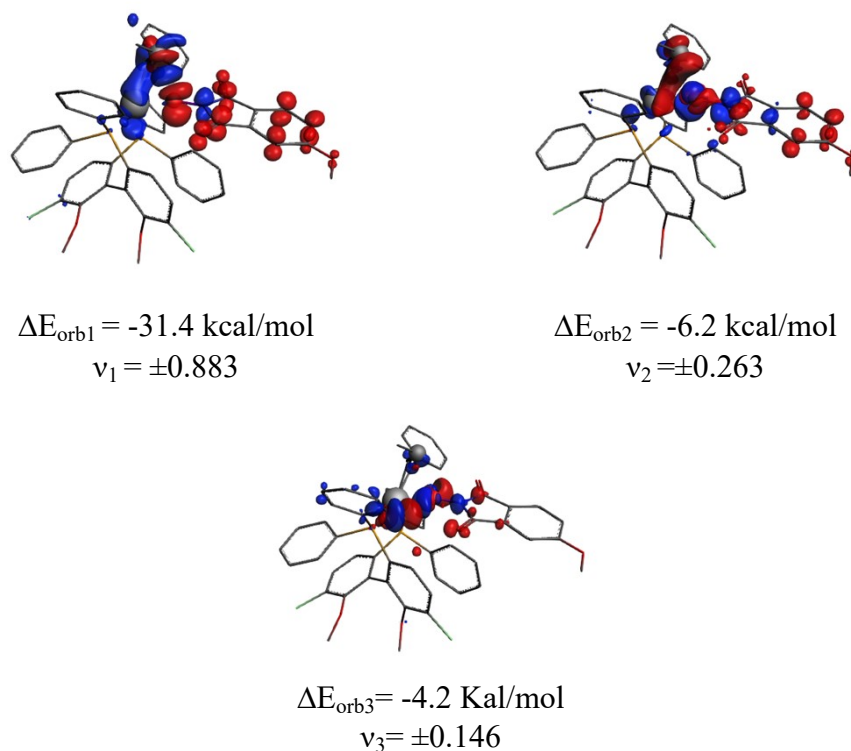


Figure S9. Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions between the two fragments of **(S)-L1/Ni-1a⁺ (S) + 2a⁺(S)** in **(R)-TS3B** together with the associated interaction energies ΔE_{orb} (in kcal/mol). The eigenvalues v are a measure for the relative amount of charge

transfer. The direction of the charge flow is from red to blue.

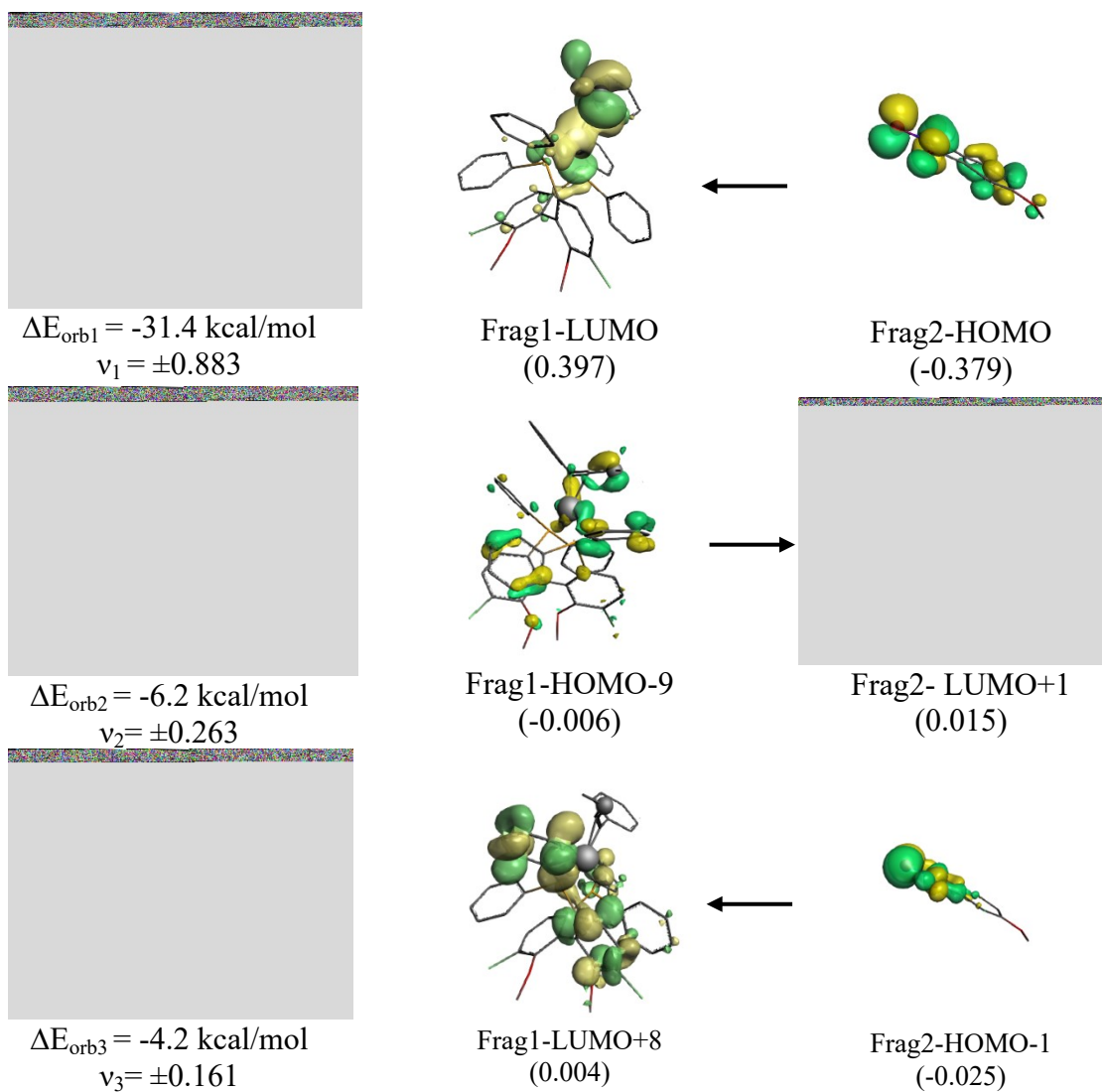


Figure S10 Plot of deformation densities $\Delta\rho$ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments, as well as the shape of the most important interacting MOs of the two fragments (S)-L1/Ni-1a⁺ (S) +2a⁻(S) in (R)-TS3B, The direction of the charge flow is red to blue.

Table S4. Coordinates and energies (in hatree) of the calculated structures at the BP86+D3BJ/def2-TZVPP(IEFPCM,solvent=1,4-Dioxane)/BP86+D3BJ/def2-SVP(IEFPCM,solvent=1,4-Dioxane) level of theory.

Ni-L				H	-2.680528	2.577954	-0.841996
Ni	-0.085199	-0.262795	-2.407602	C	-1.332951	1.059797	-0.041929
P	1.708260	-0.124278	-1.402659	C	-2.184641	-1.715898	-0.290563
P	-1.821059	-0.221902	-1.297837	C	-2.935007	-1.694389	0.903528
C	3.295573	-0.908871	-1.940122	H	-3.330748	-0.741998	1.287515
C	3.147571	-2.027958	-2.792312	C	-3.117559	-2.875860	1.638835
H	2.126000	-2.340056	-3.073463	H	-3.685341	-2.850815	2.581775
C	4.269317	-2.713351	-3.282227	C	-2.544800	-4.080506	1.194445
H	4.136335	-3.590329	-3.935526	H	-2.674694	-5.000872	1.784288
C	5.562464	-2.263546	-2.955014	C	-1.779054	-4.103172	0.015564
H	6.446866	-2.788231	-3.349519	H	-1.305681	-5.039535	-0.319104
C	5.720061	-1.131371	-2.136636	C	-1.600343	-2.924132	-0.723353
H	6.730070	-0.766534	-1.890202	H	-0.969246	-2.899310	-1.627731
C	4.595012	-0.459595	-1.626072	C	-3.469012	0.386836	-1.880964
H	4.733368	0.425333	-0.987680	C	-3.424157	1.242091	-3.005706
C	2.175688	1.535982	-0.762659	H	-2.438221	1.469727	-3.448504
C	1.570866	2.646124	-1.387489	C	-4.601609	1.774153	-3.553009
H	0.862643	2.452922	-2.210871	H	-4.549097	2.447808	-4.423075
C	1.827445	3.946521	-0.928860	C	-5.848536	1.426886	-3.000437
H	1.334343	4.806807	-1.407711	H	-6.777233	1.828934	-3.435231
C	2.699353	4.146129	0.156056	C	-5.905288	0.551716	-1.901299
H	2.896297	5.164748	0.523872	H	-6.880177	0.266675	-1.474382
C	3.299831	3.042888	0.788329	C	-4.723409	0.037669	-1.339250
H	3.968093	3.199028	1.650041	H	-4.781923	-0.646444	-0.479974
C	3.031641	1.739409	0.340016	O	1.116242	1.413630	2.647168
H	3.456419	0.875044	0.872912	C	1.470287	2.106604	3.839982
C	1.286718	-1.066504	0.143901	H	2.030073	1.370839	4.450033
C	1.822581	-2.353900	0.362564	H	0.576286	2.444992	4.402649
H	2.575123	-2.758250	-0.329764	H	2.120297	2.979626	3.631935
C	1.400836	-3.135667	1.443812	O	-0.991578	-0.769755	3.018011
H	1.793748	-4.151837	1.594589	C	-0.690348	-0.651355	4.411088
C	0.456470	-2.625742	2.346546	H	-1.136294	0.303957	4.754130
C	-0.063599	-1.321029	2.183482	H	0.405143	-0.621442	4.584176
C	0.326619	-0.551435	1.057263	H	-1.124473	-1.490072	4.993388
C	-0.310506	0.798651	0.906360	Cl	0.203447	4.531733	2.535277
C	0.149339	1.825840	1.783693	Cl	-0.117523	-3.658230	3.644932
C	-0.379835	3.132225	1.635310				
C	-1.393734	3.381518	0.694958	(S)-1a			
H	-1.791784	4.403651	0.612994	C	-1.434292	0.571499	-0.492584
C	-1.877639	2.359592	-0.123543	H	-1.807698	-0.027436	-1.349823

C	0.000388	0.341065	-0.329401	H	1.461819	2.645457	0.166772
C	1.212971	0.178070	-0.223611	H	-5.432578	1.544081	1.141820
C	2.624726	-0.016259	-0.097243	O	2.093147	0.075461	0.724971
C	3.238475	-1.196178	-0.594059	C	3.368537	-0.354914	0.688965
H	2.613514	-1.962238	-1.077046	O	3.951076	-0.742890	1.679414
C	4.622184	-1.380524	-0.467698	O	3.898798	-0.300667	-0.560501
C	5.415336	-0.398173	0.153071	C	5.254326	-0.769135	-0.667573
H	6.501950	-0.547208	0.251056	H	5.534405	-0.641448	-1.728511
C	4.816959	0.774449	0.649413	H	5.925897	-0.175417	-0.015754
H	5.434378	1.544914	1.137065	H	5.324080	-1.836237	-0.376064
C	3.434212	0.968657	0.527637				
H	2.960873	1.883128	0.915426	2a			
C	-1.783413	2.049071	-0.699704	O	-3.616251	-0.848941	0.066984
H	-2.875828	2.160948	-0.842204	O	-2.771012	1.872399	-0.008749
H	-1.268036	2.436331	-1.601052	O	-1.302432	-2.460077	-0.018247
H	-1.461580	2.644808	0.176885	O	3.553860	0.184216	0.056442
H	5.086953	-2.300115	-0.856256	N	-2.318701	-0.404128	-0.097649
O	-2.093241	0.072753	0.725316	C	-1.963562	0.963049	-0.048715
C	-3.368666	-0.357381	0.687581	C	-1.231623	-1.244576	-0.066885
O	-3.951286	-0.749153	1.676485	C	-0.060130	-0.371277	-0.055326
O	-3.898859	-0.298211	-0.561693	C	1.291975	-0.681592	-0.029045
C	-5.254374	-0.766304	-0.670696	H	1.574054	-1.568950	-0.032430
H	-5.534668	-0.633655	-1.730969	C	2.225030	0.362498	0.010636
H	-5.323939	-1.834789	-0.384239	C	1.769192	1.665902	0.043048
H	-5.925863	-0.175734	-0.015948	H	2.395517	2.352284	0.097108
				C	0.448274	1.995123	0.001749
(R)-1a				H	0.184980	2.886826	-0.009823
C	1.434324	0.569650	-0.494888	C	-0.498952	0.979984	-0.021324
H	1.807744	-0.032567	-1.349810	C	4.069442	-1.175649	0.000441
C	-0.000373	0.339927	-0.330907	H	3.506415	-1.710013	-0.565709
C	-1.212956	0.177346	-0.224477	H	4.077825	-1.551502	0.885573
C	-2.624705	-0.016479	-0.097290	H	4.961521	-1.167519	-0.351085
C	-3.433200	0.967843	0.529801	H	-3.680617	-1.353780	0.880983
H	-2.959102	1.881479	0.918630				
C	-4.815935	0.774094	0.652434	IM1A			
C	-5.415290	-0.397450	0.154730	Ni	1.234817	0.273910	-0.199937
H	-6.501894	-0.546118	0.253384	P	0.047865	-1.513810	-0.130936
C	-4.623128	-1.379194	-0.468256	P	-0.316176	1.747654	-0.054822
H	-5.088661	-2.297944	-0.857887	C	0.842287	-2.991749	-0.900292
C	-3.239432	-1.195322	-0.595453	C	1.659361	-2.761462	-2.030549
H	-2.615239	-1.960928	-1.080149	H	1.750913	-1.737756	-2.428257
C	1.783645	2.046385	-0.707543	C	2.390776	-3.808470	-2.607723
H	1.268398	2.430321	-1.610385	H	3.035035	-3.610068	-3.477983
H	2.876090	2.157572	-0.850365	C	2.333940	-5.097234	-2.048168

H	2.929147	-5.914851	-2.483898	C	1.265601	3.332154	1.596739
C	1.530142	-5.333010	-0.920636	H	1.741175	2.370900	1.850936
H	1.490182	-6.337815	-0.471063	C	1.742777	4.517715	2.177638
C	0.784788	-4.287143	-0.349040	H	2.575069	4.465823	2.895834
H	0.177581	-4.477932	0.548002	C	1.184462	5.755049	1.809898
C	-0.553876	-2.104418	1.501584	H	1.565382	6.687818	2.255059
C	0.039841	-1.550520	2.654298	C	0.150310	5.799660	0.858037
H	0.836666	-0.797582	2.536175	H	-0.280353	6.767344	0.555263
C	-0.405943	-1.934834	3.929152	C	-0.334951	4.612920	0.281251
H	0.049922	-1.487737	4.826151	H	-1.135681	4.660310	-0.471523
C	-1.443087	-2.874382	4.057335	O	-4.159485	-1.449694	1.279735
H	-1.802410	-3.164350	5.056625	C	-5.472091	-1.698017	1.784240
C	-2.036995	-3.429362	2.909316	H	-6.030016	-2.172144	0.952986
H	-2.862325	-4.151462	3.009505	H	-5.982114	-0.757561	2.077800
C	-1.597908	-3.044523	1.633732	H	-5.454788	-2.385780	2.652869
H	-2.092754	-3.443761	0.735329	O	-4.583814	0.704986	-0.866606
C	-1.507057	-1.280179	-1.110894	C	-5.976391	0.400958	-0.982591
C	-1.599690	-1.778853	-2.426255	H	-6.447650	0.725161	-0.033481
H	-0.814403	-2.440097	-2.820140	H	-6.142462	-0.687690	-1.118266
C	-2.671264	-1.418351	-3.250147	H	-6.443392	0.944409	-1.828550
H	-2.727330	-1.770489	-4.290502	Cl	-4.197196	-0.741025	4.388886
C	-3.681624	-0.576633	-2.760884	Cl	-4.932995	-0.047788	-3.872262
C	-3.651754	-0.115543	-1.423562	C	2.920826	1.084406	-0.433618
C	-2.536327	-0.443827	-0.607438	C	3.077959	-0.205512	-0.288297
C	-2.499305	0.129902	0.776984	C	3.946238	-1.360885	-0.321213
C	-3.378974	-0.437293	1.742903	C	3.694542	-2.483813	0.506067
C	-3.305478	0.023155	3.080232	H	2.846532	-2.439831	1.205749
C	-2.447497	1.080343	3.423454	C	4.492095	-3.631133	0.418945
H	-2.422009	1.421714	4.468571	C	5.556971	-3.686800	-0.499899
C	-1.621898	1.665421	2.459718	H	6.175182	-4.595002	-0.576982
H	-0.952145	2.487728	2.748766	C	5.823620	-2.577823	-1.324159
C	-1.621488	1.183400	1.134850	H	6.654447	-2.615693	-2.047175
C	-1.268158	2.168839	-1.570202	C	5.030913	-1.423738	-1.234718
C	-2.516940	2.824625	-1.532675	H	5.220025	-0.559533	-1.890119
H	-2.963686	3.099619	-0.565131	C	3.651354	2.890596	-2.000422
C	-3.217800	3.068725	-2.723298	H	4.223655	3.837197	-2.071407
H	-4.201829	3.561074	-2.687244	H	2.603506	3.080626	-2.304953
C	-2.681622	2.654418	-3.955448	H	4.087605	2.146499	-2.696886
H	-3.243283	2.829438	-4.885897	H	4.273336	-4.497131	1.062905
C	-1.441294	1.994555	-3.996691	O	5.062552	2.156972	-0.184698
H	-1.028784	1.652623	-4.958786	C	5.270631	2.033752	1.146070
C	-0.735555	1.752113	-2.807552	O	4.465264	2.270810	2.025704
H	0.224940	1.210519	-2.817333	O	6.523793	1.622031	1.424617
C	0.214293	3.368550	0.652644	C	7.388699	1.210765	0.351502

H	8.339346	0.915351	0.832517	H	-2.100902	-2.179157	-4.283931
H	6.956548	0.345341	-0.190897	C	-1.125115	-1.995517	-2.344823
H	7.568055	2.039190	-0.362769	H	-0.249921	-2.585681	-2.651627
C	3.656492	2.361257	-0.570171	C	-1.183624	-1.438372	-1.051135
H	3.236014	3.120797	0.119884	C	-0.387329	-2.107550	1.645981
				C	-1.347411	-3.140093	1.703819
IM1B				H	-1.715051	-3.599404	0.773624
Ni	1.303854	0.417162	0.077508	C	-1.873340	-3.540874	2.941510
P	-0.386650	1.741245	-0.051587	H	-2.633144	-4.337047	2.981297
P	0.298961	-1.474004	0.061598	C	-1.453365	-2.908143	4.125027
C	-0.087387	3.455013	0.565535	H	-1.883309	-3.210245	5.092307
C	0.774513	3.591583	1.678131	C	-0.501282	-1.875412	4.070847
H	1.192056	2.687128	2.149241	H	-0.184463	-1.367243	4.994973
C	1.138514	4.860592	2.148010	C	0.032314	-1.476768	2.835297
H	1.821268	4.949934	3.006761	H	0.761094	-0.651817	2.770932
C	0.667571	6.013401	1.494731	C	1.289884	-2.870530	-0.631693
H	0.973633	7.010997	1.846549	C	2.169118	-2.555524	-1.693135
C	-0.177422	5.886804	0.380030	H	2.267643	-1.506704	-2.017492
H	-0.539360	6.785761	-0.143707	C	2.923964	-3.561484	-2.316024
C	-0.556793	4.614526	-0.082691	H	3.608762	-3.301347	-3.136734
H	-1.203203	4.527111	-0.968308	C	2.831120	-4.890096	-1.863349
C	-1.231340	1.970999	-1.666733	H	3.422200	-5.681232	-2.351136
C	-0.556819	1.522786	-2.820656	C	1.991779	-5.203294	-0.780523
H	0.440067	1.064652	-2.709841	H	1.931739	-6.238637	-0.409196
C	-1.168477	1.629589	-4.079990	C	1.220427	-4.199919	-0.168264
H	-0.644280	1.264142	-4.976739	H	0.564192	-4.455024	0.677038
C	-2.454900	2.184465	-4.190805	O	-4.442641	0.247862	-1.134900
H	-2.941445	2.253063	-5.175897	C	-5.786838	-0.204284	-1.319462
C	-3.131198	2.631709	-3.041405	H	-5.833797	-1.310089	-1.397567
H	-4.148496	3.044164	-3.125389	H	-6.245582	0.240297	-2.225604
C	-2.524148	2.524451	-1.781392	H	-6.352985	0.121345	-0.424137
H	-3.070313	2.832949	-0.876890	O	-3.987609	-1.779649	1.127778
C	-1.727350	1.096951	1.058559	C	-5.290461	-2.170710	1.560471
C	-1.896773	1.635315	2.350554	H	-5.728329	-2.740271	0.717322
H	-1.353302	2.543803	2.646374	H	-5.930271	-1.291427	1.779783
C	-2.734712	1.004997	3.274306	H	-5.247595	-2.819637	2.457677
H	-2.838472	1.394617	4.297558	Cl	-4.492791	-0.673461	-4.109623
C	-3.442296	-0.155337	2.920930	Cl	-4.356141	-0.951657	4.195699
C	-3.353885	-0.676646	1.607129	C	4.121211	-0.960750	0.654513
C	-2.456615	-0.060137	0.687732	H	3.594864	-1.913496	0.858109
C	-2.325427	-0.689469	-0.666376	C	3.139019	0.122371	0.383830
C	-3.398752	-0.504948	-1.577865	C	2.953880	1.392231	0.145316
C	-3.282644	-1.025240	-2.888363	C	3.393316	2.768731	0.090489
C	-2.160676	-1.780493	-3.260747	C	2.806407	3.670819	-0.833057

H	2.048361	3.284439	-1.530988	C	1.341889	3.943559	2.705053
C	3.162449	5.024268	-0.839276	H	2.279910	4.515193	2.783963
C	4.103471	5.512810	0.086318	C	1.383399	2.591316	2.335290
H	4.371159	6.581097	0.092349	H	2.348798	2.107525	2.120751
C	4.695977	4.630444	1.008099	C	-1.373205	-0.526931	1.435300
H	5.432911	5.006733	1.735742	C	-1.788786	-1.702403	2.098904
C	4.351778	3.270666	1.008061	H	-1.155312	-2.153365	2.874323
H	4.803361	2.580631	1.737192	C	-2.998448	-2.313478	1.767736
C	5.065283	-0.615006	1.806206	H	-3.317786	-3.235883	2.274558
H	5.754821	-1.457139	2.013239	C	-3.837304	-1.773754	0.778390
H	4.475098	-0.407655	2.721318	C	-3.455766	-0.596314	0.088206
H	5.653968	0.289718	1.554308	C	-2.195804	0.001347	0.405182
H	2.687974	5.709838	-1.558420	C	-1.783231	1.177490	-0.430430
O	4.901399	-1.154062	-0.585045	C	-2.444831	2.413585	-0.215333
C	5.472823	-2.337756	-0.853322	C	-2.035217	3.553980	-0.942724
O	6.092600	-2.548495	-1.878035	C	-1.082443	3.443113	-1.967539
O	5.286002	-3.246016	0.139808	H	-0.800644	4.337830	-2.541827
C	5.879764	-4.531056	-0.091336	C	-0.496636	2.201551	-2.239165
H	5.603059	-5.152257	0.779401	H	0.230314	2.123146	-3.059372
H	5.485564	-4.981676	-1.022864	C	-0.803726	1.065638	-1.459709
H	6.982434	-4.445197	-0.171194	C	-1.236713	-1.725325	-1.924122
				C	-2.271559	-1.474936	-2.851132
				H	-2.281753	-0.527002	-3.411340
IM1C				C	-3.284030	-2.426009	-3.050544
Ni	1.560967	-0.682307	0.054586	H	-4.084190	-2.230532	-3.782279
P	0.351981	0.094041	1.677301	C	-3.280430	-3.625923	-2.314571
P	0.128882	-0.520770	-1.623571	H	-4.085224	-4.363228	-2.459518
C	0.877322	-0.635361	3.300322	C	-2.254142	-3.876700	-1.388719
C	2.166832	-1.201337	3.363724	H	-2.258230	-4.808604	-0.801670
H	2.786729	-1.192032	2.452048	C	-1.231857	-2.932427	-1.195764
C	2.654863	-1.735142	4.569035	H	-0.432006	-3.109337	-0.461324
H	3.663538	-2.175899	4.603882	C	0.979298	-0.464747	-3.248476
C	1.852217	-1.706803	5.722274	C	2.043162	0.457391	-3.433948
H	2.227701	-2.129343	6.667671	H	2.234587	1.237197	-2.684561
C	0.571795	-1.121995	5.672343	C	2.877711	0.374334	-4.558584
H	-0.050812	-1.081123	6.580279	H	3.692279	1.106244	-4.679751
C	0.089406	-0.579745	4.470351	C	2.689259	-0.642225	-5.513007
H	-0.904738	-0.106243	4.439067	H	3.351893	-0.713127	-6.389836
C	0.188150	1.849065	2.214632	C	1.645246	-1.569220	-5.333642
C	-1.042286	2.468487	2.502037	H	1.484956	-2.369633	-6.073912
H	-1.979054	1.899480	2.429978	C	0.798486	-1.482260	-4.217429
C	-1.084323	3.830201	2.846101	H	-0.007114	-2.220499	-4.089380
H	-2.057792	4.311921	3.026283	O	-3.420595	2.449106	0.741549
C	0.105240	4.571961	2.944533	C	-4.730579	2.883518	0.359219
H	0.070697	5.640876	3.208240				

H	-4.857518	3.975617	0.507713	H	3.073577	-1.508328	1.343243
H	-5.444618	2.336695	1.006113	C	3.666030	-3.603610	1.324820
H	-4.937356	2.633034	-0.701328	H	4.688626	-3.397004	1.675984
O	-4.115782	0.049075	-0.907051	C	3.270312	-4.921430	1.032721
C	-5.441888	-0.245328	-1.335373	H	3.981624	-5.753407	1.154266
H	-5.691231	0.552425	-2.061630	C	1.960657	-5.175850	0.590740
H	-6.164024	-0.216291	-0.494657	H	1.640720	-6.207774	0.374392
H	-5.500479	-1.229991	-1.839039	C	1.048976	-4.117519	0.423958
Cl	-2.658079	5.139159	-0.520494	H	0.023236	-4.330753	0.085817
Cl	-5.309166	-2.686470	0.445267	C	-0.310152	-1.180171	2.183530
C	4.012505	-2.170313	-0.707130	C	-0.070659	-0.023116	2.949894
H	5.121709	-2.122508	-0.694678	H	0.527785	0.797288	2.520238
C	3.401672	-0.870931	-0.407471	C	-0.607271	0.079082	4.244121
C	3.172665	0.391670	-0.376333	H	-0.431653	0.993856	4.831690
C	3.492761	1.780710	-0.546699	C	-1.364300	-0.975711	4.781327
C	2.447545	2.741529	-0.588739	H	-1.786898	-0.888726	5.794377
H	1.415294	2.394237	-0.449028	C	-1.574298	-2.145701	4.026922
C	2.726997	4.097112	-0.799022	H	-2.144251	-2.983354	4.459844
C	4.056025	4.527559	-0.969077	C	-1.050183	-2.249710	2.729729
H	4.278243	5.593806	-1.132482	H	-1.223454	-3.159769	2.134805
C	5.104833	3.585193	-0.928186	C	-0.999357	-1.695131	-0.614631
H	6.147061	3.917650	-1.059993	C	-0.790940	-2.532693	-1.733511
C	4.832341	2.227003	-0.719852	H	0.154670	-3.083297	-1.840482
H	5.650134	1.490432	-0.688775	C	-1.755704	-2.643616	-2.738017
C	3.513470	-2.761076	-2.026766	H	-1.581799	-3.267994	-3.626361
H	3.972458	-3.753097	-2.209157	C	-2.954946	-1.924271	-2.629232
H	3.776766	-2.076869	-2.857803	C	-3.203630	-1.090740	-1.514741
H	2.410304	-2.848855	-2.010018	C	-2.200615	-0.941562	-0.519140
H	1.897624	4.821460	-0.822876	C	-2.460514	0.067726	0.564729
O	3.770354	-3.144258	0.402993	C	-3.371523	-0.316009	1.596008
C	2.538967	-3.327166	0.865930	C	-3.659325	0.613644	2.625685
O	1.513668	-2.696192	0.577605	C	-3.091813	1.898871	2.596179
O	2.543739	-4.328503	1.752693	H	-3.348301	2.600705	3.403002
C	1.289228	-4.565129	2.425174	C	-2.208046	2.270687	1.583361
H	1.479782	-5.405987	3.114697	H	-1.764815	3.276127	1.595776
H	0.982248	-3.663083	2.990573	C	-1.864234	1.355615	0.567529
H	0.498444	-4.832243	1.696787	C	-1.121530	1.385772	-2.226874
				C	-2.444567	1.732232	-2.573830
IM1D				H	-3.102286	2.199721	-1.825306
Ni	1.317320	0.498299	-0.289945	C	-2.936916	1.433997	-3.852766
P	0.408942	-1.283675	0.486286	H	-3.977979	1.683083	-4.109289
P	-0.437016	1.730708	-0.549661	C	-2.114215	0.785601	-4.791390
C	1.452808	-2.791774	0.678746	H	-2.508930	0.536882	-5.788753
C	2.764729	-2.546636	1.143455	C	-0.796107	0.439197	-4.449652

H	-0.152678	-0.075903	-5.180287	C	3.643903	2.074526	1.934368
C	-0.298435	0.738706	-3.170960	O	2.498520	2.402567	2.189261
H	0.730282	0.463963	-2.884410	O	4.361815	1.326114	2.794276
C	-0.301296	3.573614	-0.519478	C	5.637606	0.801570	2.388752
C	0.405686	4.148406	0.562580	H	6.016617	0.232793	3.257486
H	0.844324	3.497764	1.335282	H	5.527284	0.126251	1.516711
C	0.601047	5.538065	0.623704	H	6.347792	1.616608	2.132240
H	1.151445	5.970418	1.474607	C	3.562148	2.717027	-0.386973
C	0.121272	6.367356	-0.406428	H	2.824860	3.496662	-0.108689
H	0.283946	7.455874	-0.362601				
C	-0.556786	5.797501	-1.498019	TS1A			
H	-0.928234	6.438613	-2.313608	Ni	1.368958	0.563065	-0.282674
C	-0.771036	4.409193	-1.555063	P	0.409432	-1.375873	-0.043663
H	-1.303083	3.975757	-2.414847	P	-0.414884	1.833140	-0.357481
O	-3.831195	-1.586399	1.446739	C	1.384653	-2.784286	-0.728262
C	-4.739421	-2.241889	2.327618	C	1.993622	-2.598429	-1.990932
H	-5.004654	-3.189488	1.809353	H	1.843439	-1.647984	-2.527460
H	-5.657218	-1.640511	2.494453	C	2.816376	-3.590535	-2.540863
H	-4.265062	-2.471060	3.306004	H	3.290520	-3.426220	-3.520588
O	-4.328227	-0.320635	-1.408589	C	3.066280	-4.773581	-1.822575
C	-5.587706	-0.981734	-1.235603	H	3.731704	-5.543967	-2.242365
H	-6.330076	-0.195867	-1.091014	C	2.479030	-4.959350	-0.560492
H	-5.569342	-1.618370	-0.321309	H	2.680771	-5.877980	0.012856
H	-5.847818	-1.633330	-2.129068	C	1.638803	-3.972486	-0.015267
Cl	-4.691799	0.267331	4.012508	H	1.195104	-4.121065	0.980170
Cl	-4.101127	-1.996402	-3.953869	C	-0.099597	-1.924842	1.634438
C	2.891173	1.440292	-0.749835	C	0.338964	-1.179975	2.748621
C	3.090614	0.173890	-0.985957	H	0.977646	-0.290493	2.602848
C	3.898882	-0.961869	-1.368997	C	-0.084291	-1.550795	4.036266
C	3.282258	-2.108503	-1.932245	H	0.239247	-0.954756	4.903870
H	2.195496	-2.079922	-2.098987	C	-0.928152	-2.659362	4.217807
C	4.030595	-3.248794	-2.246062	H	-1.263998	-2.938059	5.228733
C	5.415714	-3.272808	-1.997782	C	-1.357873	-3.405501	3.104874
H	6.005758	-4.173722	-2.227888	H	-2.024208	-4.271736	3.243192
C	6.046928	-2.137562	-1.455548	C	-0.954136	-3.035106	1.813413
H	7.132331	-2.148289	-1.265438	H	-1.323184	-3.591779	0.938093
C	5.300875	-0.988090	-1.153220	C	-1.187410	-1.478164	-0.980122
H	5.791592	-0.097164	-0.731005	C	-1.282544	-2.190253	-2.192346
C	4.556110	3.234879	-1.411616	H	-0.435750	-2.796338	-2.543314
H	5.143832	4.080660	-0.992252	C	-2.440696	-2.120193	-2.974900
H	4.006827	3.588040	-2.308367	H	-2.503201	-2.643277	-3.940202
H	5.248743	2.422867	-1.719018	C	-3.530135	-1.352273	-2.540127
H	3.530897	-4.133184	-2.670610	C	-3.488621	-0.679586	-1.297509
O	4.351009	2.397595	0.828913	C	-2.299037	-0.723915	-0.525427

C	-2.294648	0.033509	0.769097	C	4.185619	-0.679753	-0.848279
C	-3.047244	-0.536048	1.841162	C	4.262090	-1.735369	0.096639
C	-3.016861	0.107835	3.102300	H	3.553110	-1.736775	0.936570
C	-2.328451	1.322479	3.260000	C	5.231941	-2.733868	-0.035439
H	-2.331735	1.801306	4.249919	C	6.122219	-2.718121	-1.126588
C	-1.633848	1.898482	2.195345	H	6.870095	-3.518391	-1.240498
H	-1.098293	2.844294	2.350414	C	6.053834	-1.677983	-2.071508
C	-1.593847	1.252553	0.943778	H	6.751020	-1.660965	-2.924245
C	-1.376592	1.747754	-1.919193	C	5.104673	-0.655426	-1.928525
C	-2.695438	2.242276	-2.010096	H	5.041960	0.161317	-2.664090
H	-3.183715	2.666329	-1.119563	C	4.859414	3.214342	-0.740300
C	-3.396591	2.151177	-3.220954	H	5.241520	3.998634	-0.058300
H	-4.433128	2.516484	-3.281382	H	4.917497	3.611352	-1.779126
C	-2.787762	1.565469	-4.345768	H	5.508030	2.318714	-0.680196
H	-3.346804	1.478649	-5.290162	H	5.282844	-3.544705	0.707299
C	-1.475158	1.071595	-4.258117	O	3.637682	2.765980	1.580641
H	-1.002259	0.600022	-5.133683	C	3.054040	1.729402	2.066402
C	-0.768874	1.164222	-3.047804	O	1.824231	1.521123	2.157834
H	0.254105	0.764198	-2.952655	O	3.857995	0.698613	2.508515
C	-0.210117	3.649198	-0.088482	C	5.268502	0.832025	2.315383
C	0.571552	4.075327	1.011394	H	5.728255	-0.048512	2.803254
H	1.019497	3.316634	1.675099	H	5.530499	0.823725	1.236859
C	0.816504	5.442584	1.216612	H	5.656727	1.765550	2.771052
H	1.431433	5.755642	2.075041	C	3.431207	2.882696	-0.428590
C	0.306779	6.399622	0.321211	H	2.736955	3.735503	-0.345162
H	0.507136	7.471230	0.479437				
C	-0.447427	5.978657	-0.787432	TS1B			
H	-0.838285	6.718354	-1.504188	Ni	1.470631	-0.053669	-0.822803
C	-0.705617	4.612427	-0.994384	P	0.511675	-1.449122	0.528065
H	-1.288270	4.299855	-1.872624	P	-0.317074	1.016964	-1.534957
O	-3.674477	-1.693391	1.504992	C	1.344843	-3.082004	0.683658
C	-4.714883	-2.297181	2.268302	C	1.811891	-3.670486	-0.515036
H	-5.175126	-3.043175	1.591516	H	1.669148	-3.136477	-1.465036
H	-5.482101	-1.558691	2.577820	C	2.485643	-4.899890	-0.484840
H	-4.319416	-2.812041	3.166113	H	2.854865	-5.342659	-1.424396
O	-4.503209	0.092233	-0.819632	C	2.716884	-5.544065	0.742606
C	-5.804687	-0.481514	-0.656014	H	3.260480	-6.499497	0.765734
H	-6.229990	-0.045987	0.270284	C	2.273279	-4.954632	1.939167
H	-5.746023	-1.583537	-0.544333	H	2.470293	-5.448030	2.904114
H	-6.464286	-0.238979	-1.514127	C	1.586487	-3.727576	1.910499
Cl	-3.752996	-0.559066	4.557310	H	1.262540	-3.265876	2.854122
Cl	-4.916707	-1.173900	-3.598429	C	0.361145	-0.756533	2.220700
C	2.881471	1.624933	-0.733242	C	0.966695	0.490863	2.482498
C	3.166096	0.329787	-0.711825	H	1.525437	1.027051	1.692512

C	0.798738	1.099433	3.733191	C	-0.722380	2.731498	-3.795081
H	1.232703	2.101816	3.885528	H	-1.355892	1.938042	-4.223907
C	0.045443	0.459811	4.733642	O	-3.215821	-0.288020	2.531970
H	-0.090584	0.941468	5.716401	C	-4.175033	-0.159686	3.577962
C	-0.551894	-0.787124	4.473689	H	-4.756857	-1.097319	3.555367
H	-1.154215	-1.282561	5.253768	H	-4.862241	0.700650	3.407156
C	-0.413686	-1.388559	3.217147	H	-3.699701	-0.053919	4.571033
H	-0.936800	-2.333075	2.995679	O	-4.455647	-0.197309	-0.277400
C	-1.229434	-1.906421	0.117884	C	-5.715515	-0.394940	0.372595
C	-1.541228	-3.195494	-0.362270	H	-5.937881	0.535570	0.931501
H	-0.772433	-3.980330	-0.380186	H	-5.677284	-1.245190	1.088987
C	-2.821697	-3.487128	-0.839859	H	-6.523460	-0.577473	-0.360518
H	-3.059492	-4.479617	-1.252207	Cl	-2.761649	2.454393	4.202940
C	-3.809912	-2.492991	-0.831811	Cl	-5.359892	-2.829833	-1.578705
C	-3.544148	-1.210482	-0.295863	C	3.601769	2.156823	-1.121867
C	-2.236333	-0.909851	0.161309	H	3.109732	2.887879	-1.785545
C	-1.994974	0.472557	0.691791	C	3.196370	0.826248	-1.175949
C	-2.543814	0.758596	1.978954	C	3.296213	-0.426354	-0.777024
C	-2.294842	2.027629	2.560181	C	4.197589	-1.546420	-0.567430
C	-1.587715	3.004420	1.841487	C	4.376699	-2.068702	0.739423
H	-1.388382	3.974371	2.317247	H	3.844381	-1.598452	1.578158
C	-1.094254	2.735607	0.562740	C	5.219005	-3.168801	0.947625
H	-0.545049	3.524640	0.032338	C	5.874314	-3.782229	-0.139301
C	-1.275488	1.464251	-0.020663	H	6.518252	-4.656856	0.027280
C	-1.479801	0.030507	-2.560729	C	5.690038	-3.276671	-1.439449
C	-2.801973	0.467341	-2.806409	H	6.196820	-3.750112	-2.290744
H	-3.169396	1.394059	-2.340178	C	4.863832	-2.161730	-1.657455
C	-3.654738	-0.309164	-3.603265	H	4.709700	-1.763405	-2.669055
H	-4.691983	0.019018	-3.776459	C	4.906091	2.566113	-0.493260
C	-3.199734	-1.512457	-4.162705	H	4.859399	3.624356	-0.141952
H	-3.876487	-2.124014	-4.779469	H	5.716212	2.502210	-1.269304
C	-1.884419	-1.949493	-3.924632	H	5.191455	1.896240	0.341986
H	-1.526316	-2.897569	-4.350389	H	5.350374	-3.562145	1.963938
C	-1.026687	-1.178538	-3.122967	O	2.307472	2.663861	0.517015
H	0.002689	-1.511344	-2.904507	C	2.238215	3.769592	1.176526
C	-0.136554	2.568941	-2.523049	O	1.782086	3.933566	2.313780
C	0.699543	3.591020	-2.025025	O	2.715141	4.853997	0.442336
H	1.215772	3.444933	-1.064370	C	2.641076	6.111367	1.114109
C	0.907832	4.769857	-2.758761	H	3.106521	6.855379	0.435757
H	1.559575	5.548936	-2.336249	H	1.590409	6.411132	1.321840
C	0.303119	4.929733	-4.016497	H	3.191262	6.094045	2.079807
H	0.472429	5.852128	-4.595953				
C	-0.502484	3.908291	-4.536804	TS1C			
H	-0.966404	4.018346	-5.529867	Ni	-1.503727	-0.708598	0.212606

P	-0.689314	0.225189	-1.535009	H	4.767888	-2.878696	2.452793
P	0.248796	-0.844704	1.558337	C	3.666049	-3.939157	0.900939
C	-1.503475	-0.397690	-3.079405	H	4.471030	-4.668307	0.720340
C	-2.754513	-1.031141	-2.940417	C	2.470931	-4.013049	0.166654
H	-3.178359	-1.150942	-1.931960	H	2.339771	-4.798340	-0.594385
C	-3.464439	-1.465349	-4.073208	C	1.445222	-3.079181	0.391261
H	-4.437594	-1.964652	-3.946843	H	0.503490	-3.120553	-0.177933
C	-2.927765	-1.264023	-5.355755	C	-0.296149	-1.097242	3.289162
H	-3.477696	-1.608507	-6.245790	C	-1.293658	-0.233906	3.816038
C	-1.692651	-0.603296	-5.503788	H	-1.609057	0.653150	3.247285
H	-1.281572	-0.421824	-6.509595	C	-1.902258	-0.513137	5.047953
C	-0.987382	-0.162726	-4.372862	H	-2.667449	0.174563	5.441941
H	-0.033682	0.374797	-4.494401	C	-1.556865	-1.673806	5.766116
C	-0.839171	2.023046	-1.900182	H	-2.045837	-1.898834	6.726851
C	0.254345	2.886074	-2.084327	C	-0.583171	-2.544921	5.243902
H	1.278754	2.493797	-2.102846	H	-0.305419	-3.456727	5.796572
C	0.043212	4.267127	-2.246287	C	0.044697	-2.259803	4.020588
H	0.913268	4.934114	-2.350678	H	0.801201	-2.952279	3.621583
C	-1.261744	4.786710	-2.269913	O	3.009341	2.795996	-0.912573
H	-1.425289	5.869074	-2.391907	C	4.375513	3.215923	-0.792062
C	-2.361609	3.916603	-2.143552	H	4.457761	4.239043	-0.371130
H	-3.388485	4.312920	-2.168454	H	4.786775	3.206662	-1.819027
C	-2.152621	2.545787	-1.947433	H	4.943773	2.502550	-0.162344
H	-3.013482	1.871731	-1.815445	O	4.198672	0.161704	0.179975
C	1.092484	-0.250429	-1.697734	C	5.542925	-0.233719	0.446903
C	1.429974	-1.285271	-2.599289	H	5.853667	0.388730	1.308091
H	0.680872	-1.674294	-3.301068	H	6.211311	-0.032770	-0.414178
C	2.706998	-1.844648	-2.597610	H	5.606425	-1.303307	0.724262
H	2.964495	-2.653285	-3.297007	Cl	2.457180	5.108215	1.020650
C	3.693286	-1.395898	-1.705061	Cl	5.255686	-2.202660	-1.825022
C	3.391447	-0.374484	-0.771099	C	-3.916394	-1.945950	1.440925
C	2.070108	0.179701	-0.760843	H	-5.023420	-1.942266	1.469268
C	1.800994	1.164634	0.342485	C	-3.299232	-0.720180	1.148355
C	2.334095	2.473147	0.233038	C	-2.822617	0.456152	0.895619
C	2.089586	3.409245	1.265947	C	-2.937823	1.889375	1.077678
C	1.489231	3.007208	2.467631	C	-1.768384	2.688117	1.067775
H	1.348525	3.740913	3.274735	H	-0.803274	2.194074	0.911297
C	1.044079	1.687798	2.609714	C	-1.844000	4.075772	1.232188
H	0.575038	1.381492	3.554979	C	-3.097576	4.693829	1.384604
C	1.136697	0.770897	1.541123	H	-3.165069	5.787576	1.496181
C	1.620050	-2.056010	1.345539	C	-4.271503	3.913770	1.387069
C	2.822598	-1.981638	2.081157	H	-5.253479	4.398900	1.505198
H	2.960528	-1.176606	2.819970	C	-4.196223	2.521031	1.242502
C	3.836785	-2.927764	1.865757	H	-5.108679	1.904790	1.244396

C	-3.269403	-2.883537	2.434775	H	1.228877	-3.051042	3.801763
H	-3.758467	-3.876433	2.415383	C	2.684739	-1.772093	2.836142
H	-3.367728	-2.456624	3.455950	C	3.010821	-0.994226	1.702922
H	-2.188807	-2.988458	2.225082	C	2.068931	-0.872204	0.645995
H	-0.920319	4.674220	1.214156	C	2.425249	0.064115	-0.471605
O	-3.939089	-2.974082	-0.083609	C	3.420521	-0.378906	-1.394703
C	-2.799514	-3.217089	-0.641018	C	3.772642	0.476744	-2.467520
O	-1.696203	-2.654913	-0.447211	C	3.193248	1.753134	-2.572725
O	-2.892598	-4.210951	-1.561257	H	3.499384	2.396524	-3.410469
C	-1.704919	-4.458146	-2.331059	C	2.241140	2.190526	-1.651505
H	-1.985116	-5.226359	-3.074708	H	1.800915	3.191204	-1.763029
H	-1.367786	-3.534203	-2.843244	C	1.832033	1.345878	-0.599454
H	-0.883557	-4.834381	-1.687487	C	0.957184	1.525111	2.150121
				C	2.251259	1.914125	2.558226
TS1D				H	2.940725	2.368585	1.830405
Ni	-1.423323	0.593171	0.025661	C	2.674007	1.676194	3.874048
P	-0.458806	-1.248760	-0.553111	H	3.692824	1.958840	4.180430
P	0.361853	1.788235	0.429109	C	1.809853	1.048364	4.789494
C	-1.523869	-2.751535	-0.653079	H	2.149987	0.847266	5.817096
C	-2.829740	-2.527514	-1.142765	C	0.521717	0.658957	4.385744
H	-3.129287	-1.503233	-1.416892	H	-0.151963	0.155084	5.096579
C	-3.735917	-3.590100	-1.262148	C	0.094280	0.895572	3.068945
H	-4.754546	-3.399690	-1.633454	H	-0.904470	0.579578	2.727784
C	-3.352018	-4.888430	-0.882005	C	0.231498	3.623571	0.288917
H	-4.070137	-5.720404	-0.953529	C	-0.387619	4.141834	-0.874562
C	-2.047706	-5.122667	-0.413562	H	-0.762601	3.442811	-1.638815
H	-1.737640	-6.140543	-0.128161	C	-0.574341	5.525941	-1.020167
C	-1.131427	-4.061281	-0.309297	H	-1.055204	5.915916	-1.931331
H	-0.110550	-4.259566	0.050830	C	-0.172412	6.407683	-0.000198
C	0.441346	-1.367507	-2.161574	H	-0.328339	7.492381	-0.111649
C	0.303795	-0.320554	-3.093937	C	0.415676	5.895370	1.168975
H	-0.344575	0.534928	-2.850046	H	0.719884	6.577231	1.979058
C	0.988756	-0.387242	-4.318970	C	0.618828	4.511915	1.314827
H	0.894814	0.440164	-5.039685	H	1.075112	4.123188	2.237007
C	1.794203	-1.497421	-4.622884	O	3.878869	-1.627520	-1.118909
H	2.336323	-1.541384	-5.580135	C	4.945394	-2.278131	-1.804026
C	1.907249	-2.555365	-3.701531	H	5.113297	-3.218139	-1.243485
H	2.525887	-3.434357	-3.943187	H	5.874335	-1.673028	-1.794250
C	1.234835	-2.491613	-2.472222	H	4.673519	-2.518318	-2.850540
H	1.341093	-3.310210	-1.744152	O	4.160141	-0.268403	1.599095
C	0.844741	-1.588910	0.703644	C	5.413384	-0.961750	1.617986
C	0.560755	-2.375247	1.841537	H	6.114656	-0.356741	1.010327
H	-0.391694	-2.918492	1.910026	H	5.315880	-1.968182	1.161672
C	1.465591	-2.462589	2.903622	H	5.809784	-1.063661	2.649209

Cl	4.893522	0.036355	-3.755026	H	1.302932	-4.208814	0.487046
Cl	3.760249	-1.816518	4.219604	C	-0.239691	-2.285695	1.310672
C	-2.908889	1.557698	0.756172	C	0.036618	-1.813950	2.609768
C	-3.045030	0.264360	0.918474	H	0.657276	-0.911245	2.723118
C	-3.853443	-0.856972	1.341931	C	-0.533901	-2.458811	3.719516
C	-3.254646	-1.977526	1.968308	H	-0.339934	-2.072098	4.732022
H	-2.177881	-1.936397	2.184292	C	-1.365465	-3.577059	3.539569
C	-4.010705	-3.110851	2.287573	H	-1.817116	-4.074699	4.411925
C	-5.379657	-3.158285	1.964604	C	-1.633773	-4.053087	2.242746
H	-5.970443	-4.059380	2.191665	H	-2.288796	-4.926963	2.098687
C	-5.991477	-2.050095	1.349996	C	-1.083636	-3.403331	1.127585
H	-7.064224	-2.080405	1.101411	H	-1.322349	-3.752110	0.110876
C	-5.241734	-0.901718	1.056303	C	-1.030519	-1.252345	-1.226800
H	-5.716849	-0.031899	0.576899	C	-1.024140	-1.748861	-2.545814
C	-4.775521	3.268472	0.956615	H	-0.156883	-2.307780	-2.921819
H	-5.193888	4.101830	0.358588	C	-2.107786	-1.527475	-3.403133
H	-4.627236	3.628880	1.997066	H	-2.084792	-1.881059	-4.444163
H	-5.502234	2.433537	0.980781	C	-3.230045	-0.825872	-2.941857
H	-3.526252	-3.974799	2.768233	C	-3.297764	-0.379108	-1.602880
O	-3.921364	2.602674	-1.334351	C	-2.181700	-0.574783	-0.748766
C	-3.184449	1.771068	-2.013086	C	-2.299100	-0.053725	0.651305
O	-1.944055	1.689421	-2.013697	C	-3.133891	-0.791315	1.543525
O	-3.868028	0.860282	-2.774249	C	-3.210007	-0.369241	2.893643
C	-5.298117	0.852619	-2.688984	C	-2.547289	0.798372	3.309980
H	-5.637739	0.055376	-3.376521	H	-2.634429	1.101521	4.363434
H	-5.636697	0.625551	-1.657176	C	-1.774870	1.545094	2.418860
H	-5.728888	1.826752	-2.998011	H	-1.261892	2.449021	2.772521
C	-3.446494	2.822072	0.402617	C	-1.631326	1.117434	1.084208
H	-2.706030	3.630919	0.266583	C	-1.151292	2.082922	-1.636089
				C	-2.450808	2.616259	-1.775355
IM2A				H	-3.024879	2.899691	-0.880211
Ni	1.455710	0.600882	0.142533	C	-3.022813	2.742123	-3.049307
P	0.461670	-1.376875	-0.125967	H	-4.045794	3.134819	-3.153159
P	-0.354818	1.881228	0.000531	C	-2.302041	2.339936	-4.188578
C	1.501290	-2.625878	-0.995086	H	-2.760240	2.423909	-5.186040
C	2.136740	-2.241507	-2.199549	C	-1.006504	1.812776	-4.052768
H	1.977150	-1.227229	-2.597525	H	-0.446213	1.486835	-4.942955
C	2.989068	-3.126657	-2.872928	C	-0.430131	1.684828	-2.778548
H	3.477620	-2.809536	-3.806874	H	0.576227	1.254449	-2.648806
C	3.247356	-4.400351	-2.335244	C	-0.102221	3.612093	0.582204
H	3.932795	-5.089453	-2.852639	C	0.599347	3.833597	1.792304
C	2.640860	-4.781460	-1.127350	H	0.937994	2.978498	2.397050
H	2.847931	-5.772556	-0.693699	C	0.911954	5.140627	2.195576
C	1.768939	-3.902521	-0.461038	H	1.463018	5.289540	3.137301

C	0.550535	6.241296	1.398017	H	2.381102	3.885992	-0.472402
H	0.806464	7.265005	1.714265				
C	-0.127690	6.025189	0.186774	IM2B			
H	-0.404904	6.877687	-0.453515	Ni	1.114755	1.108328	-0.917203
C	-0.451982	4.719700	-0.222138	P	0.915250	-1.004920	-0.451744
H	-0.968531	4.567142	-1.180385	P	-0.956917	1.650100	-0.595682
O	-3.725636	-1.867331	0.962365	C	2.004984	-2.040954	-1.515172
C	-4.809470	-2.595882	1.531305	C	1.987783	-1.798076	-2.907438
H	-5.209343	-3.213297	0.703521	H	1.342057	-1.002643	-3.312361
H	-5.606976	-1.923248	1.907230	C	2.795298	-2.554468	-3.769441
H	-4.471004	-3.258856	2.351885	H	2.766556	-2.363524	-4.853734
O	-4.350926	0.313231	-1.088998	C	3.652726	-3.539518	-3.246733
C	-5.659028	-0.268270	-1.131922	H	4.297624	-4.124349	-3.921103
H	-6.162358	0.011262	-0.184825	C	3.701489	-3.756580	-1.860112
H	-5.603336	-1.373980	-1.199649	H	4.391869	-4.504908	-1.441291
H	-6.245319	0.119060	-1.990134	C	2.878885	-3.014743	-0.995621
Cl	-4.051686	-1.271277	4.151191	H	2.930513	-3.182490	0.089551
Cl	-4.516752	-0.445370	-4.069473	C	1.176079	-1.647814	1.252073
C	2.804805	1.804091	-0.533599	C	1.705774	-0.787640	2.229349
C	3.144900	0.498621	-0.514038	H	1.994502	0.240976	1.971522
C	4.188911	-0.449149	-0.785877	C	1.869744	-1.241662	3.547571
C	4.292212	-1.625546	0.004308	H	2.273464	-0.551190	4.303847
H	3.590031	-1.744452	0.840440	C	1.513121	-2.555860	3.891949
C	5.281633	-2.574012	-0.270237	H	1.634955	-2.908863	4.928017
C	6.159700	-2.385337	-1.355016	C	0.991572	-3.421334	2.911642
H	6.923215	-3.145507	-1.583367	H	0.712069	-4.453334	3.176859
C	6.064959	-1.225963	-2.148973	C	0.811177	-2.968391	1.595824
H	6.754017	-1.080092	-2.995666	H	0.370889	-3.634520	0.837799
C	5.101387	-0.252381	-1.857201	C	-0.757864	-1.722737	-0.809496
H	5.015638	0.656088	-2.472808	C	-0.979629	-2.604850	-1.885256
C	4.484006	3.591801	-1.157638	H	-0.139193	-2.946289	-2.504067
H	4.904975	4.327008	-0.435872	C	-2.273207	-3.039317	-2.195627
H	4.410217	4.129281	-2.131244	H	-2.455620	-3.695121	-3.059284
H	5.206789	2.760129	-1.271540	C	-3.360487	-2.609268	-1.421639
H	5.357683	-3.480140	0.349794	C	-3.159762	-1.781674	-0.292931
O	2.763455	1.919364	3.645796	C	-1.850133	-1.327303	0.001648
C	2.499792	1.050692	2.809112	C	-1.664466	-0.435180	1.188752
O	1.388996	0.910380	2.163490	C	-1.772796	-1.051512	2.474124
O	3.429643	0.065172	2.493742	C	-1.475151	-0.271442	3.618099
C	4.705467	0.202577	3.114167	C	-1.152999	1.089380	3.480809
H	5.329416	-0.625252	2.724017	H	-0.922642	1.667245	4.387323
H	5.176060	1.175471	2.858758	C	-1.097737	1.697496	2.226390
H	4.631559	0.134396	4.220464	H	-0.818486	2.754600	2.165472
C	3.136986	3.112554	-0.699881	C	-1.344171	0.938276	1.064993

C	-2.238808	0.986860	-1.728938	C	6.069214	-1.357495	-1.710111
C	-3.609271	1.063292	-1.397749	H	6.676831	-1.853347	-2.483311
H	-3.914845	1.468971	-0.421430	C	5.016949	-0.516368	-2.091749
C	-4.573940	0.596826	-2.300600	H	4.783303	-0.355648	-3.154058
H	-5.639964	0.637073	-2.030154	C	1.428354	4.021401	-2.175976
C	-4.178679	0.056702	-3.538707	H	1.845356	4.156880	-1.159910
H	-4.937780	-0.320664	-4.240911	H	0.415515	4.464713	-2.209991
C	-2.815773	-0.018954	-3.870433	H	2.060788	4.572946	-2.906431
H	-2.503474	-0.453844	-4.832509	H	5.774556	-1.103240	1.702353
C	-1.846065	0.446780	-2.966787	O	1.577709	2.533165	0.636957
H	-0.771083	0.373706	-3.196218	C	2.137137	2.636747	1.771804
C	-1.392535	3.448538	-0.568375	O	3.051427	1.969365	2.289246
C	-0.753568	4.354022	0.310912	O	1.575973	3.693162	2.518993
H	0.027113	4.003843	0.998137	C	2.103262	3.872321	3.829787
C	-1.045971	5.725948	0.250905	H	1.586055	4.753152	4.258993
H	-0.537105	6.409131	0.948946	H	1.918036	2.982677	4.470425
C	-1.948668	6.227422	-0.701084	H	3.198996	4.052090	3.810053
H	-2.166928	7.305956	-0.749709				
C	-2.558236	5.339774	-1.603448	IM2C			
H	-3.255667	5.716278	-2.368334	Ni	1.703945	0.533099	0.151251
C	-2.285278	3.963480	-1.539066	P	0.040270	0.751107	1.620020
H	-2.770071	3.292356	-2.260406	P	0.786227	-0.953189	-1.214945
O	-2.106990	-2.365219	2.410217	C	0.611469	0.877028	3.370159
C	-2.472869	-3.167870	3.529447	C	1.990666	0.928732	3.643854
H	-2.868304	-4.105368	3.092801	H	2.733663	0.867610	2.830654
H	-3.260728	-2.686254	4.142948	C	2.430690	1.097944	4.970416
H	-1.598050	-3.401705	4.167365	H	3.512458	1.139630	5.172736
O	-4.164416	-1.305313	0.490652	C	1.504275	1.216823	6.018278
C	-5.060549	-2.227402	1.122810	H	1.853594	1.346749	7.055041
H	-5.309512	-1.796958	2.113011	C	0.123033	1.186661	5.740633
H	-4.578687	-3.215698	1.268353	H	-0.608684	1.298909	6.556399
H	-5.989999	-2.358247	0.532159	C	-0.323403	1.027396	4.421239
Cl	-1.412860	-0.915400	5.255452	H	-1.402952	1.027467	4.201701
Cl	-4.981885	-3.038912	-1.927978	C	-1.002833	2.266735	1.598201
C	1.383177	2.551920	-2.532961	C	-2.397001	2.260093	1.423711
H	0.748306	2.287248	-3.401530	H	-2.945582	1.314009	1.331768
C	2.458838	1.714058	-2.263788	C	-3.102804	3.475203	1.363118
C	3.083416	0.911959	-1.487541	H	-4.191071	3.456696	1.195416
C	4.212875	0.108257	-1.105344	C	-2.426079	4.696494	1.514623
C	4.503951	-0.096474	0.266799	H	-2.980494	5.646686	1.463617
H	3.918103	0.448356	1.025927	C	-1.035968	4.702782	1.736907
C	5.557996	-0.944496	0.634187	H	-0.498277	5.655274	1.860877
C	6.336102	-1.585351	-0.347119	C	-0.325332	3.496655	1.766705
H	7.155844	-2.259204	-0.051429	H	0.766596	3.502198	1.911512

C	-1.116081	-0.691952	1.612707	C	-4.071633	-3.576728	-1.093062
C	-1.090612	-1.579974	2.709860	H	-4.435010	-3.365708	-2.117142
H	-0.491385	-1.344178	3.598683	H	-4.936287	-3.668394	-0.406013
C	-1.800883	-2.778826	2.668625	H	-3.497443	-4.523280	-1.094155
H	-1.770419	-3.475890	3.518454	Cl	-4.567306	2.198967	-2.640712
C	-2.555784	-3.135189	1.540072	Cl	-3.365148	-4.696552	1.623324
C	-2.602699	-2.274301	0.416392	C	4.201924	1.369142	-1.526534
C	-1.858409	-1.050046	0.459164	H	4.591522	2.227461	-2.111337
C	-1.898323	-0.245184	-0.808861	C	3.012435	1.529525	-0.889995
C	-3.106750	0.423643	-1.132619	C	1.849020	2.152883	-0.658790
C	-3.196141	1.147417	-2.345653	C	1.052579	3.293485	-1.027772
C	-2.168528	1.079925	-3.296093	C	-0.343547	3.148484	-1.239701
H	-2.274550	1.621442	-4.247037	H	-0.796226	2.164054	-1.087735
C	-1.002759	0.360725	-3.005555	C	-1.123908	4.237754	-1.639098
H	-0.205523	0.312464	-3.758678	C	-0.533630	5.506229	-1.784641
C	-0.832997	-0.263444	-1.753036	H	-1.150012	6.372418	-2.072306
C	0.373531	-2.680531	-0.753797	C	0.848679	5.670870	-1.560476
C	-0.390286	-3.489743	-1.624393	H	1.309427	6.664796	-1.674788
H	-0.744264	-3.082186	-2.584037	C	1.644419	4.573013	-1.209504
C	-0.700775	-4.807263	-1.256920	H	2.726544	4.690466	-1.045257
H	-1.286904	-5.443183	-1.939142	C	5.033254	0.127817	-1.480696
C	-0.264299	-5.316228	-0.018794	H	5.880677	0.235495	-0.767136
H	-0.523339	-6.345359	0.273854	H	5.464149	-0.100631	-2.478908
C	0.495574	-4.509198	0.843673	H	4.425144	-0.733765	-1.145427
H	0.832014	-4.903915	1.815041	H	-2.201814	4.097103	-1.810697
C	0.822636	-3.192119	0.479067	O	4.470273	0.482760	1.758991
H	1.424797	-2.541853	1.131794	C	3.998458	-0.615334	1.447132
C	1.842863	-1.131206	-2.694869	O	2.797538	-0.896404	1.056345
C	2.204364	0.011910	-3.451272	O	4.853133	-1.705711	1.528502
H	1.767847	0.992399	-3.217564	C	4.344920	-2.972301	1.121402
C	3.129522	-0.094964	-4.502495	H	5.203441	-3.672761	1.135317
H	3.388627	0.800974	-5.087854	H	3.560358	-3.346597	1.814502
C	3.745463	-1.325448	-4.782447	H	3.908403	-2.936607	0.100061
H	4.483708	-1.402518	-5.595805				
C	3.419490	-2.458185	-4.012785	IM2D			
H	3.902190	-3.425819	-4.221423	Ni	-1.535361	0.626045	-0.260772
C	2.476523	-2.365046	-2.979230	P	-0.380770	-1.209893	-0.818281
H	2.227192	-3.256670	-2.385443	P	0.162422	1.737296	0.630259
O	-4.118387	0.365763	-0.221594	C	-1.424633	-2.705859	-1.082015
C	-5.403655	-0.116894	-0.639706	C	-2.753197	-2.455620	-1.490792
H	-6.079592	0.719572	-0.909258	H	-3.076986	-1.412827	-1.639133
H	-5.824375	-0.672510	0.221112	C	-3.643319	-3.520787	-1.692778
H	-5.304767	-0.805157	-1.503161	H	-4.680290	-3.312976	-1.998442
O	-3.246757	-2.460788	-0.763077	C	-3.219940	-4.844242	-1.482266

H	-3.924671	-5.679328	-1.620272	C	-0.626797	4.191032	-0.455873
C	-1.890955	-5.101368	-1.101094	H	-0.770746	3.604307	-1.377773
H	-1.549410	-6.137723	-0.950557	C	-0.967076	5.552125	-0.413430
C	-0.992459	-4.038240	-0.910007	H	-1.332140	6.044401	-1.328424
H	0.044616	-4.255493	-0.613670	C	-0.866886	6.273934	0.789850
C	0.705772	-1.207195	-2.313295	H	-1.142375	7.339941	0.821117
C	0.688927	-0.095465	-3.179666	C	-0.429869	5.624247	1.956946
H	0.035695	0.758974	-2.942102	H	-0.364144	6.177712	2.907054
C	1.526268	-0.079276	-4.307510	C	-0.076704	4.264461	1.922608
H	1.525603	0.800625	-4.969541	H	0.256382	3.764810	2.843910
C	2.369261	-1.168337	-4.583482	O	4.004847	-1.264698	-0.950526
H	3.028167	-1.148296	-5.465379	C	5.165216	-1.774967	-1.602136
C	2.375292	-2.283784	-3.725517	H	5.352096	-2.755609	-1.123549
H	3.030078	-3.143365	-3.939851	H	6.045630	-1.118225	-1.453201
C	1.551522	-2.302562	-2.590096	H	4.992691	-1.922559	-2.686117
H	1.583380	-3.165287	-1.908047	O	3.929019	-0.223041	1.887680
C	0.814348	-1.628262	0.528748	C	5.232807	-0.810914	1.978309
C	0.520789	-2.603614	1.505485	H	5.922556	-0.130931	1.440307
H	-0.367440	-3.239392	1.399299	H	5.254678	-1.807180	1.491156
C	1.342034	-2.778820	2.624127	H	5.559989	-0.911656	3.033271
H	1.089992	-3.517034	3.399010	Cl	5.119966	0.736026	-3.294028
C	2.491293	-1.990041	2.774406	Cl	3.445122	-2.150627	4.234798
C	2.841868	-1.036634	1.792462	C	-3.080066	1.453316	0.538264
C	1.981428	-0.833593	0.680107	C	-2.975380	0.125737	0.737389
C	2.373995	0.246734	-0.283087	C	-3.695230	-1.037241	1.179164
C	3.478416	-0.029147	-1.145236	C	-3.021886	-2.176280	1.687455
C	3.858282	0.960205	-2.086010	H	-1.935136	-2.116623	1.826542
C	3.193793	2.198966	-2.119240	C	-3.724630	-3.342799	2.002821
H	3.520044	2.945360	-2.857903	C	-5.114732	-3.408541	1.788168
C	2.138555	2.476591	-1.249821	H	-5.665618	-4.335426	2.011083
H	1.637816	3.453109	-1.298465	C	-5.799385	-2.282735	1.291085
C	1.712201	1.499514	-0.327487	H	-6.887644	-2.328767	1.126887
C	0.596894	1.264605	2.346877	C	-5.106221	-1.097871	1.010742
C	1.807165	1.696758	2.932621	H	-5.634220	-0.217247	0.614595
H	2.510199	2.309560	2.348361	C	-4.935876	2.927419	1.414603
C	2.129278	1.309219	4.241048	H	-5.742077	3.310161	0.748230
H	3.083887	1.629482	4.685614	H	-4.774381	3.716277	2.183542
C	1.248836	0.491116	4.971837	H	-5.305827	2.015610	1.923892
H	1.512171	0.174766	5.992783	H	-3.184420	-4.217467	2.397276
C	0.042275	0.063882	4.392475	O	-2.843015	2.762290	-3.376672
H	-0.645545	-0.584255	4.957434	C	-2.538257	1.827500	-2.636931
C	-0.284978	0.449700	3.082797	O	-1.443527	1.696658	-1.956395
H	-1.219444	0.109106	2.611027	O	-3.397845	0.745063	-2.458547
C	-0.155307	3.541923	0.711959	C	-4.671889	0.862144	-3.086556

H	-5.208290	-0.083941	-2.877895	H	-0.850010	2.903932	-4.073089
H	-5.247668	1.716936	-2.671465	C	-0.459071	1.064421	-2.974888
H	-4.575119	1.009499	-4.182601	H	0.242458	0.690859	-3.731817
C	-3.672255	2.667919	0.643576	C	-0.708223	0.315233	-1.807060
H	-3.200631	3.529588	0.136925	C	-0.999018	-2.434433	-1.027218
				C	-2.014379	-2.702867	-1.970634
IM3A				H	-2.020922	-2.171898	-2.935000
Ni	1.753514	-0.490395	0.114409	C	-3.021541	-3.631446	-1.667045
P	0.316299	0.241256	1.712493	H	-3.813032	-3.841217	-2.403563
P	0.288140	-1.171200	-1.372686	C	-3.026570	-4.285215	-0.421266
C	0.646927	-0.410134	3.407538	H	-3.828321	-4.998968	-0.178378
C	1.023478	-1.762442	3.551717	C	-2.017809	-4.015316	0.519362
H	1.210071	-2.366278	2.651102	H	-2.027881	-4.512133	1.501380
C	1.203204	-2.312114	4.829825	C	-1.002393	-3.095265	0.216189
H	1.507263	-3.365773	4.930488	H	-0.224932	-2.852395	0.954744
C	1.019307	-1.516202	5.974935	C	1.129251	-1.765724	-2.881847
H	1.168609	-1.946677	6.977747	C	2.066276	-0.930506	-3.541923
C	0.654374	-0.166047	5.834881	H	2.193331	0.114285	-3.231206
H	0.513283	0.464598	6.726926	C	2.859096	-1.437347	-4.583596
C	0.466288	0.387272	4.556604	H	3.578632	-0.773427	-5.087448
H	0.171778	1.442271	4.453581	C	2.760361	-2.787661	-4.958339
C	0.337122	2.049634	2.009629	H	3.396832	-3.186748	-5.763312
C	-0.814128	2.855946	1.943652	C	1.845487	-3.628530	-4.296719
H	-1.795677	2.409929	1.727963	H	1.762150	-4.688623	-4.583078
C	-0.703578	4.245680	2.126894	C	1.036514	-3.125107	-3.268084
H	-1.604606	4.874481	2.050993	H	0.332176	-3.793635	-2.751683
C	0.545946	4.827399	2.398879	O	-3.192985	2.451295	-0.137993
H	0.629457	5.916727	2.537204	C	-4.533014	2.781227	-0.530441
C	1.693834	4.017261	2.486792	H	-4.682082	3.879824	-0.538122
H	2.676325	4.469012	2.692588	H	-5.210024	2.320578	0.217056
C	1.595315	2.635101	2.280133	H	-4.767666	2.373848	-1.534170
H	2.492744	1.996724	2.315886	O	-3.953278	-0.365428	-1.159699
C	-1.477767	-0.206158	1.515685	C	-5.283360	-0.652013	-1.587313
C	-2.120774	-0.915174	2.554512	H	-5.375132	-0.164914	-2.577174
H	-1.618333	-1.057849	3.519256	H	-6.040228	-0.229383	-0.896581
C	-3.381869	-1.477029	2.360352	H	-5.452559	-1.741194	-1.696362
H	-3.866490	-2.053883	3.161331	Cl	-2.609326	4.424516	-2.410034
C	-4.041941	-1.357226	1.127254	Cl	-5.556037	-2.241555	0.973086
C	-3.460974	-0.597834	0.083694	C	4.459644	-0.436332	-1.540853
C	-2.166223	-0.019555	0.293837	H	4.988315	0.314210	-2.164784
C	-1.657035	0.790999	-0.861655	C	3.359993	0.014691	-0.877633
C	-2.302436	2.037875	-1.081609	C	2.528865	1.019207	-0.571265
C	-1.971079	2.802744	-2.223613	C	2.389762	2.438877	-0.737188
C	-1.080673	2.301375	-3.183007	C	1.117890	3.062090	-0.773135

H	0.227317	2.438884	-0.659551	C	1.532860	-3.468096	2.958121
C	1.002565	4.443944	-0.947466	H	1.567145	-4.552150	3.150547
C	2.158980	5.239069	-1.049036	C	1.350572	-2.996722	1.648814
H	2.070587	6.330993	-1.162466	H	1.225871	-3.710311	0.819252
C	3.432811	4.636975	-1.002863	C	-0.459328	-1.815004	-0.883861
H	4.338926	5.258643	-1.078837	C	-0.436000	-2.624619	-2.037182
C	3.553021	3.248450	-0.871938	H	0.517977	-2.871930	-2.521538
H	4.543328	2.769424	-0.835609	C	-1.625255	-3.095598	-2.607723
C	5.009492	-1.828874	-1.542996	H	-1.606143	-3.692982	-3.530853
H	6.088558	-1.831533	-1.797303	C	-2.860501	-2.758414	-2.038284
H	4.497090	-2.450113	-2.316915	C	-2.922718	-2.017905	-0.832450
H	4.874973	-2.334824	-0.566925	C	-1.709990	-1.560353	-0.253821
H	0.002876	4.901677	-0.988108	C	-1.766299	-0.834417	1.049268
O	3.567110	-0.719927	2.133490	C	-2.083303	-1.591403	2.206329
C	3.707863	-1.878879	1.770781	C	-1.897470	-1.014157	3.479373
O	4.480748	-2.819060	1.857293	C	-1.470404	0.315588	3.611849
O	2.372317	-2.265120	0.859395	H	-1.311024	0.739655	4.613540
C	2.433815	-3.471563	0.115655	C	-1.239249	1.090036	2.469662
H	3.257039	-4.091346	0.528686	H	-0.868514	2.122298	2.598133
H	1.476961	-4.030179	0.204991	C	-1.408358	0.528569	1.183210
H	2.629983	-3.282964	-0.961802	C	-2.044810	0.989347	-1.677797
				C	-3.448218	1.102891	-1.616286
				H	-3.930909	1.511832	-0.716420
IM3B				C	-4.230556	0.668221	-2.696442
Ni	1.160005	1.212817	-0.574095	H	-5.327661	0.733998	-2.636293
P	1.089931	-0.946639	-0.303824	C	-3.618538	0.136028	-3.845159
P	-0.957947	1.531333	-0.293715	H	-4.236890	-0.212377	-4.686461
C	2.397925	-1.755217	-1.324760	C	-2.217736	0.039523	-3.915070
C	2.474489	-1.376151	-2.685126	H	-1.734508	-0.382883	-4.809645
H	1.751257	-0.648972	-3.087102	C	-1.433690	0.468683	-2.834893
C	3.470253	-1.905710	-3.518162	H	-0.336397	0.383098	-2.848967
H	3.512040	-1.606595	-4.577173	C	-1.683960	3.187824	0.074249
C	4.422054	-2.800718	-2.996366	C	-2.754830	3.345482	0.981815
H	5.212930	-3.207060	-3.645939	H	-3.120079	2.486930	1.562693
C	4.374486	-3.151024	-1.637929	C	-3.358873	4.600870	1.155263
H	5.135280	-3.822999	-1.212118	H	-4.185982	4.709011	1.874068
C	3.368812	-2.632360	-0.804553	C	-2.910563	5.711512	0.420998
H	3.364271	-2.890922	0.262873	H	-3.381970	6.696439	0.563312
C	1.317661	-1.608030	1.396998	C	-1.858401	5.557028	-0.497161
C	1.451585	-0.694532	2.461956	H	-1.501094	6.418725	-1.081979
H	1.412247	0.391495	2.259519	C	-1.250701	4.303877	-0.669179
C	1.607445	-1.175786	3.773161	H	-0.430420	4.196228	-1.386736
H	1.689671	-0.458759	4.604642	O	-2.631105	-2.841108	2.084347
C	1.652835	-2.556884	4.024006	C	-1.754086	-3.970030	2.092829
H	1.775525	-2.928412	5.053370				

H	-1.107491	-3.975650	1.190439	H	-3.553444	-1.908160	-1.907829
H	-2.402881	-4.866469	2.086585	C	-4.298702	-1.378357	-3.881663
H	-1.116748	-3.974618	3.000493	H	-5.045352	-2.187852	-3.882602
O	-4.083790	-1.589601	-0.269639	C	-4.188067	-0.512221	-4.980444
C	-5.048229	-2.545509	0.203862	H	-4.847760	-0.637203	-5.853743
H	-5.925636	-1.951163	0.520128	C	-3.235969	0.526284	-4.960866
H	-4.632052	-3.089301	1.074388	H	-3.152184	1.217647	-5.814236
H	-5.355802	-3.254032	-0.590698	C	-2.398630	0.689922	-3.848951
Cl	-2.191544	-1.989550	4.900897	H	-1.668091	1.513914	-3.829536
Cl	-4.323877	-3.181026	-2.902573	C	-2.070174	1.793949	-0.920718
C	1.535568	2.847361	-1.989929	C	-1.338558	2.952499	-1.226390
H	1.447240	3.756191	-1.360746	H	-0.337214	2.882824	-1.669135
C	2.622553	2.060475	-1.654012	C	-1.887414	4.218810	-0.958358
C	3.177858	1.206307	-0.879250	H	-1.288555	5.119203	-1.165608
C	4.323131	0.489636	-0.392261	C	-3.183181	4.330101	-0.428289
C	4.391295	0.112888	0.971623	H	-3.609779	5.322453	-0.214008
H	3.581502	0.427106	1.642854	C	-3.939215	3.169957	-0.176170
C	5.471344	-0.644793	1.440960	H	-4.957791	3.249442	0.233082
C	6.503613	-1.025774	0.563468	C	-3.383456	1.906333	-0.411849
H	7.349235	-1.627334	0.932241	H	-3.963664	0.997161	-0.188082
C	6.454123	-0.633182	-0.787164	C	0.256234	0.195836	-1.932733
H	7.259147	-0.930116	-1.477568	C	0.477404	-0.490044	-3.150476
C	5.373610	0.117512	-1.267694	H	-0.364473	-0.946162	-3.687319
H	5.311314	0.399672	-2.328749	C	1.762357	-0.615153	-3.676721
C	0.935924	2.883145	-3.376599	H	1.930546	-1.166905	-4.612839
H	1.101866	1.933205	-3.920637	C	2.869438	-0.058282	-3.016757
H	1.394567	3.703051	-3.973418	C	2.690773	0.649225	-1.802715
H	-0.155977	3.072547	-3.345228	C	1.370420	0.741192	-1.246134
H	5.506446	-0.940674	2.501059	C	1.316081	1.403450	0.099556
O	0.483452	3.762338	2.690154	C	1.496134	2.808432	0.172487
C	1.119554	3.392587	1.690805	C	1.529885	3.430988	1.441874
O	1.428378	2.202029	1.341898	C	1.561311	2.663134	2.615029
O	1.586197	4.362733	0.785036	H	1.624734	3.169054	3.589212
C	1.306927	5.713243	1.149677	C	1.475438	1.268537	2.533238
H	0.224910	5.864648	1.343084	H	1.514720	0.677859	3.458122
H	1.865635	6.008658	2.063876	C	1.305805	0.628608	1.288914
H	1.632858	6.342812	0.297974	C	2.907107	-1.541080	0.559995
				C	3.992927	-0.981158	1.269007
IM3C				H	3.800403	-0.343924	2.146006
Ni	-1.673807	-1.461611	0.246751	C	5.311920	-1.231090	0.863016
P	-1.463273	0.091606	-1.245526	H	6.150597	-0.794458	1.428304
P	1.144995	-1.205904	1.076242	C	5.563069	-2.029871	-0.269010
C	-2.495830	-0.198829	-2.752902	H	6.598683	-2.220481	-0.592098
C	-3.454935	-1.225751	-2.765293	C	4.489113	-2.576108	-0.989608

H	4.675716	-3.188839	-1.884516	H	-1.283459	4.126575	2.385560
C	3.167280	-2.335043	-0.573701	O	-3.722828	-3.624330	-0.816435
H	2.330624	-2.754568	-1.147376	C	-2.660064	-4.140280	-1.130751
C	1.186097	-1.848267	2.803875	O	-2.173179	-5.191150	-1.494173
C	0.276784	-1.384508	3.786428	O	-1.458575	-2.940226	-1.020013
H	-0.375230	-0.527216	3.575741	C	-0.147887	-3.399758	-1.288043
C	0.186235	-2.021781	5.034621	H	-0.206107	-4.266095	-1.977227
H	-0.526135	-1.641845	5.783735	H	0.434952	-2.584279	-1.761407
C	0.988187	-3.139180	5.323334	H	0.380935	-3.724147	-0.361000
H	0.909844	-3.641585	6.300050				
C	1.893410	-3.608924	4.355012	TS2A			
H	2.529674	-4.481962	4.569877	Ni	1.728687	-0.533647	0.070912
C	1.993981	-2.969667	3.109025	P	0.339745	0.269968	1.683587
H	2.703229	-3.351659	2.359055	P	0.240997	-1.186060	-1.390513
O	1.598984	3.489622	-1.003861	C	0.717588	-0.322360	3.392189
C	2.725246	4.353764	-1.211722	C	1.168848	-1.649662	3.559455
H	2.993072	4.267851	-2.283080	H	1.380199	-2.255293	2.659695
H	3.588434	4.034760	-0.593303	C	1.399075	-2.153513	4.849767
H	2.474045	5.407130	-0.974380	H	1.760375	-3.187011	4.972307
O	3.635636	1.233469	-1.029923	C	1.188873	-1.340989	5.978351
C	4.992163	1.466962	-1.408625	H	1.375310	-1.737498	6.989115
H	5.401293	2.111864	-0.607549	C	0.748125	-0.015853	5.812322
H	5.061653	1.994952	-2.380695	H	0.585747	0.627627	6.691613
H	5.571276	0.525024	-1.446849	C	0.511230	0.494285	4.524728
Cl	1.465310	5.179261	1.565176	H	0.158863	1.529293	4.400708
Cl	4.438622	-0.365392	-3.747383	C	0.344031	2.086435	1.939968
C	-2.432923	-2.984572	1.766080	C	-0.816209	2.879298	1.874718
H	-3.394913	-3.336657	1.344715	H	-1.796047	2.418665	1.685378
C	-2.383724	-1.658556	2.093818	C	-0.719943	4.273852	2.027541
C	-2.216899	-0.406732	1.787394	H	-1.629562	4.889988	1.950141
C	-2.490602	0.907992	2.337364	C	0.525479	4.875732	2.272355
C	-1.655966	2.018165	2.077908	H	0.598179	5.968576	2.387201
H	-0.788957	1.884364	1.427392	C	1.683152	4.080125	2.363568
C	-1.948843	3.279396	2.610250	H	2.662982	4.546719	2.547870
C	-3.092532	3.459238	3.406953	C	1.597280	2.693441	2.184796
H	-3.331676	4.452864	3.817392	H	2.504181	2.069198	2.221518
C	-3.937649	2.364271	3.671673	C	-1.451665	-0.200612	1.535672
H	-4.837609	2.498652	4.292460	C	-2.056830	-0.911734	2.595417
C	-3.641628	1.099307	3.145612	H	-1.524386	-1.043892	3.545641
H	-4.304326	0.241867	3.339753	C	-3.314933	-1.492429	2.439769
C	-1.457623	-4.063347	2.142175	H	-3.767165	-2.076006	3.254710
H	-1.311025	-4.746134	1.279751	C	-4.008438	-1.386444	1.224305
H	-1.877705	-4.681913	2.965823	C	-3.467969	-0.621681	0.163208
H	-0.481318	-3.665434	2.466869	C	-2.174490	-0.029665	0.330395

C	-1.701492	0.771263	-0.847867	C	3.335611	-0.042239	-0.938299
C	-2.352678	2.015954	-1.064043	C	2.498593	0.963836	-0.633171
C	-2.039543	2.776105	-2.214793	C	2.393060	2.389486	-0.798609
C	-1.174895	2.265563	-3.193010	C	1.130365	3.029048	-0.862250
H	-0.962341	2.863177	-4.090931	H	0.230000	2.418654	-0.753969
C	-0.554121	1.027334	-2.992860	C	1.035498	4.410370	-1.055510
H	0.128173	0.645496	-3.763349	C	2.203663	5.189064	-1.148920
C	-0.775267	0.288204	-1.812635	H	2.131621	6.280539	-1.277608
C	-1.014203	-2.456525	-0.975303	C	3.468157	4.570813	-1.074289
C	-2.072995	-2.742291	-1.864005	H	4.383560	5.179676	-1.144059
H	-2.137706	-2.215812	-2.828645	C	3.567727	3.182127	-0.923474
C	-3.051267	-3.680841	-1.502546	H	4.550799	2.689871	-0.867569
H	-3.880141	-3.902051	-2.193092	C	5.042033	-1.821166	-1.643419
C	-2.980636	-4.327375	-0.255014	H	6.143176	-1.752775	-1.770303
H	-3.759352	-5.049713	0.033621	H	4.665342	-2.435880	-2.497047
C	-1.926909	-4.039992	0.629619	H	4.824303	-2.375417	-0.712046
H	-1.877741	-4.534777	1.611656	H	0.042309	4.880246	-1.116133
C	-0.939708	-3.109021	0.270930	O	3.788259	-0.620276	2.174546
H	-0.115102	-2.854003	0.954692	C	3.998470	-1.768754	1.945886
C	1.049224	-1.792556	-2.910612	O	4.568763	-2.814066	1.947086
C	1.978320	-0.964773	-3.590878	O	2.218106	-2.271877	0.851052
H	2.115157	0.080712	-3.285653	C	2.387249	-3.405830	0.046998
C	2.746432	-1.479281	-4.647317	H	3.151220	-4.077520	0.506630
H	3.458727	-0.820980	-5.168694	H	1.443872	-3.999410	-0.053078
C	2.631400	-2.830064	-5.016015	H	2.729187	-3.174146	-0.989042
H	3.247835	-3.235091	-5.833631				
C	1.726968	-3.664077	-4.331650	TS2B			
H	1.632773	-4.724938	-4.611861	Ni	1.324905	0.786577	-0.611677
C	0.942808	-3.153024	-3.287732	P	0.815361	-1.266897	-0.166719
H	0.247447	-3.815532	-2.751743	P	-0.650492	1.644084	-0.389824
O	-3.227914	2.432034	-0.106940	C	1.942267	-2.406489	-1.075203
C	-4.563719	2.796439	-0.479617	C	2.149837	-2.134525	-2.447796
H	-4.685750	3.898315	-0.490254	H	1.619889	-1.295849	-2.926033
H	-5.239775	2.356986	0.281236	C	3.045295	-2.909403	-3.197509
H	-4.825753	2.392150	-1.477991	H	3.194920	-2.688740	-4.265837
O	-4.002848	-0.415755	-1.067699	C	3.767792	-3.946627	-2.579607
C	-5.380683	-0.588470	-1.394556	H	4.486603	-4.542357	-3.163439
H	-5.518473	-0.054765	-2.354918	C	3.591682	-4.197975	-1.210905
H	-6.046213	-0.144044	-0.627223	H	4.179340	-4.982575	-0.710590
H	-5.639487	-1.657141	-1.528570	C	2.680263	-3.434074	-0.460186
Cl	-2.662571	4.405775	-2.391053	H	2.576233	-3.622445	0.616623
Cl	-5.503061	-2.306153	1.097673	C	0.821559	-1.789066	1.591191
C	4.411508	-0.464051	-1.657415	C	1.071166	-0.797535	2.561421
H	4.847075	0.276234	-2.361750	H	1.268266	0.236004	2.239014

C	1.046465	-1.128112	3.925186	C	-0.016077	4.386764	-0.384542
H	1.221479	-0.343598	4.677113	H	0.954726	4.033547	-0.768080
C	0.798516	-2.451934	4.325542	O	-3.322713	-2.169213	2.074967
H	0.779243	-2.710535	5.395476	C	-2.680030	-3.444860	2.140462
C	0.571399	-3.447580	3.357916	H	-2.002788	-3.594601	1.273691
H	0.382691	-4.486889	3.669756	H	-3.488576	-4.199395	2.109542
C	0.568695	-3.116888	1.993155	H	-2.103392	-3.551393	3.081737
H	0.359313	-3.891354	1.239306	O	-4.366723	-0.729065	-0.420370
C	-0.861664	-1.795219	-0.798518	C	-5.535097	-1.431857	0.038369
C	-0.964161	-2.645769	-1.917738	H	-6.273572	-0.648644	0.291795
H	-0.068675	-3.129108	-2.329608	H	-5.283321	-2.015665	0.945480
C	-2.196616	-2.858692	-2.548058	H	-5.957569	-2.090444	-0.746399
H	-2.264532	-3.488087	-3.447231	Cl	-2.917448	-1.231941	4.861665
C	-3.349449	-2.221640	-2.070926	Cl	-4.824292	-2.342535	-3.005461
C	-3.303310	-1.429847	-0.897465	C	2.164503	2.461202	-1.767492
C	-2.050547	-1.230224	-0.261628	H	2.807155	3.445573	-0.537652
C	-2.020166	-0.435698	1.001133	C	2.966563	1.406719	-1.501416
C	-2.554387	-1.040338	2.167753	C	3.276592	0.388075	-0.745799
C	-2.363959	-0.417308	3.418918	C	4.257555	-0.556123	-0.300123
C	-1.743968	0.838389	3.508948	C	4.245252	-1.051743	1.031806
H	-1.613358	1.311117	4.492780	H	3.485756	-0.673326	1.729140
C	-1.304616	1.473145	2.342752	C	5.182413	-2.002065	1.454974
H	-0.834375	2.462351	2.418518	C	6.165876	-2.476040	0.567203
C	-1.434411	0.849612	1.081976	H	6.901679	-3.225207	0.899090
C	-1.731664	1.279984	-1.838568	C	6.203975	-1.978489	-0.749774
C	-3.095079	1.629450	-1.908429	H	6.968321	-2.344476	-1.453985
H	-3.582332	2.142547	-1.068283	C	5.263030	-1.037360	-1.183819
C	-3.846984	1.290943	-3.043385	H	5.273288	-0.671606	-2.221413
H	-4.917452	1.543975	-3.082360	C	1.622636	2.841299	-3.119747
C	-3.243698	0.613386	-4.117525	H	1.407786	1.982308	-3.795563
H	-3.841180	0.339800	-5.000576	H	2.365666	3.491754	-3.634826
C	-1.880628	0.275978	-4.057938	H	0.693834	3.442714	-3.030434
H	-1.403159	-0.258611	-4.893609	H	5.146690	-2.373633	2.491573
C	-1.128029	0.612054	-2.923729	O	1.843378	4.731370	2.437264
H	-0.061799	0.344679	-2.843184	C	1.898729	3.630612	2.010047
C	-0.987739	3.425090	-0.052108	O	1.757800	2.462252	1.855422
C	-2.222157	3.845472	0.497388	O	3.228529	3.990828	0.254313
H	-2.978803	3.105001	0.797944	C	3.420192	5.324499	-0.154465
C	-2.476534	5.210948	0.694381	H	3.076310	6.017114	0.647370
H	-3.438795	5.528842	1.125612	H	4.495095	5.547648	-0.357953
C	-1.502725	6.168569	0.354403	H	2.847369	5.567044	-1.082105
H	-1.702052	7.239178	0.518658				
C	-0.272335	5.752865	-0.178452	TS2C			
H	0.503810	6.492642	-0.426621	Ni	-1.719263	-1.283848	0.465201

P	-1.438398	0.033675	-1.232286	H	6.079655	-0.984152	1.497654
P	1.053815	-1.107609	1.233631	C	5.390368	-2.436163	0.024961
C	-2.540272	-0.402090	-2.650256	H	6.406922	-2.743747	-0.267167
C	-3.593429	-1.310540	-2.449616	C	4.272985	-3.020477	-0.592375
H	-3.697783	-1.814808	-1.480924	H	4.406811	-3.781567	-1.376064
C	-4.506222	-1.567989	-3.487967	C	2.975304	-2.628963	-0.216882
H	-5.326495	-2.283272	-3.319681	H	2.104182	-3.079957	-0.709972
C	-4.368516	-0.921716	-4.727081	C	1.071074	-1.500726	3.035183
H	-5.081005	-1.127672	-5.541546	C	0.208606	-0.840321	3.944863
C	-3.321573	-0.000257	-4.924720	H	-0.386453	0.021468	3.616821
H	-3.216616	0.519624	-5.890101	C	0.091018	-1.285901	5.271553
C	-2.415567	0.267736	-3.888227	H	-0.583631	-0.754213	5.960943
H	-1.611003	1.004641	-4.039382	C	0.817837	-2.404220	5.714277
C	-1.918759	1.806516	-1.160537	H	0.718315	-2.755923	6.753042
C	-1.113552	2.853476	-1.636778	C	1.675715	-3.068686	4.819495
H	-0.129532	2.647638	-2.076188	H	2.253523	-3.944622	5.154485
C	-1.563127	4.182440	-1.543350	C	1.803712	-2.621152	3.494981
H	-0.905217	4.997784	-1.882093	H	2.475025	-3.154211	2.804682
C	-2.835540	4.463587	-1.019289	O	1.854060	3.197952	-1.492636
H	-3.184381	5.505287	-0.942304	C	3.043316	3.932494	-1.814101
C	-3.667354	3.409678	-0.597050	H	3.285262	3.691170	-2.867664
H	-4.667969	3.621453	-0.190286	H	3.887249	3.621918	-1.165469
C	-3.208592	2.087817	-0.657089	H	2.884275	5.024794	-1.710154
H	-3.846852	1.265022	-0.297883	O	3.721156	0.809358	-1.198295
C	0.263506	-0.083832	-1.949089	C	5.080420	0.902992	-1.622981
C	0.418248	-0.949884	-3.056469	H	5.542719	1.634202	-0.932340
H	-0.461690	-1.416710	-3.517736	H	5.160555	1.275319	-2.664031
C	1.685129	-1.248283	-3.556459	H	5.604687	-0.066725	-1.527694
H	1.802753	-1.941868	-4.401546	Cl	1.852127	5.240209	0.808590
C	2.837630	-0.692309	-2.978279	Cl	4.373449	-1.229759	-3.645170
C	2.725514	0.195272	-1.880069	C	-2.586391	-2.529541	2.038016
C	1.422131	0.466692	-1.344851	H	-3.555459	-2.872945	1.627866
C	1.425669	1.314485	-0.106069	C	-2.492013	-1.179435	2.280278
C	1.707247	2.698814	-0.232074	C	-2.218505	0.016581	1.859508
C	1.791015	3.491731	0.935912	C	-2.381362	1.405451	2.240551
C	1.771036	2.898827	2.206537	C	-1.485385	2.408830	1.806400
H	1.874920	3.532232	3.099280	H	-0.658107	2.128441	1.150361
C	1.581217	1.517086	2.323177	C	-1.667729	3.746981	2.175577
H	1.578369	1.062958	3.323016	C	-2.759453	4.113403	2.981028
C	1.360263	0.720245	1.181858	H	-2.911527	5.166975	3.263654
C	2.782639	-1.644501	0.771533	C	-3.663951	3.126889	3.420205
C	3.912533	-1.051181	1.377124	H	-4.523234	3.406810	4.050123
H	3.774782	-0.268393	2.138945	C	-3.478429	1.785769	3.058080
C	5.206913	-1.450369	1.013205	H	-4.187349	1.012028	3.391177

C	-1.709142	-3.615030	2.599289	H	-3.755089	-1.726446	3.457868
H	-1.519231	-4.376124	1.814252	C	-4.034528	-1.132670	1.403299
H	-2.226676	-4.136256	3.434565	C	-3.493112	-0.458272	0.282539
H	-0.742490	-3.233486	2.970558	C	-2.169998	0.083873	0.379331
H	-0.956487	4.506083	1.816525	C	-1.694853	0.785510	-0.860859
O	-4.135579	-3.643458	-0.386755	C	-2.294889	2.041555	-1.145010
C	-3.186622	-4.277028	-0.744447	C	-1.971773	2.713918	-2.346428
O	-2.607112	-5.242280	-1.131391	C	-1.156307	2.103046	-3.309177
O	-1.659800	-2.853532	-0.653779	H	-0.937104	2.632791	-4.247219
C	-0.409922	-3.457705	-0.805680	C	-0.592823	0.849416	-3.044965
H	-0.524057	-4.397990	-1.391342	H	0.050223	0.385634	-3.804212
H	0.300728	-2.799101	-1.356197	C	-0.818376	0.197998	-1.815037
H	0.076186	-3.730287	0.167873	C	-1.166882	-2.475215	-0.804315
				C	-2.259683	-2.757592	-1.652320
				H	-2.322076	-2.285468	-2.644996
IM4A				C	-3.271450	-3.626415	-1.216133
Ni	1.667566	-0.645687	0.077523	H	-4.124367	-3.850224	-1.876115
P	0.385779	0.370981	1.652360	C	-3.200897	-4.203114	0.065528
P	0.136167	-1.294422	-1.322459	H	-4.005832	-4.869044	0.412401
C	0.789295	-0.084449	3.399227	C	-2.111049	-3.920643	0.906744
C	1.255831	-1.389933	3.667776	H	-2.059713	-4.364429	1.912882
H	1.440657	-2.071106	2.814090	C	-1.087829	-3.062282	0.473930
C	1.518044	-1.778087	4.992482	H	-0.223922	-2.814010	1.113506
H	1.888418	-2.795728	5.196162	C	0.886384	-2.035323	-2.811353
C	1.323865	-0.874378	6.052307	C	1.835357	-1.298339	-3.564567
H	1.534545	-1.181797	7.089110	H	2.023002	-0.241458	-3.334229
C	0.865446	0.428067	5.783858	C	2.554560	-1.917211	-4.599382
H	0.714000	1.142609	6.608587	H	3.281876	-1.328383	-5.179816
C	0.597435	0.824200	4.463013	C	2.372966	-3.283431	-4.871368
H	0.233417	1.842414	4.259026	H	2.951476	-3.769928	-5.672149
C	0.463877	2.200801	1.764740	C	1.451057	-4.028423	-4.111364
C	-0.663912	3.033613	1.652145	H	1.305470	-5.100896	-4.315007
H	-1.664931	2.601491	1.515058	C	0.714173	-3.412848	-3.089882
C	-0.509613	4.430805	1.693548	H	0.003743	-4.005234	-2.494836
H	-1.395222	5.075196	1.577522	O	-3.137443	2.557448	-0.206541
C	0.762028	4.998320	1.877353	C	-4.474499	2.911845	-0.586155
H	0.880367	6.092873	1.905132	H	-4.572958	4.008570	-0.716490
C	1.887500	4.164867	2.019906	H	-5.139485	2.574388	0.233948
H	2.887688	4.603515	2.157744	H	-4.769943	2.403973	-1.526233
C	1.743377	2.773369	1.950277	O	-4.052206	-0.281985	-0.942016
H	2.624907	2.117672	2.028672	C	-5.409635	-0.560925	-1.277302
C	-1.421594	-0.043589	1.574498	H	-5.544476	-0.138477	-2.291701
C	-2.018654	-0.675701	2.687214	H	-6.117712	-0.073310	-0.577612
H	-1.461337	-0.779789	3.626737	H	-5.609983	-1.649926	-1.303173
C	-3.303489	-1.208953	2.599121				

Cl	-2.525117	4.356986	-2.608423	H	2.379119	-3.729608	0.748852
Cl	-5.587135	-1.963278	1.395851	C	0.732578	-1.753184	1.647520
C	4.314112	-0.842433	-1.728360	C	1.043337	-0.724257	2.559643
H	4.725225	-0.185742	-2.524676	H	1.291070	0.277761	2.177217
C	3.296496	-0.320590	-0.989304	C	1.015758	-0.977067	3.939665
C	2.518772	0.747432	-0.740535	H	1.239687	-0.162609	4.645288
C	2.499405	2.164461	-0.997071	C	0.702977	-2.262155	4.414220
C	1.275219	2.870984	-1.101230	H	0.680931	-2.460296	5.496915
H	0.341440	2.324669	-0.942430	C	0.415254	-3.296415	3.504994
C	1.258464	4.237718	-1.395737	H	0.177038	-4.305773	3.875730
C	2.468426	4.938575	-1.552181	C	0.416619	-3.042155	2.123884
H	2.458294	6.019913	-1.761229	H	0.161822	-3.845208	1.415426
C	3.695508	4.254511	-1.437535	C	-0.963693	-1.790937	-0.742018
H	4.644017	4.802146	-1.556645	C	-1.109753	-2.672706	-1.832061
C	3.716011	2.877062	-1.184795	H	-0.239785	-3.213098	-2.227355
H	4.669491	2.333326	-1.099226	C	-2.352143	-2.846195	-2.454863
C	4.902353	-2.215385	-1.632872	H	-2.452155	-3.501338	-3.332378
H	6.001408	-2.194346	-1.794690	C	-3.471836	-2.138830	-1.998399
H	4.481885	-2.876895	-2.429200	C	-3.385015	-1.311849	-0.851847
H	4.693344	-2.692631	-0.657644	C	-2.122529	-1.150495	-0.224556
H	0.293300	4.758769	-1.485719	C	-2.050863	-0.313746	1.008795
O	3.914353	-0.448036	2.198005	C	-2.609427	-0.850342	2.197140
C	4.205815	-1.582798	2.078980	C	-2.388896	-0.190955	3.424552
O	4.650555	-2.673468	2.036359	C	-1.712178	1.037511	3.468065
O	1.980912	-2.336142	0.992945	H	-1.557395	1.539041	4.433984
C	2.182871	-3.509974	0.266799	C	-1.246044	1.607714	2.279223
H	2.908843	-4.172835	0.801393	H	-0.724839	2.573097	2.317920
H	1.241808	-4.108579	0.132642	C	-1.405852	0.944919	1.042315
H	2.590356	-3.345825	-0.758971	C	-1.683976	1.291543	-1.889942
				C	-3.033018	1.691819	-1.967577
IM4B				H	-3.498581	2.246128	-1.141694
Ni	1.344278	0.684232	-0.662875	C	-3.801703	1.349153	-3.089979
P	0.739236	-1.322186	-0.134017	H	-4.861595	1.642578	-3.133654
P	-0.582060	1.648436	-0.454630	C	-3.229919	0.614980	-4.143905
C	1.805201	-2.554288	-0.992417	H	-3.841200	0.337558	-5.016247
C	2.024749	-2.349213	-2.374705	C	-1.881259	0.225461	-4.076931
H	1.536309	-1.505692	-2.887200	H	-1.428376	-0.353508	-4.896574
C	2.881811	-3.196114	-3.090472	C	-1.111765	0.566465	-2.955550
H	3.042091	-3.026584	-4.166551	H	-0.056294	0.260051	-2.870708
C	3.554067	-4.240377	-2.429130	C	-0.815321	3.453763	-0.161144
H	4.244042	-4.892772	-2.986576	C	-2.037831	3.960782	0.339522
C	3.365817	-4.427400	-1.051864	H	-2.854107	3.275771	0.614156
H	3.915138	-5.218306	-0.518993	C	-2.203581	5.340966	0.527764
C	2.492182	-3.590494	-0.334536	H	-3.157735	5.726554	0.920056

C	-1.150744	6.226784	0.231015	H	3.109053	5.429274	-1.219716
H	-1.280167	7.308951	0.389597				
C	0.068609	5.724226	-0.250093	IM4C			
H	0.905813	6.406765	-0.461378	Ni	-1.324720	-0.927721	1.010302
C	0.235723	4.343164	-0.450377	P	-1.387989	-0.396662	-1.083513
H	1.194924	3.922901	-0.795412	P	0.986896	-0.378327	1.585604
O	-3.427994	-1.946247	2.147381	C	-2.696017	-1.364722	-1.944564
C	-2.842058	-3.246673	2.248144	C	-3.823811	-1.744188	-1.191159
H	-2.174538	-3.450872	1.384975	H	-3.817110	-1.573519	-0.104258
H	-3.683222	-3.965265	2.239779	C	-4.927867	-2.339364	-1.822699
H	-2.268679	-3.351755	3.191603	H	-5.803918	-2.634986	-1.224309
O	-4.413816	-0.547300	-0.397210	C	-4.906077	-2.569413	-3.209416
C	-5.610111	-1.181104	0.089463	H	-5.766910	-3.045902	-3.704204
H	-6.313004	-0.357722	0.315230	C	-3.786080	-2.180179	-3.965964
H	-5.380704	-1.741696	1.016921	H	-3.770462	-2.346001	-5.054754
H	-6.063671	-1.849086	-0.669647	C	-2.690050	-1.563590	-3.340360
Cl	-2.975257	-0.926709	4.896329	H	-1.832459	-1.227250	-3.943707
Cl	-4.953531	-2.219272	-2.926250	C	-1.838004	1.230204	-1.817505
C	2.254076	2.281909	-1.864758	C	-1.032450	1.929488	-2.732311
H	3.021862	3.277687	-0.644485	H	-0.081738	1.504481	-3.077531
C	3.006624	1.201021	-1.574994	C	-1.442193	3.184699	-3.216046
C	3.272636	0.189301	-0.789586	H	-0.783439	3.737180	-3.903994
C	4.213625	-0.782045	-0.318914	C	-2.678379	3.725173	-2.824387
C	4.186534	-1.238259	1.027425	H	-2.996681	4.709703	-3.201786
H	3.445818	-0.809119	1.715503	C	-3.515117	2.998349	-1.956848
C	5.085665	-2.212818	1.476684	H	-4.489870	3.409079	-1.651917
C	6.046010	-2.753127	0.601536	C	-3.095124	1.762365	-1.449550
H	6.752062	-3.521271	0.954012	H	-3.741963	1.209359	-0.751058
C	6.099404	-2.296514	-0.729819	C	0.237095	-0.923702	-1.755911
H	6.845764	-2.714034	-1.424678	C	0.326666	-2.208703	-2.333791
C	5.196232	-1.331157	-1.189719	H	-0.581981	-2.798060	-2.511394
H	5.218494	-0.997078	-2.237815	C	1.574258	-2.769262	-2.611031
C	1.718037	2.678328	-3.212246	H	1.650260	-3.785424	-3.024383
H	1.444502	1.827448	-3.877494	C	2.759724	-2.067102	-2.335332
H	2.490512	3.280005	-3.743014	C	2.707164	-0.761793	-1.786407
H	0.827475	3.334300	-3.116444	C	1.427704	-0.212115	-1.456018
H	5.038323	-2.551305	2.524155	C	1.461039	1.110450	-0.744646
O	2.242582	4.863889	2.336192	C	1.778039	2.271513	-1.495151
C	2.117476	3.732901	2.028706	C	1.841722	3.521888	-0.838127
O	1.853784	2.584364	1.932320	C	1.769369	3.598960	0.560308
O	3.473787	3.830986	0.103947	H	1.862112	4.577368	1.053537
C	3.808197	5.095931	-0.413522	C	1.548009	2.435829	1.306178
H	3.760183	5.850606	0.402768	H	1.502577	2.506027	2.401126
H	4.841158	5.124787	-0.840389	C	1.340810	1.196289	0.667825

C	2.722819	-1.073551	1.443940	C	-3.773105	4.068440	2.193940
C	3.835055	-0.233724	1.680241	H	-4.628733	4.535346	2.707335
H	3.676134	0.820213	1.954555	C	-3.553531	2.691190	2.328586
C	5.141653	-0.729371	1.566189	H	-4.228079	2.073463	2.941549
H	5.997095	-0.062342	1.758774	C	-1.495296	-2.246742	3.962137
C	5.359448	-2.069469	1.194769	H	-0.909128	-3.123083	3.612562
H	6.385837	-2.456552	1.093765	H	-2.139883	-2.606492	4.794781
C	4.261099	-2.907860	0.948679	H	-0.797694	-1.488031	4.358952
H	4.418080	-3.954374	0.645696	H	-1.136215	4.849001	0.131427
C	2.950975	-2.412830	1.080589	O	-3.913968	-4.099268	0.952384
H	2.095945	-3.068934	0.877870	C	-3.312118	-4.448788	0.001263
C	1.019038	0.116449	3.362545	O	-2.795046	-4.907228	-0.949335
C	0.147658	1.113155	3.866423	O	-1.336198	-2.711426	0.292211
H	-0.457569	1.719569	3.180953	C	-0.299140	-3.575716	0.604267
C	0.040129	1.339119	5.248401	H	-0.611770	-4.636227	0.430424
H	-0.641756	2.123047	5.614055	H	0.603048	-3.419286	-0.042442
C	0.786915	0.569291	6.156357	H	0.046879	-3.513108	1.670804
H	0.695828	0.743416	7.239920				
C	1.655071	-0.424135	5.667295	IM5			
H	2.249636	-1.032520	6.367201	Ni	-1.423651	1.071736	-0.636181
C	1.772476	-0.646834	4.286603	P	-1.034341	-0.710646	0.533467
H	2.451042	-1.431868	3.920554	P	0.717585	1.582856	-0.870880
O	1.962193	2.118270	-2.838382	C	-2.407357	-1.260803	1.624343
C	3.177697	2.597065	-3.428762	C	-2.825074	-0.397439	2.663909
H	3.427853	1.893281	-4.246749	H	-2.284485	0.542853	2.846908
H	4.002303	2.601961	-2.687328	C	-3.949842	-0.714101	3.439165
H	3.052552	3.618265	-3.842412	H	-4.264192	-0.033442	4.245664
O	3.743596	0.046971	-1.456677	C	-4.688226	-1.879939	3.168145
C	5.079975	-0.105341	-1.931198	H	-5.582456	-2.117651	3.765199
H	5.579633	0.853398	-1.692443	C	-4.296978	-2.724690	2.117555
H	5.109893	-0.274168	-3.026820	H	-4.885409	-3.624173	1.880418
H	5.606879	-0.927436	-1.410262	C	-3.162959	-2.417224	1.347085
Cl	1.946135	5.003031	-1.771569	H	-2.881499	-3.070085	0.509115
Cl	4.262088	-2.939807	-2.614640	C	-0.750129	-2.118450	-0.614584
C	-2.341010	-1.714016	2.834695	C	-0.865251	-1.907185	-2.002002
H	-3.083700	-2.419445	2.414308	H	-1.114077	-0.899584	-2.369947
C	-2.506035	-0.381401	2.538493	C	-0.618848	-2.959313	-2.896784
C	-2.217651	0.651556	1.808862	H	-0.693003	-2.782325	-3.980675
C	-2.459302	2.070093	1.668595	C	-0.260981	-4.227429	-2.408683
C	-1.604157	2.874465	0.878687	H	-0.058405	-5.050316	-3.110950
H	-0.779593	2.396634	0.342467	C	-0.141596	-4.440477	-1.023203
C	-1.817686	4.253086	0.757868	H	0.152767	-5.430094	-0.640308
C	-2.905539	4.856943	1.410774	C	-0.380118	-3.389329	-0.125400
H	-3.083990	5.938978	1.309291	H	-0.258496	-3.546227	0.957253

C	0.471512	-0.783042	1.610850	C	5.207535	-1.315275	1.607663
C	0.359185	-0.714320	3.014927	H	5.897388	-0.747327	2.264064
H	-0.625922	-0.782975	3.494167	H	5.745096	-1.624845	0.689124
C	1.488512	-0.530188	3.817774	H	4.857870	-2.219499	2.146763
H	1.394015	-0.427918	4.908520	Cl	3.167018	-3.911377	-2.973636
C	2.756374	-0.428886	3.227177	Cl	4.124021	0.001771	4.233915
C	2.912901	-0.592227	1.832450	C	-2.962537	3.255251	1.538015
C	1.761157	-0.758010	1.019511	H	-2.749426	3.123912	2.620027
C	1.994274	-0.906181	-0.452511	C	-3.168374	2.168357	0.788936
C	2.522568	-2.157222	-0.896278	C	-3.237304	1.130630	-0.005897
C	2.696543	-2.362605	-2.285806	C	-4.331500	0.226348	-0.343869
C	2.412305	-1.331632	-3.199234	C	-4.189585	-0.701820	-1.402111
H	2.557017	-1.525572	-4.271855	H	-3.265957	-0.674155	-1.996319
C	1.916180	-0.105661	-2.757106	C	-5.189233	-1.645974	-1.673813
H	1.665216	0.673218	-3.491619	C	-6.356744	-1.682111	-0.890291
C	1.699807	0.119182	-1.379181	H	-7.138845	-2.431052	-1.092420
C	1.450715	2.185406	0.711214	C	-6.518827	-0.753195	0.155888
C	2.840896	2.372246	0.856854	H	-7.428900	-0.777385	0.776720
H	3.523306	2.109915	0.035301	C	-5.520862	0.191582	0.425864
C	3.360809	2.847615	2.068841	H	-5.632052	0.902134	1.259363
H	4.448776	2.965169	2.187353	C	-2.971104	4.672921	1.017554
C	2.496636	3.151996	3.136969	H	-3.223762	4.697191	-0.060373
H	2.909042	3.514374	4.091391	H	-1.971034	5.144231	1.147917
C	1.110303	2.982634	2.986895	H	-3.698360	5.309150	1.569018
H	0.429212	3.219688	3.819349	H	-5.051295	-2.364780	-2.497240
C	0.585943	2.499816	1.776235	O	-2.067087	2.123390	-2.070749
H	-0.499482	2.355976	1.645693	C	-1.697227	1.602611	-3.302790
C	1.227707	2.938674	-2.002805	H	-0.589280	1.426337	-3.421582
C	2.537766	3.053477	-2.518765	H	-2.192734	0.623904	-3.555489
H	3.279036	2.260376	-2.336097	H	-1.982197	2.311618	-4.121828
C	2.898673	4.181402	-3.272534				
H	3.921259	4.265428	-3.673285	IM6A			
C	1.959418	5.201702	-3.511533	Ni	0.579174	-0.728705	0.173070
H	2.246435	6.086304	-4.101904	P	-0.460270	0.877293	1.146615
C	0.655697	5.087625	-2.998656	P	-1.131069	-1.345516	-1.103169
H	-0.084919	5.879717	-3.192200	C	0.275811	1.536660	2.703591
C	0.285201	3.962657	-2.242861	C	0.522854	0.651423	3.778848
H	-0.746132	3.822222	-1.878618	H	0.205430	-0.397598	3.711076
O	2.727817	-3.053998	0.101643	C	1.215353	1.088125	4.917185
C	3.663580	-4.128988	0.019959	H	1.405933	0.382127	5.740242
H	3.890318	-4.401827	1.069050	C	1.688003	2.410105	4.992784
H	4.598875	-3.820736	-0.490111	H	2.248604	2.746915	5.878750
H	3.235548	-5.006900	-0.502741	C	1.453053	3.293702	3.927492
O	4.105245	-0.506115	1.182133	H	1.829545	4.327471	3.970993

C	0.753635	2.860354	2.788866	H	1.628951	-1.966416	-5.160781
H	0.603619	3.554822	1.950467	C	0.208553	-3.604880	-4.937180
C	-0.605100	2.351718	0.062040	H	0.543271	-4.126387	-5.847876
C	0.107800	2.365911	-1.153443	C	-0.811347	-4.157634	-4.144817
H	0.735012	1.501734	-1.431105	H	-1.277133	-5.114313	-4.429110
C	0.004418	3.477556	-2.005591	C	-1.239653	-3.495487	-2.980418
H	0.553970	3.480940	-2.959461	H	-2.030606	-3.939931	-2.358588
C	-0.802468	4.570356	-1.646905	O	-4.302270	2.647435	-0.331581
H	-0.892206	5.434294	-2.323251	C	-5.550962	3.280136	-0.625258
C	-1.511193	4.555614	-0.431285	H	-6.157928	3.204681	0.298562
H	-2.157344	5.403916	-0.157983	H	-6.080729	2.767943	-1.454302
C	-1.416211	3.448529	0.423740	H	-5.415502	4.347971	-0.888607
H	-1.993921	3.420513	1.360109	O	-5.336458	-0.267853	-0.184405
C	-2.212049	0.462394	1.580869	C	-6.731995	0.016763	-0.052893
C	-2.539687	0.082485	2.899182	H	-7.052037	0.434631	-1.027712
H	-1.807652	0.197634	3.708031	H	-6.920958	0.763442	0.745279
C	-3.790204	-0.464800	3.194616	H	-7.316638	-0.899433	0.162729
H	-4.029076	-0.803991	4.212923	Cl	-3.950845	3.991554	-3.155456
C	-4.747318	-0.626606	2.181693	Cl	-6.222607	-1.487927	2.579426
C	-4.485335	-0.167939	0.869590	C	1.453719	-2.855284	2.932861
C	-3.197133	0.360114	0.567260	H	0.862958	-2.707930	3.863154
C	-2.968636	0.780330	-0.851921	C	1.810058	-1.772000	2.242479
C	-3.603582	1.977050	-1.285326	C	2.005983	-0.697613	1.509428
C	-3.386135	2.421732	-2.611015	C	3.134260	0.242214	1.547680
C	-2.637810	1.646885	-3.510543	C	3.064046	1.500571	0.906021
H	-2.501088	2.009737	-4.539508	H	2.155440	1.762402	0.348897
C	-2.040799	0.456773	-3.086569	C	4.139362	2.398589	0.949527
H	-1.442138	-0.129276	-3.797314	C	5.325560	2.050805	1.616626
C	-2.172132	0.030829	-1.749383	H	6.180381	2.745115	1.635902
C	-2.298690	-2.419445	-0.184402	C	5.420033	0.794546	2.246626
C	-3.572202	-2.747111	-0.696773	H	6.351801	0.502990	2.756440
H	-3.892743	-2.345663	-1.670042	C	4.338819	-0.094361	2.218125
C	-4.445769	-3.542311	0.059704	H	4.414438	-1.081710	2.700241
H	-5.445542	-3.782754	-0.333447	C	1.778761	-4.278559	2.549720
C	-4.056095	-4.007188	1.328749	H	0.843628	-4.857564	2.377614
H	-4.751129	-4.615630	1.927549	H	2.330225	-4.799898	3.363392
C	-2.788597	-3.679935	1.840308	H	2.387961	-4.303307	1.626549
H	-2.485817	-4.032794	2.838382	H	4.051950	3.371943	0.441058
C	-1.907430	-2.889219	1.086251	O	1.706999	-1.998981	-0.903718
H	-0.917698	-2.608520	1.486088	O	3.955658	-3.475059	0.153655
C	-0.647065	-2.273947	-2.606847	O	2.664522	0.408125	-2.047592
C	0.402288	-1.734094	-3.387620	O	8.067545	1.462290	-1.214147
H	0.914688	-0.816659	-3.059341	N	2.986982	-1.644180	-0.971213
C	0.813345	-2.392827	-4.555835	C	4.058458	-2.390170	-0.399715

C	3.403529	-0.421573	-1.513850	C	-3.644220	-0.448176	3.263429
C	4.875290	-0.356495	-1.261789	H	-3.839189	-0.781856	4.292841
C	5.763136	0.684955	-1.510845	C	-4.642649	-0.617769	2.292480
H	5.405265	1.607986	-1.984711	C	-4.436630	-0.168091	0.967372
C	7.105457	0.510049	-1.081101	C	-3.163354	0.360193	0.607689
C	7.512860	-0.696980	-0.461644	C	-2.991876	0.765490	-0.823616
H	8.564726	-0.783082	-0.150989	C	-3.646997	1.955024	-1.246332
C	6.595276	-1.734650	-0.224440	C	-3.478903	2.386437	-2.583584
H	6.905560	-2.661103	0.282125	C	-2.760794	1.604719	-3.501539
C	5.268344	-1.546608	-0.620070	H	-2.662404	1.957468	-4.538360
C	7.703069	2.711466	-1.790466	C	-2.143818	0.421627	-3.086848
H	6.904504	3.214379	-1.201692	H	-1.568045	-0.169533	-3.812118
H	7.357283	2.594070	-2.841438	C	-2.224512	0.010015	-1.741171
H	8.614591	3.337203	-1.777159	C	-2.284381	-2.427300	-0.154298
				C	-3.579595	-2.754459	-0.609200
				H	-3.941697	-2.356719	-1.569301
IM6B				C	-4.421214	-3.543461	0.188751
Ni	0.598148	-0.733155	0.092697	H	-5.437490	-3.783816	-0.159494
P	-0.405249	0.888166	1.074428	C	-3.978522	-4.001389	1.442834
P	-1.154385	-1.356266	-1.121704	H	-4.648539	-4.604085	2.074973
C	0.376861	1.576733	2.595501	C	-2.689448	-3.674526	1.897381
C	0.683738	0.700827	3.661886	H	-2.346159	-4.021831	2.884135
H	0.398969	-0.357503	3.598316	C	-1.839402	-2.891454	1.100852
C	1.406716	1.154831	4.773914	H	-0.831189	-2.612455	1.451600
H	1.645594	0.454545	5.589321	C	-0.720958	-2.288253	-2.638512
C	1.849476	2.487953	4.830745	C	0.312682	-1.758659	-3.446740
H	2.434989	2.839883	5.694421	H	0.850796	-0.853047	-3.127057
C	1.554041	3.363643	3.773745	C	0.676968	-2.414856	-4.631830
H	1.907970	4.405863	3.802094	H	1.480884	-1.997198	-5.258102
C	0.824492	2.911874	2.661630	C	0.040978	-3.613976	-5.003342
H	0.629071	3.600583	1.827900	H	0.339153	-4.133514	-5.927767
C	-0.588064	2.342422	-0.031696	C	-0.962980	-4.156828	-4.184219
C	0.091247	2.336473	-1.266596	H	-1.452510	-5.103785	-4.461062
H	0.711797	1.467642	-1.545847	C	-1.344596	-3.496978	-3.002400
C	-0.035904	3.433431	-2.134376	H	-2.123158	-3.933525	-2.359643
H	0.487549	3.421192	-3.102723	O	-4.311916	2.634156	-0.274686
C	-0.833240	4.532081	-1.772043	C	-5.571152	3.262838	-0.529854
H	-0.941515	5.384696	-2.459973	H	-6.144798	3.196132	0.415635
C	-1.508976	4.537505	-0.537782	H	-6.129388	2.741891	-1.334362
H	-2.148313	5.389965	-0.261522	H	-5.446543	4.328072	-0.808467
C	-1.390185	3.444817	0.332776	O	-5.331495	-0.278373	-0.048748
H	-1.943853	3.431763	1.283849	C	-6.719405	0.011908	0.139636
C	-2.138056	0.473489	1.579171	H	-7.079461	0.424816	-0.823293
C	-2.408807	0.100413	2.912457	H	-6.871962	0.764096	0.940436
H	-1.643274	0.221751	3.688897				

H	-7.297178	-0.900941	0.385796	Ni	-0.371454	1.425865	1.023718
Cl	-4.065755	3.949877	-3.122923	P	-1.025599	1.122063	-1.011373
Cl	-6.098646	-1.478808	2.756453	P	-1.042365	-0.487501	1.879818
C	1.817113	-3.009934	2.600683	C	-1.463237	2.650623	-1.939227
C	1.989424	-1.814618	2.039497	C	-2.286071	3.586805	-1.271392
C	2.080399	-0.685576	1.369211	H	-2.620754	3.373749	-0.243462
C	3.164249	0.306935	1.422942	C	-2.646501	4.789832	-1.892207
C	3.067432	1.545039	0.748217	H	-3.280933	5.512241	-1.356849
H	2.165314	1.760444	0.161825	C	-2.162398	5.088769	-3.178323
C	4.111132	2.480123	0.790571	H	-2.427226	6.043498	-3.658758
C	5.291133	2.192053	1.495380	C	-1.319245	4.178320	-3.835349
H	6.119221	2.917956	1.521000	H	-0.920130	4.416422	-4.833970
C	5.413078	0.955774	2.160318	C	-0.970056	2.962941	-3.220936
H	6.340698	0.710422	2.701121	H	-0.296821	2.263956	-3.737998
C	4.364072	0.030253	2.129376	C	0.172009	0.221002	-2.077636
H	4.461100	-0.940700	2.640305	C	1.425898	-0.092707	-1.520625
H	4.002273	3.436363	0.254494	H	1.612726	0.212141	-0.482276
O	1.667051	-2.030775	-1.010707	C	2.364050	-0.827590	-2.261045
O	3.842033	-3.574581	0.083473	H	3.335218	-1.088908	-1.813968
O	2.708351	0.339187	-2.149516	C	2.052149	-1.245347	-3.566024
O	8.082005	1.313758	-1.077640	H	2.783956	-1.827718	-4.146428
N	2.959379	-1.725669	-1.080163	C	0.795752	-0.941962	-4.122584
C	3.992618	-2.491022	-0.461084	H	0.546331	-1.284293	-5.139423
C	3.415113	-0.508067	-1.599420	C	-0.150953	-0.220072	-3.378685
C	4.876485	-0.468935	-1.286364	H	-1.150312	-0.023313	-3.796267
C	5.787795	0.561397	-1.490973	C	-2.540127	0.074582	-1.202925
H	5.463441	1.489025	-1.979398	C	-3.776678	0.642583	-1.569285
C	7.104855	0.371302	-0.994511	H	-3.831899	1.701789	-1.856579
C	7.467439	-0.840997	-0.358139	C	-4.949058	-0.120237	-1.546776
H	8.501121	-0.938991	0.005484	H	-5.921803	0.329880	-1.792621
C	6.527439	-1.868982	-0.169444	C	-4.893193	-1.470253	-1.172370
H	6.802402	-2.799537	0.349943	C	-3.657557	-2.084623	-0.865866
C	5.223313	-1.665499	-0.627997	C	-2.474775	-1.300577	-0.861266
C	7.761588	2.563445	-1.678909	C	-1.192809	-2.000747	-0.516120
H	6.937171	3.076418	-1.136657	C	-0.668627	-2.874719	-1.520031
H	7.472144	2.443161	-2.746469	C	0.572281	-3.512354	-1.280823
H	8.677292	3.180343	-1.619259	C	1.233540	-3.332855	-0.054639
C	1.081998	-3.294114	3.887368	H	2.200360	-3.831525	0.104372
H	0.653131	-2.375488	4.335451	C	0.699472	-2.509558	0.936262
H	0.251492	-4.015326	3.717612	H	1.267138	-2.376102	1.863987
H	1.750703	-3.762221	4.643405	C	-0.512913	-1.825826	0.715477
H	2.258287	-3.870901	2.059423	C	-2.867370	-0.691419	1.991986
				C	-3.453752	-1.952338	2.233503
TS3A				H	-2.814795	-2.844110	2.322579

C	-4.847205	-2.070872	2.327398	H	-1.136949	5.429162	2.064818
H	-5.302289	-3.059384	2.492474	C	2.943840	2.719268	3.317026
C	-5.662779	-0.933172	2.183391	H	3.701303	1.918468	3.451843
H	-6.757754	-1.031228	2.241807	H	2.991998	3.363024	4.224988
C	-5.081571	0.323754	1.945902	H	3.209049	3.326830	2.432151
H	-5.718580	1.213239	1.820970	H	1.119630	6.008905	-2.373065
C	-3.685251	0.445379	1.852284	O	2.024441	0.516230	1.745082
H	-3.209388	1.418367	1.645478	O	3.298376	2.337657	-0.039697
C	-0.522309	-0.988773	3.590115	O	3.703085	-1.782887	2.078973
C	0.845076	-1.153063	3.915101	O	8.175577	-1.919679	-1.234013
H	1.616823	-0.975470	3.151826	N	3.211522	0.341919	1.204207
C	1.231311	-1.481211	5.224674	C	3.781334	1.254917	0.259258
H	2.301608	-1.619929	5.445344	C	3.978515	-0.837915	1.346431
C	0.270982	-1.615698	6.241934	C	5.131449	-0.669190	0.405259
H	0.578035	-1.865634	7.269900	C	6.167044	-1.558048	0.122949
C	-1.085332	-1.414135	5.936693	H	6.217497	-2.524454	0.642360
H	-1.850149	-1.498900	6.725037	C	7.120437	-1.157270	-0.852845
C	-1.481062	-1.106996	4.623783	C	7.004808	0.101572	-1.497326
H	-2.548184	-0.957326	4.409438	H	7.766446	0.363087	-2.246842
O	-1.438188	-2.931093	-2.639182	C	5.951711	0.979609	-1.192911
C	-1.315762	-3.923974	-3.653210	H	5.859306	1.951754	-1.700109
H	-2.240820	-3.837972	-4.255996	C	5.013038	0.581057	-0.234950
H	-1.248794	-4.945323	-3.226338	C	8.343621	-3.199554	-0.630393
H	-0.437093	-3.741270	-4.303039	H	7.474412	-3.863342	-0.832558
O	-3.533964	-3.384790	-0.482927	H	8.489515	-3.116771	0.469007
C	-4.032528	-4.420051	-1.336979	H	9.250246	-3.638795	-1.085309
H	-3.303415	-5.253549	-1.286628				
H	-4.111774	-4.071076	-2.386805	TS3B			
H	-5.026081	-4.778500	-0.998430	Ni	-0.369133	1.370285	1.117478
Cl	1.420064	-4.489367	-2.478381	P	-1.105191	1.234822	-0.900556
Cl	-6.391643	-2.365139	-1.005392	P	-0.897729	-0.658578	1.781565
C	1.569978	2.133645	3.182884	C	-1.648360	2.812950	-1.678192
H	1.248897	1.411992	3.954257	C	-2.434409	3.680087	-0.886471
C	0.619946	2.641597	2.319102	H	-2.674591	3.393361	0.149951
C	0.206889	3.216660	1.214241	C	-2.875538	4.907638	-1.398277
C	0.096384	4.494407	0.536571	H	-3.477335	5.578573	-0.766831
C	0.727114	4.666752	-0.720211	C	-2.514820	5.295349	-2.700994
H	1.301982	3.829083	-1.140216	H	-2.843162	6.268988	-3.096869
C	0.625143	5.888210	-1.396729	C	-1.715770	4.448178	-3.485759
C	-0.116553	6.949813	-0.845756	H	-1.415977	4.754640	-4.500324
H	-0.205924	7.903628	-1.388875	C	-1.282850	3.210984	-2.978563
C	-0.747193	6.783694	0.399698	H	-0.642462	2.562739	-3.594000
H	-1.328904	7.610100	0.838738	C	0.136332	0.521549	-2.051381
C	-0.640895	5.567412	1.091770	C	1.439733	0.330459	-1.553985

H	1.641846	0.617371	-0.511660	H	-1.624028	-1.900160	6.564390
C	2.423797	-0.253259	-2.367230	C	-1.271438	-1.414932	4.480624
H	3.438755	-0.413939	-1.972754	H	-2.317633	-1.120134	4.320001
C	2.106635	-0.644369	-3.678865	O	-1.413999	-2.661877	-2.982824
H	2.874620	-1.113287	-4.312977	C	-1.680058	-3.886278	-3.670795
C	0.802065	-0.464223	-4.174120	H	-2.720157	-3.815825	-4.047653
H	0.547037	-0.799435	-5.191362	H	-1.597781	-4.759064	-2.990628
C	-0.186575	0.111966	-3.362746	H	-0.989643	-4.031255	-4.526218
H	-1.219298	0.205006	-3.731589	O	-3.382952	-3.392354	-0.735295
C	-2.578449	0.146205	-1.164877	C	-4.174643	-4.443183	-1.290767
C	-3.844258	0.707641	-1.428606	H	-3.504572	-5.323011	-1.352992
H	-3.944873	1.786033	-1.612066	H	-4.539512	-4.187695	-2.306543
C	-4.986581	-0.095716	-1.426554	H	-5.041680	-4.688143	-0.645859
H	-5.982864	0.341281	-1.587289	Cl	1.385748	-4.005836	-3.179252
C	-4.886428	-1.472980	-1.174133	Cl	-6.391048	-2.366143	-1.004862
C	-3.620572	-2.079397	-0.988069	C	1.719961	2.039272	3.172871
C	-2.462838	-1.249825	-0.961619	C	0.728640	2.558376	2.364501
C	-1.138984	-1.921802	-0.752510	C	0.223588	3.153056	1.315460
C	-0.636845	-2.657812	-1.863477	C	0.078689	4.469847	0.720637
C	0.644861	-3.245195	-1.781222	C	0.621706	4.721996	-0.562308
C	1.385775	-3.165990	-0.593994	H	1.158029	3.912646	-1.078262
H	2.384788	-3.622413	-0.545753	C	0.476108	5.982290	-1.154803
C	0.874069	-2.475261	0.507064	C	-0.217762	7.008286	-0.486792
H	1.499099	-2.413433	1.402973	H	-0.340550	7.994070	-0.962035
C	-0.379628	-1.833498	0.444724	C	-0.757014	6.765876	0.788664
C	-2.712157	-0.950763	1.930068	H	-1.299764	7.564316	1.319652
C	-3.232878	-2.250411	2.108426	C	-0.611299	5.507199	1.391623
H	-2.551794	-3.114953	2.116082	H	-1.039513	5.306944	2.385900
C	-4.613885	-2.437131	2.257614	H	0.899618	6.162887	-2.154974
H	-5.019193	-3.453355	2.381638	O	2.095479	0.387257	1.807575
C	-5.482552	-1.329979	2.232171	O	3.415430	2.411278	0.303226
H	-6.568076	-1.480451	2.335977	O	3.771041	-1.955795	1.858620
C	-4.966252	-0.034936	2.058799	O	8.296331	-1.684034	-1.361907
H	-5.644710	0.831790	2.028142	N	3.283378	0.260365	1.242740
C	-3.582254	0.154893	1.911532	C	3.881221	1.289809	0.447128
H	-3.155936	1.160056	1.756824	C	4.049618	-0.922729	1.253134
C	-0.339252	-1.345152	3.416076	C	5.217948	-0.643207	0.357775
C	1.004728	-1.691329	3.681010	C	6.256230	-1.493556	-0.016726
H	1.786658	-1.526017	2.929404	H	6.292074	-2.520248	0.371708
C	1.383427	-2.168979	4.946303	C	7.233871	-0.972547	-0.908612
H	2.435569	-2.448834	5.114187	C	7.137742	0.361103	-1.382710
C	0.447534	-2.258400	5.989296	H	7.917631	0.715033	-2.073146
H	0.751125	-2.621767	6.983881	C	6.081340	1.198405	-0.986918
C	-0.879046	-1.858898	5.753904	H	6.005319	2.230529	-1.360894

C	5.119920	0.681717	-0.111686	C	-3.495040	-0.715282	0.774025
C	8.448640	-3.032172	-0.926361	C	-3.313975	-1.275436	-0.605093
H	7.585068	-3.661237	-1.235478	C	-4.468550	-1.345431	-1.438312
H	8.566197	-3.093971	0.177838	C	-4.313766	-1.805332	-2.769641
H	9.366642	-3.411501	-1.411420	C	-3.067277	-2.271174	-3.219781
C	1.486792	1.402278	4.503379	H	-2.985808	-2.637735	-4.253504
H	0.469631	0.977461	4.585815	C	-1.950198	-2.245798	-2.381071
H	2.225067	0.602186	4.702558	H	-0.984702	-2.614527	-2.755189
H	1.614787	2.172488	5.299102	C	-2.055526	-1.725100	-1.075439
H	2.745423	2.394360	2.958675	C	-0.916256	-2.132941	1.561219
				C	-1.560884	-3.381193	1.692256
IM7A				H	-1.856077	-3.942952	0.792706
Ni	-0.040205	0.696533	-0.169820	C	-1.872185	-3.878492	2.966406
P	-2.001874	1.556548	-0.040534	H	-2.395738	-4.841913	3.064810
P	-0.535674	-1.384180	-0.072963	C	-1.545402	-3.133252	4.113671
C	-2.044864	3.266434	0.651469	H	-1.807966	-3.517344	5.111347
C	-1.104738	3.565817	1.664103	C	-0.904480	-1.888953	3.986482
H	-0.425619	2.774373	2.020410	H	-0.662373	-1.297280	4.883044
C	-0.996056	4.866540	2.174209	C	-0.589978	-1.388539	2.712980
H	-0.247970	5.087556	2.950809	H	-0.112542	-0.402294	2.591839
C	-1.808721	5.892694	1.660571	C	0.749387	-2.490809	-0.802925
H	-1.705427	6.920906	2.041021	C	1.402004	-2.031000	-1.970970
C	-2.737360	5.605894	0.646337	H	1.099046	-1.067533	-2.413636
H	-3.367787	6.408381	0.231594	C	2.456382	-2.763716	-2.535923
C	-2.859022	4.298288	0.144299	H	2.964629	-2.385110	-3.435668
H	-3.574365	4.088957	-0.664787	C	2.890172	-3.955047	-1.925355
C	-3.049815	1.622604	-1.549128	H	3.732852	-4.519201	-2.354619
C	-2.423624	1.379234	-2.788807	C	2.257181	-4.410634	-0.756945
H	-1.339107	1.180832	-2.807140	H	2.600218	-5.336015	-0.267656
C	-3.182684	1.358865	-3.969509	C	1.188639	-3.685951	-0.198516
H	-2.692499	1.150103	-4.933094	H	0.708088	-4.045074	0.723609
C	-4.568583	1.587455	-3.917653	O	-5.603965	-0.880750	-0.854681
H	-5.166071	1.557930	-4.841682	C	-6.913854	-1.285120	-1.249646
C	-5.195793	1.836012	-2.683474	H	-7.561328	-1.086819	-0.373278
H	-6.283665	2.002542	-2.641417	H	-6.952822	-2.365514	-1.497669
C	-4.441827	1.848260	-1.500108	H	-7.280950	-0.700002	-2.115979
H	-4.939001	1.996894	-0.529365	O	-4.529059	-2.776745	1.307274
C	-3.039783	0.576954	1.143304	C	-5.872552	-3.214995	1.531459
C	-3.237962	1.029531	2.463522	H	-6.166729	-3.803817	0.639625
H	-2.900650	2.034469	2.755535	H	-6.563762	-2.354228	1.642202
C	-3.838684	0.202947	3.419860	H	-5.945544	-3.854457	2.434541
H	-3.959892	0.538137	4.460235	Cl	-5.612025	-1.758679	-3.957023
C	-4.274041	-1.081100	3.060583	Cl	-4.911815	-2.133746	4.310495
C	-4.143595	-1.540870	1.729606	C	3.084294	0.140509	0.008524

H	3.179335	-0.612825	-0.803706	C	-0.456819	3.396918	1.700761
C	1.832841	0.898025	-0.142730	H	0.144967	2.509132	1.952103
C	1.284595	2.071738	-0.308060	C	-0.111473	4.647625	2.230244
C	1.417743	3.512202	-0.328881	H	0.743962	4.730866	2.917856
C	0.487223	4.317693	-1.030462	C	-0.826340	5.795648	1.845906
H	-0.310536	3.820750	-1.602518	H	-0.538851	6.782724	2.240383
C	0.566573	5.714742	-0.976986	C	-1.894276	5.680649	0.941085
C	1.575299	6.336280	-0.217521	H	-2.450590	6.577653	0.625888
H	1.629522	7.435174	-0.163265	C	-2.251562	4.424865	0.419870
C	2.516538	5.547241	0.470921	H	-3.075385	4.351398	-0.305007
H	3.314676	6.029098	1.058470	C	-3.103617	1.892142	-1.234391
C	2.447447	4.147651	0.413271	C	-2.755992	1.643863	-2.577489
H	3.183093	3.521114	0.941034	H	-1.735071	1.295729	-2.805730
C	3.189267	-0.548505	1.369131	C	-3.710978	1.805779	-3.593904
H	4.137054	-1.115287	1.464413	H	-3.440129	1.593888	-4.639907
H	2.352507	-1.267433	1.467137	C	-5.014699	2.220611	-3.272669
H	3.121246	0.195277	2.187247	H	-5.767326	2.334615	-4.067772
H	-0.173048	6.324814	-1.518669	C	-5.364641	2.471436	-1.933362
O	4.175315	1.131053	-0.201496	H	-6.390529	2.782060	-1.680505
O	5.897041	1.645668	2.009226	C	-4.414853	2.304571	-0.914531
O	5.530549	-0.686671	-1.997885	H	-4.698175	2.461921	0.137410
O	10.715658	-2.078178	-0.503836	C	-2.714544	0.664294	1.365490
N	5.410224	0.582232	-0.026893	C	-2.556689	1.012158	2.722916
C	6.230020	0.922246	1.086327	H	-2.027989	1.936066	2.996589
C	6.033251	-0.260723	-0.969316	C	-3.048405	0.182004	3.736438
C	7.395090	-0.509031	-0.386565	H	-2.890600	0.431482	4.795846
C	8.428487	-1.294725	-0.895302	C	-3.735289	-0.996011	3.407366
H	8.295770	-1.829646	-1.845355	C	-3.970048	-1.337897	2.055559
C	9.627573	-1.359046	-0.136957	C	-3.424497	-0.518219	1.032130
C	9.745082	-0.646133	1.086251	C	-3.617116	-0.969518	-0.382920
H	10.694459	-0.730324	1.635645	C	-4.914992	-0.825079	-0.952373
C	8.689952	0.136363	1.576236	C	-5.098252	-1.182992	-2.310935
H	8.785563	0.685832	2.524876	C	-4.042748	-1.746508	-3.046388
C	7.508695	0.199998	0.825478	H	-4.222965	-2.024592	-4.095072
C	10.664955	-2.817624	-1.721716	C	-2.783992	-1.924498	-2.466406
H	10.506805	-2.150313	-2.597062	H	-1.971102	-2.362897	-3.062043
H	9.860878	-3.585518	-1.698567	C	-2.552013	-1.517595	-1.136966
H	11.644934	-3.319404	-1.818726	C	-0.993805	-2.424366	1.129375
				C	-1.824493	-3.556181	1.266508
				H	-2.403702	-3.919157	0.403712
IM7B				C	-1.959157	-4.179687	2.516223
Ni	-0.013958	0.499513	-0.361661	H	-2.626887	-5.048283	2.624753
P	-1.812117	1.607948	0.041574	C	-1.270532	-3.676080	3.634052
P	-0.831667	-1.487609	-0.444120	H	-1.394603	-4.155080	4.617489
C	-1.537579	3.270067	0.797341				

C	-0.442234	-2.548089	3.501420	H	2.944059	-1.915798	-1.404040
H	0.084933	-2.142965	4.379314	H	0.437671	6.106745	-1.602564
C	-0.304207	-1.922056	2.252588	O	4.189861	0.433135	-0.741800
H	0.316403	-1.018269	2.133519	O	5.495135	1.565442	1.530603
C	0.071301	-2.608163	-1.596520	O	6.036366	-1.373049	-2.033355
C	0.630137	-2.010081	-2.748526	O	11.114899	-1.613367	0.233008
H	0.512936	-0.924469	-2.901961	N	5.432951	0.091920	-0.295412
C	1.362202	-2.779728	-3.665012	C	6.049764	0.759994	0.798084
H	1.796660	-2.302080	-4.556928	C	6.309906	-0.741285	-1.027910
C	1.567712	-4.150985	-3.424865	C	7.605534	-0.649949	-0.272036
H	2.159548	-4.752405	-4.132560	C	8.807224	-1.308817	-0.527732
C	1.028889	-4.747080	-2.271741	H	8.887430	-1.991901	-1.384074
H	1.198239	-5.817233	-2.073186	C	9.889060	-1.050577	0.355453
C	0.276563	-3.981748	-1.363085	C	9.729056	-0.156789	1.448524
H	-0.133744	-4.453846	-0.457844	H	10.598357	0.009333	2.101924
O	-5.833360	-0.271155	-0.118295	C	8.508768	0.490748	1.685639
C	-7.236049	-0.508870	-0.230186	H	8.390045	1.181701	2.533792
H	-7.651277	-0.317005	0.778467	C	7.443874	0.236534	0.810631
H	-7.452585	-1.556683	-0.522457	C	11.344924	-2.520463	-0.843070
H	-7.712373	0.176821	-0.958639	H	11.203069	-2.026542	-1.829113
O	-4.626357	-2.460685	1.651200	H	10.675662	-3.406158	-0.778838
C	-5.930394	-2.744666	2.165937	H	12.395556	-2.850219	-0.748643
H	-6.497956	-3.219688	1.341061				
H	-6.451140	-1.815592	2.477408	(S)-3a			
H	-5.885427	-3.439413	3.029002	O	0.463758	-0.028440	-0.304369
Cl	-6.596075	-0.881042	-3.183408	O	-0.857479	2.463000	0.197844
Cl	-4.230560	-2.068593	4.704435	O	-1.540038	-2.085429	-0.497213
C	3.117816	-0.274706	0.014367	O	-6.812045	-0.321095	-0.240374
H	3.357612	-0.131777	1.094901	N	-0.877676	0.135511	-0.099799
C	1.879675	0.488183	-0.252274	C	1.212536	0.002569	0.976152
C	1.452546	1.707534	-0.460208	H	0.970075	0.975097	1.462222
C	1.755083	3.122810	-0.497524	C	2.623018	-0.008421	0.605018
C	0.886544	4.033449	-1.147727	C	3.818549	-0.031631	0.325587
H	0.003045	3.633267	-1.667943	C	5.210554	-0.048839	-0.002531
C	1.131703	5.411423	-1.104981	C	5.877682	1.148437	-0.373253
C	2.253052	5.906459	-0.413416	H	5.308906	2.089722	-0.406087
H	2.440606	6.991168	-0.369404	C	7.241821	1.126800	-0.694297
C	3.135223	5.010166	0.219497	C	7.962051	-0.081095	-0.651145
H	4.019605	5.392835	0.754249	H	9.033676	-0.093690	-0.904243
C	2.897372	3.628638	0.176468	C	7.310269	-1.273025	-0.285019
H	3.586247	2.924759	0.669348	H	7.870777	-2.220308	-0.251443
C	3.103315	-1.758657	-0.321289	C	5.946165	-1.262541	0.036863
H	2.276099	-2.249403	0.228416	H	5.430585	-2.191960	0.321586
H	4.053316	-2.243698	-0.021580	C	0.819339	-1.168281	1.879097

H	-0.255129	-1.109279	2.143041	C	-1.636942	1.540594	-0.450676
H	1.405982	-1.129216	2.818378	C	-1.672624	-0.808787	-0.044571
H	1.014367	-2.129994	1.366907	C	-3.082115	-0.302080	-0.128230
C	-1.475396	1.422602	0.045833	C	-4.272148	-1.016117	0.008880
C	-1.806263	-0.912394	-0.304819	H	-4.245907	-2.097174	0.200743
C	-3.140046	-0.227898	-0.216274	C	-5.483717	-0.285707	-0.114797
C	-4.411006	-0.794604	-0.303293	C	-5.458813	1.113867	-0.361296
H	-4.520917	-1.874790	-0.468527	H	-6.425027	1.632651	-0.447712
C	-5.521489	0.080994	-0.172428	C	-4.248675	1.808567	-0.490816
C	-5.321007	1.471393	0.044294	H	-4.235178	2.892406	-0.680330
H	-6.214741	2.105846	0.138462	C	-3.054064	1.084707	-0.374551
C	-4.032742	2.015296	0.133191	C	-6.812755	-2.242841	0.230725
H	-3.883307	3.092378	0.301668	H	-6.336932	-2.522677	1.195932
C	-2.938193	1.149991	-0.002905	H	-6.347900	-2.831157	-0.590312
C	-7.086389	-1.703362	-0.461878	H	-7.892899	-2.471900	0.276938
H	-6.679610	-2.334958	0.357801	H	8.088297	1.560758	-0.128242
H	-6.668719	-2.049921	-1.432254				
H	-8.187148	-1.799030	-0.483673	(R)-IM1A			
H	7.748671	2.061276	-0.981500	Ni	1.302894	0.478191	-0.608654
				P	0.401917	-1.409363	-0.083505
(R)-3a				P	-0.467763	1.714641	-0.506363
O	0.471683	0.303064	-0.379744	C	1.301768	-2.917062	-0.650424
O	-1.165401	2.644333	-0.655042	C	1.924720	-2.853708	-1.916584
O	-1.249936	-1.937587	0.145031	H	1.828497	-1.933915	-2.516008
O	-6.714013	-0.840758	-0.012219	C	2.699185	-3.924183	-2.384923
N	-0.883264	0.351733	-0.209797	H	3.191926	-3.854229	-3.366768
C	1.177206	0.198650	0.921659	C	2.876903	-5.065825	-1.583624
H	0.799841	-0.726736	1.414083	H	3.505378	-5.897107	-1.939499
C	2.586407	0.024379	0.588601	C	2.265122	-5.134107	-0.321038
C	3.782093	-0.105381	0.340754	H	2.410165	-6.020922	0.315970
C	5.173544	-0.263123	0.049887	C	1.479821	-4.066044	0.144971
C	6.052791	0.850122	0.108577	H	1.027307	-4.118829	1.145849
H	5.649099	1.837372	0.378904	C	0.191981	-1.639973	1.727509
C	7.415713	0.690164	-0.176550	C	0.867239	-0.741188	2.579575
C	7.924024	-0.574719	-0.524769	H	1.489087	0.062130	2.151096
H	8.995266	-0.696037	-0.749074	C	0.714222	-0.847127	3.971652
C	7.060839	-1.684072	-0.586994	H	1.234679	-0.130997	4.626081
H	7.455297	-2.675181	-0.860373	C	-0.110885	-1.845214	4.516665
C	5.696508	-1.535201	-0.302532	H	-0.243799	-1.916264	5.607363
H	5.016429	-2.398806	-0.350440	C	-0.789369	-2.739155	3.667955
C	0.915195	1.424354	1.799192	H	-1.459307	-3.502844	4.092095
H	1.475524	1.328903	2.750372	C	-0.642273	-2.637155	2.276738
H	-0.162805	1.503211	2.042542	H	-1.214156	-3.302371	1.612052
H	1.236306	2.345567	1.276398	C	-1.293281	-1.646842	-0.781720

C	-1.480924	-2.464073	-1.915472	H	-6.425428	0.256911	0.318988
H	-0.659497	-3.093541	-2.285970	H	-6.229372	-1.345261	-0.495932
C	-2.702254	-2.457107	-2.592562	H	-6.362660	0.160660	-1.484377
H	-2.846171	-3.061029	-3.500372	Cl	-3.360543	-0.400703	4.805088
C	-3.764172	-1.653303	-2.145711	Cl	-5.200788	-1.609671	-3.161690
C	-3.630025	-0.876299	-0.969025	C	2.931788	1.405893	-0.935576
C	-2.367680	-0.858130	-0.306245	C	3.166339	0.126651	-0.788264
C	-2.243566	0.001319	0.915288	C	4.125984	-0.953612	-0.767045
C	-2.888053	-0.473908	2.089338	C	4.149909	-1.875988	0.308769
C	-2.746864	0.248325	3.295493	H	3.435178	-1.742013	1.134069
C	-2.051710	1.465532	3.319386	C	5.060564	-2.938771	0.314074
H	-1.962679	2.015625	4.267275	C	5.959556	-3.111646	-0.755635
C	-1.453414	1.949554	2.152061	H	6.663971	-3.958117	-0.755504
H	-0.909995	2.902665	2.192262	C	5.948158	-2.201195	-1.827443
C	-1.513824	1.218277	0.948108	H	6.647518	-2.330898	-2.668981
C	-1.641015	1.567994	-1.916905	C	5.043889	-1.128362	-1.834295
C	-2.949532	2.093663	-1.861796	H	5.017579	-0.421939	-2.678726
H	-3.294976	2.606761	-0.951270	C	3.100280	3.823559	-1.700238
C	-3.818081	1.928307	-2.950867	H	3.178362	3.564890	-2.775628
H	-4.842209	2.330105	-2.900498	H	3.657484	4.764545	-1.520727
C	-3.390365	1.230509	-4.094949	H	2.034504	3.974942	-1.451913
H	-4.080461	1.084812	-4.940025	H	5.060164	-3.650189	1.154512
C	-2.089081	0.702557	-4.151194	O	3.723862	3.159463	0.536406
H	-1.757837	0.142415	-5.039425	C	3.658191	2.252560	1.549394
C	-1.214402	0.874563	-3.066741	O	2.749416	2.240909	2.360339
H	-0.197702	0.448108	-3.082327	O	4.690143	1.396659	1.695980
C	-0.258951	3.536521	-0.296633	C	5.896390	1.523491	0.927969
C	0.619289	3.976540	0.720467	H	6.702187	1.093667	1.551636
H	1.148859	3.250048	1.358027	H	5.817824	0.936755	-0.009207
C	0.877212	5.345253	0.889303	H	6.117650	2.585526	0.704379
H	1.568864	5.667246	1.683287	C	3.686325	2.686952	-0.879311
C	0.290964	6.289728	0.028182	H	4.741369	2.514178	-1.190695
H	0.507010	7.362842	0.151243				
C	-0.557583	5.854848	-1.004396	(R)-IM1B			
H	-1.007308	6.585400	-1.695570	Ni	-1.308321	0.278549	-0.139500
C	-0.837137	4.486147	-1.165296	P	0.350851	1.646858	0.026132
H	-1.496765	4.159080	-1.982074	P	-0.205553	-1.574340	-0.168479
O	-3.537566	-1.667325	1.987302	C	0.029199	3.353467	-0.600164
C	-4.886467	-1.782312	2.449455	C	-0.784744	3.470576	-1.749757
H	-5.403367	-2.468552	1.749041	H	-1.164882	2.557143	-2.235025
H	-5.400479	-0.799086	2.440561	C	-1.149086	4.731596	-2.241048
H	-4.930789	-2.202368	3.474794	H	-1.795863	4.806071	-3.128594
O	-4.562436	-0.059662	-0.413106	C	-0.723742	5.894860	-1.575458
C	-5.968001	-0.268349	-0.542090	H	-1.030357	6.885647	-1.945492

C	0.076573	5.787166	-0.426403	H	-2.232243	-1.940350	1.823820
H	0.402570	6.694220	0.106825	C	-2.822355	-4.031015	1.834743
C	0.454079	4.523432	0.059593	H	-3.594162	-3.876204	2.603452
H	1.061886	4.451229	0.973253	C	-2.649407	-5.291948	1.237447
C	1.099087	1.896343	1.686602	H	-3.263804	-6.145827	1.564289
C	0.382192	1.414400	2.800864	C	-1.707368	-5.455039	0.206252
H	-0.588604	0.918086	2.635637	H	-1.578292	-6.437721	-0.274726
C	0.920560	1.537587	4.091776	C	-0.934325	-4.364103	-0.226987
H	0.364647	1.144250	4.956992	H	-0.215583	-4.498213	-1.048423
C	2.174243	2.145548	4.274900	O	4.385583	0.312426	1.309984
H	2.602803	2.229399	5.285357	C	5.712145	0.188357	1.822309
C	2.891821	2.628460	3.165548	H	6.377388	0.584183	1.030066
H	3.882296	3.088445	3.307249	H	5.974908	-0.869890	2.026501
C	2.360033	2.501823	1.873550	H	5.852441	0.781011	2.747936
H	2.941387	2.837763	1.001456	O	4.201736	-1.675328	-1.010644
C	1.782167	1.084711	-1.009444	C	5.627571	-1.737130	-1.105424
C	2.012712	1.655638	-2.277872	H	5.980490	-2.261509	-0.195095
H	1.439111	2.537381	-2.596920	H	6.074511	-0.722182	-1.137016
C	2.949965	1.095875	-3.152341	H	5.951678	-2.301306	-2.003176
H	3.103111	1.512514	-4.158515	Cl	4.244878	-0.672973	4.352251
C	3.691716	-0.028287	-2.759716	Cl	4.756085	-0.778523	-3.936026
C	3.532248	-0.581897	-1.468075	C	-4.281265	-0.930337	-0.613895
C	2.546314	-0.037944	-0.602333	C	-3.173391	0.042214	-0.397225
C	2.354285	-0.700899	0.727278	C	-2.917979	1.306568	-0.196515
C	3.362518	-0.487521	1.712001	C	-3.370733	2.680337	-0.169503
C	3.174060	-1.034358	3.004401	C	-2.836281	3.602401	0.764721
C	2.061853	-1.847245	3.276771	H	-2.091799	3.242438	1.490765
H	1.951546	-2.269302	4.286317	C	-3.228726	4.946085	0.748682
C	1.100848	-2.089588	2.292435	C	-4.156316	5.402674	-0.206334
H	0.236120	-2.725536	2.528605	H	-4.452042	6.463327	-0.228017
C	1.221257	-1.500313	1.016911	C	-4.698383	4.498194	-1.137593
C	0.579856	-2.046939	-1.762948	H	-5.424146	4.849205	-1.888799
C	1.610744	-3.006448	-1.851367	C	-4.315128	3.149082	-1.118619
H	1.988851	-3.490868	-0.938336	H	-4.723783	2.441172	-1.856587
C	2.194834	-3.297425	-3.093065	H	-2.794184	5.649439	1.475954
H	3.014261	-4.030051	-3.153475	O	-4.562482	-1.521668	0.710129
C	1.759336	-2.629127	-4.251365	C	-5.720653	-2.136268	0.974490
H	2.233068	-2.845146	-5.221342	O	-5.935618	-2.701557	2.030727
C	0.737184	-1.668324	-4.166580	O	-6.609512	-2.046771	-0.049693
H	0.406562	-1.131931	-5.069789	C	-7.877511	-2.678355	0.188494
C	0.147855	-1.377672	-2.925681	H	-8.469132	-2.524697	-0.731956
H	-0.639498	-0.610942	-2.834980	H	-7.746068	-3.761338	0.385979
C	-1.099364	-3.097459	0.371664	H	-8.390043	-2.217518	1.056818
C	-2.054736	-2.940114	1.399096	C	-3.933491	-2.025278	-1.618326

H	-3.043760	-2.586888	-1.275150	H	-3.474068	3.164174	2.678764
H	-4.783426	-2.721067	-1.758549	C	-2.159741	2.526326	1.065777
H	-3.692323	-1.560631	-2.595711	H	-1.717368	3.524127	0.945209
H	-5.199784	-0.390509	-0.929173	C	-1.715733	1.452430	0.266576
(R)-IM1D				C	-0.826332	0.901381	-2.426860
Ni	1.578493	0.680059	0.013426	C	-2.076389	1.264522	-2.974699
P	0.535011	-1.052804	0.996609	H	-2.714789	1.989962	-2.447782
P	-0.252590	1.620347	-0.839176	C	-2.511207	0.680338	-4.173673
C	1.656776	-2.447990	1.434062	H	-3.487990	0.962951	-4.596643
C	3.011994	-2.107327	1.635695	C	-1.709954	-0.274248	-4.825951
H	3.316074	-1.052681	1.539622	H	-2.062654	-0.745114	-5.756199
C	3.952459	-3.101521	1.944619	C	-0.463972	-0.633478	-4.284280
H	5.008983	-2.826316	2.085606	H	0.163237	-1.385466	-4.787393
C	3.550961	-4.443941	2.051434	C	-0.020018	-0.043863	-3.090675
H	4.292598	-5.227232	2.273925	H	0.947892	-0.324870	-2.647895
C	2.197182	-4.785239	1.881766	C	-0.055505	3.410097	-1.175916
H	1.874203	-5.833533	1.982049	C	0.329719	4.264001	-0.112856
C	1.250398	-3.791329	1.583399	H	0.505002	3.839600	0.887493
H	0.194375	-4.072628	1.456691	C	0.575709	5.623110	-0.357280
C	-0.433678	-0.807559	2.548795	H	0.877547	6.274719	0.477469
C	-0.349010	0.424683	3.227294	C	0.479997	6.140387	-1.661520
H	0.284484	1.223159	2.810754	H	0.688484	7.204988	-1.851856
C	-1.100852	0.626921	4.396844	C	0.131181	5.288859	-2.724862
H	-1.044551	1.596769	4.915586	H	0.067107	5.682999	-3.751449
C	-1.931917	-0.390930	4.892760	C	-0.139332	3.931280	-2.486398
H	-2.530087	-0.222524	5.801611	H	-0.409417	3.273783	-3.325578
C	-2.013553	-1.621108	4.215722	O	-3.865361	-1.269152	1.476319
H	-2.678781	-2.415313	4.588779	C	-5.281319	-1.465133	1.409405
C	-1.266549	-1.831405	3.048250	H	-5.443805	-2.410987	0.854465
H	-1.364786	-2.781944	2.503142	H	-5.777791	-0.635305	0.865491
C	-0.733491	-1.748973	-0.158020	H	-5.726585	-1.551528	2.421305
C	-0.470127	-2.890591	-0.944164	O	-3.939509	-0.625001	-1.493362
H	0.427452	-3.494231	-0.762912	C	-5.153330	-0.987170	-2.148832
C	-1.345394	-3.269701	-1.963320	H	-5.909355	-0.269625	-1.775606
H	-1.123166	-4.139931	-2.597743	H	-5.467133	-2.019301	-1.892781
C	-2.515682	-2.536091	-2.217046	H	-5.068951	-0.892544	-3.249355
C	-2.849624	-1.427212	-1.402047	Cl	-4.892526	0.841693	3.495863
C	-1.927985	-1.023477	-0.387037	Cl	-3.465037	-3.042874	-3.609497
C	-2.314913	0.175002	0.425481	C	3.040160	1.300308	-1.090528
C	-3.353098	-0.012218	1.376260	C	2.878741	-0.035700	-1.038705
C	-3.735762	1.070380	2.199767	C	3.588868	-1.253360	-1.331388
C	-3.152806	2.335437	2.031418	C	2.918194	-2.473614	-1.586968
				H	1.823462	-2.460366	-1.652854
				C	3.634452	-3.663483	-1.750926

C	5.037788	-3.663653	-1.638630	C	-1.155002	-3.308215	3.223175
H	5.600845	-4.604261	-1.741434	H	-1.815896	-4.168316	3.414779
C	5.719727	-2.455070	-1.399389	C	-0.804695	-2.977410	1.906082
H	6.818228	-2.449865	-1.317361	H	-1.208249	-3.560279	1.063917
C	5.009701	-1.254436	-1.269083	C	-1.120628	-1.529264	-0.964896
H	5.533978	-0.307561	-1.069295	C	-1.194875	-2.237856	-2.181178
H	3.095888	-4.603665	-1.947828	H	-0.328387	-2.810167	-2.540263
O	3.035311	3.379575	2.574988	C	-2.359198	-2.207311	-2.956273
C	2.727239	2.316936	2.034574	H	-2.406959	-2.727115	-3.924166
O	1.589630	2.023791	1.490151	C	-3.475802	-1.484342	-2.512420
O	3.632235	1.262294	1.958095	C	-3.453960	-0.818080	-1.265699
C	4.944236	1.543324	2.440415	C	-2.257427	-0.820508	-0.501909
H	5.527368	0.610896	2.312070	C	-2.267104	-0.066931	0.792942
H	5.418016	2.364378	1.861452	C	-2.997211	-0.656856	1.868772
H	4.930713	1.836984	3.510899	C	-2.968553	-0.020494	3.133133
C	3.736375	2.378739	-1.534625	C	-2.308245	1.208926	3.291227
H	4.537730	2.176984	-2.275728	H	-2.311602	1.683453	4.283153
C	3.520446	3.803935	-1.132397	C	-1.637535	1.804531	2.221933
H	2.917784	4.353631	-1.893459	H	-1.125668	2.762975	2.377446
H	2.979216	3.883090	-0.171366	C	-1.591055	1.165197	0.967017
H	4.486434	4.345360	-1.048464	C	-1.449976	1.705781	-1.893478
				C	-2.790695	2.143884	-1.945054
(R)-TS1A				H	-3.274883	2.533169	-1.036660
Ni	1.393812	0.589890	-0.359427	C	-3.516500	2.040409	-3.140245
P	0.484367	-1.369772	-0.049396	H	-4.568675	2.362166	-3.170339
P	-0.456554	1.805137	-0.352678	C	-2.911118	1.497578	-4.288131
C	1.470148	-2.782867	-0.710207	H	-3.488892	1.400344	-5.220099
C	2.087076	-2.613498	-1.970839	C	-1.576629	1.060322	-4.239815
H	1.942443	-1.669454	-2.520150	H	-1.105229	0.623301	-5.133884
C	2.912592	-3.613669	-2.502221	C	-0.845317	1.166146	-3.045599
H	3.395329	-3.461597	-3.479685	H	0.197129	0.812562	-2.984184
C	3.152741	-4.789356	-1.769009	C	-0.342553	3.618296	-0.029016
H	3.819869	-5.565881	-2.174507	C	0.435488	4.043503	1.072870
C	2.553143	-4.960448	-0.510724	H	0.954822	3.289915	1.691233
H	2.746883	-5.873415	0.074185	C	0.603274	5.413530	1.326713
C	1.713468	-3.964380	0.017309	H	1.219884	5.728818	2.182904
H	1.264852	-4.099732	1.012210	C	0.026182	6.372098	0.475558
C	0.035151	-1.868989	1.658979	H	0.171491	7.446766	0.669474
C	0.518301	-1.089973	2.730829	C	-0.721604	5.951921	-0.638081
H	1.150750	-0.204497	2.538365	H	-1.163124	6.694892	-1.321206
C	0.152276	-1.425385	4.045772	C	-0.909640	4.582043	-0.890968
H	0.513118	-0.804761	4.880758	H	-1.488618	4.268748	-1.771397
C	-0.680137	-2.529303	4.294568	O	-3.595144	-1.833298	1.545102
H	-0.973009	-2.778443	5.326272	C	-4.690522	-2.393585	2.265518

H	-5.157914	-3.118553	1.570896	H	1.371846	-3.287265	-1.571397
H	-5.435866	-1.622233	2.547604	C	1.965591	-5.148959	-0.614349
H	-4.354194	-2.925332	3.177517	H	2.287487	-5.617528	-1.556635
O	-4.490537	-0.087445	-0.772589	C	2.110021	-5.836137	0.604035
C	-5.785528	-0.684366	-0.649332	H	2.536903	-6.851050	0.616554
H	-6.226662	-0.293227	0.289252	C	1.729729	-5.216706	1.805932
H	-5.714937	-1.789447	-0.584601	H	1.856605	-5.744773	2.764048
H	-6.438657	-0.413616	-1.503652	C	1.198380	-3.915784	1.795793
Cl	-3.668983	-0.724720	4.586290	H	0.923193	-3.429945	2.743047
Cl	-4.869869	-1.355065	-3.568224	C	0.380096	-0.810678	2.143875
C	2.970152	1.603062	-0.852733	C	1.127474	0.364255	2.367940
C	3.200620	0.303556	-0.692535	H	1.700342	0.841824	1.553965
C	4.219030	-0.715154	-0.776912	C	1.084905	0.993430	3.622841
C	4.288686	-1.735145	0.204672	H	1.628672	1.943977	3.744837
H	3.571663	-1.710158	1.036791	C	0.318062	0.437533	4.660304
C	5.266214	-2.731386	0.118400	H	0.276000	0.934648	5.641814
C	6.173949	-2.744094	-0.958315	C	-0.430824	-0.733693	4.437438
H	6.928616	-3.542506	-1.034235	H	-1.056610	-1.150755	5.242124
C	6.114714	-1.735289	-1.936814	C	-0.415260	-1.352174	3.178412
H	6.825566	-1.740168	-2.778325	H	-1.055222	-2.226770	2.985625
C	5.154320	-0.717570	-1.842807	C	-1.398053	-1.795955	0.078251
H	5.093839	0.073168	-2.606490	C	-1.828619	-3.033222	-0.443580
C	3.030179	4.143492	-1.113252	H	-1.128837	-3.877686	-0.510690
H	3.346620	4.369151	-2.158189	C	-3.136772	-3.190039	-0.909723
H	3.405768	4.962542	-0.470201	H	-3.466995	-4.138319	-1.357939
H	1.927025	4.118564	-1.080964	C	-4.036027	-2.114976	-0.848455
H	5.312223	-3.516850	0.888269	C	-3.654058	-0.885578	-0.261626
O	3.573462	3.085974	1.375118	C	-2.315094	-0.721446	0.184645
C	3.179713	1.987526	1.901801	C	-1.941423	0.605798	0.771386
O	2.008993	1.672255	2.210231	C	-2.445363	0.882048	2.076835
O	4.121321	0.995868	2.130492	C	-2.058627	2.082882	2.717519
C	5.482640	1.266115	1.794566	C	-1.256378	3.018780	2.047475
H	6.106670	0.607450	2.429660	H	-0.948897	3.934399	2.571525
H	5.683577	1.017755	0.729692	C	-0.804773	2.763199	0.752334
H	5.734950	2.330132	1.972217	H	-0.162505	3.504704	0.263613
C	3.624352	2.835415	-0.719209	C	-1.122164	1.552255	0.106027
H	4.728764	2.802327	-0.667257	C	-1.503432	0.269625	-2.494834
				C	-2.784460	0.829955	-2.688924
(R)-TS1B				H	-3.056787	1.764714	-2.176050
Ni	1.456542	-0.188865	-0.864958	C	-3.720385	0.173544	-3.500527
P	0.387179	-1.513658	0.451093	H	-4.725318	0.602471	-3.633060
P	-0.234320	1.094409	-1.455130	C	-3.385755	-1.045001	-4.119254
C	1.042312	-3.226686	0.577622	H	-4.128409	-1.566486	-4.742457
C	1.444340	-3.848179	-0.625706	C	-2.113320	-1.607753	-3.923620

H	-1.855200	-2.569365	-4.393812	C	3.939258	5.718891	1.215050
C	-1.172511	-0.950719	-3.113966	H	4.591230	6.310148	0.542864
H	-0.177336	-1.387311	-2.926638	H	3.018191	6.295588	1.446406
C	0.034977	2.692799	-2.343653	H	4.466282	5.522186	2.172711
C	0.966026	3.604545	-1.798126	C	3.966933	2.657801	-2.149100
H	1.543026	3.314911	-0.904576	H	3.150612	2.469436	-2.869608
C	1.191471	4.845186	-2.415354	H	3.901993	3.690538	-1.753242
H	1.910720	5.544555	-1.961364	H	4.942653	2.573575	-2.681693
C	0.525319	5.175123	-3.607742	H	4.716184	1.846908	-0.230615
H	0.707260	6.145208	-4.096795				
C	-0.362697	4.249567	-4.183601	(R)-TS1D			
H	-0.873394	4.488118	-5.130061	Ni	1.391904	0.719198	-0.242513
C	-0.612237	3.016697	-3.556927	P	0.645543	-1.131042	0.590058
H	-1.312842	2.308189	-4.020583	P	-0.546243	1.739024	-0.467613
O	-3.198798	-0.112818	2.618817	C	1.838394	-2.524096	0.771746
C	-4.292198	0.147937	3.499243	C	3.139032	-2.154736	1.179546
H	-4.996380	-0.696874	3.364895	H	3.365578	-1.089658	1.345884
H	-4.806255	1.097223	3.243560	C	4.129728	-3.129590	1.359038
H	-3.966360	0.187919	4.557519	H	5.143518	-2.827742	1.663624
O	-4.450516	0.212578	-0.176609	C	3.834455	-4.484587	1.125313
C	-5.787177	0.110197	0.323734	H	4.617906	-5.249347	1.244750
H	-5.978130	1.039653	0.896061	C	2.535076	-4.861338	0.744779
H	-5.900800	-0.763177	0.997926	H	2.294359	-5.923219	0.577337
H	-6.524149	0.028298	-0.500215	C	1.535148	-3.886958	0.578852
Cl	-2.466779	2.427686	4.391033	H	0.518545	-4.194794	0.291079
Cl	-5.604981	-2.302746	-1.610090	C	-0.099010	-1.137187	2.276591
C	3.966974	1.681823	-1.024015	C	0.091172	-0.004057	3.090951
C	3.363632	0.443523	-1.053955	H	0.672949	0.847685	2.701825
C	3.201373	-0.820142	-0.738865	C	-0.456340	0.016785	4.385585
C	3.965722	-2.046054	-0.571999	H	-0.316794	0.905969	5.020525
C	4.143364	-2.597356	0.719573	C	-1.184931	-1.084108	4.865602
H	3.704764	-2.081748	1.586754	H	-1.626713	-1.056479	5.873866
C	4.852795	-3.793890	0.884039	C	-1.358982	-2.220998	4.054408
C	5.396070	-4.458945	-0.230357	H	-1.939564	-3.080373	4.424034
H	5.946466	-5.403224	-0.096991	C	-0.811378	-2.252203	2.764583
C	5.227081	-3.914240	-1.515191	H	-0.968392	-3.131391	2.121463
H	5.650324	-4.428036	-2.392997	C	-0.689611	-1.708674	-0.540984
C	4.513504	-2.718773	-1.689656	C	-0.382232	-2.555864	-1.628270
H	4.364629	-2.294505	-2.694450	H	0.606843	-3.026376	-1.702337
H	4.974686	-4.216586	1.893237	C	-1.322781	-2.791921	-2.630697
O	2.628038	2.524842	0.554213	H	-1.076485	-3.427743	-3.493400
C	2.853037	3.591690	1.232742	C	-2.597199	-2.202003	-2.574422
O	2.445440	3.872917	2.367606	C	-2.953485	-1.378357	-1.479321
O	3.639483	4.507382	0.523033	C	-1.968828	-1.107615	-0.479553

C	-2.361759	-0.158300	0.611456	C	3.843279	-0.771321	-1.526829
C	-3.254782	-0.654311	1.596711	C	3.352707	-2.006223	-2.012584
C	-3.638916	0.184863	2.666017	H	2.275636	-2.096453	-2.208461
C	-3.211922	1.519720	2.710453	C	4.216094	-3.087384	-2.224607
H	-3.536383	2.159545	3.543915	C	5.588205	-2.959906	-1.939458
C	-2.357359	2.012731	1.719456	H	6.264299	-3.817152	-2.083142
H	-2.031619	3.060090	1.774548	C	6.094080	-1.733508	-1.470100
C	-1.893070	1.180636	0.679818	H	7.168754	-1.627496	-1.252296
C	-1.269450	1.356218	-2.117376	C	5.234278	-0.642217	-1.279055
C	-2.612446	1.657446	-2.430111	H	5.621226	0.319152	-0.907160
H	-3.255362	2.136609	-1.675825	H	3.815396	-4.044081	-2.593772
C	-3.132543	1.316139	-3.687547	O	4.083267	2.771775	0.723535
H	-4.182756	1.546563	-3.926634	C	3.305925	2.116280	1.535421
C	-2.320798	0.664584	-4.634206	O	2.063796	2.126228	1.574084
H	-2.737272	0.380808	-5.612895	O	3.944637	1.285829	2.423710
C	-0.983730	0.363213	-4.324312	C	5.365674	1.145048	2.317040
H	-0.349882	-0.157456	-5.058993	H	5.673894	0.518945	3.175621
C	-0.456515	0.710904	-3.070366	H	5.646429	0.637028	1.370494
H	0.583365	0.468046	-2.798168	H	5.877991	2.127279	2.361191
C	-0.631140	3.574415	-0.355404	C	3.498457	2.857302	-1.015500
C	-0.134694	4.184858	0.822778	H	4.536164	2.857965	-1.403251
H	0.281523	3.557085	1.623862	C	2.796670	4.179630	-1.099469
C	-0.103996	5.583398	0.937973	H	2.502932	4.362875	-2.156216
H	0.282520	6.043772	1.860882	H	1.876439	4.173451	-0.490486
C	-0.532925	6.392539	-0.129675	H	3.455728	5.006365	-0.772231
H	-0.495924	7.489859	-0.043097				
C	-0.991502	5.792238	-1.314924	(R)-IM2A			
H	-1.313844	6.418155	-2.162257	Ni	1.454345	0.778537	0.061955
C	-1.045507	4.392200	-1.427885	P	0.635615	-1.294153	-0.170547
H	-1.404008	3.934177	-2.361383	P	-0.501688	1.851035	0.019782
O	-3.620493	-1.961614	1.482896	C	1.765646	-2.448333	-1.059373
C	-5.007947	-2.309998	1.510080	C	2.358619	-2.001150	-2.263792
H	-5.137848	-3.149764	0.798141	H	2.112937	-0.999580	-2.650280
H	-5.642559	-1.459155	1.187051	C	3.280092	-2.803893	-2.949631
H	-5.326078	-2.633250	2.522167	H	3.735378	-2.437063	-3.882254
O	-4.129197	-0.731320	-1.274865	C	3.647555	-4.056723	-2.426908
C	-5.368288	-1.118145	-1.864862	H	4.386605	-4.679915	-2.953980
H	-6.148932	-0.627775	-1.251322	C	3.079991	-4.500359	-1.221470
H	-5.513335	-2.217220	-1.834409	H	3.371689	-5.474881	-0.799078
H	-5.452189	-0.768092	-2.912669	C	2.142019	-3.704221	-0.541384
Cl	-4.585776	-0.444870	4.000769	H	1.711935	-4.057565	0.407014
Cl	-3.648262	-2.488855	-3.957695	C	0.064963	-2.258444	1.287085
C	2.808711	1.626198	-1.177628	C	0.342789	-1.756764	2.574776
C	2.952597	0.322001	-1.201599	H	0.875425	-0.796479	2.663961

C	-0.114912	-2.453457	3.705448	C	-1.267761	4.609080	0.077799
H	0.079295	-2.046762	4.710079	H	-1.908790	4.395748	-0.789069
C	-0.834560	-3.650989	3.557137	O	-3.477643	-2.239240	1.003306
H	-1.197275	-4.190372	4.445975	C	-4.426093	-3.111725	1.610288
C	-1.105033	-4.155042	2.271157	H	-4.777263	-3.769220	0.791432
H	-1.671391	-5.092399	2.152446	H	-5.288128	-2.556359	2.032030
C	-0.668030	-3.456301	1.135803	H	-3.963662	-3.730741	2.404161
H	-0.909165	-3.830044	0.128562	O	-4.362787	-0.159248	-0.997314
C	-0.882843	-1.314699	-1.240892	C	-5.590020	-0.897516	-1.021788
C	-0.844081	-1.767157	-2.575423	H	-6.118375	-0.663512	-0.076306
H	0.074878	-2.208445	-2.983598	H	-5.398284	-1.989021	-1.068573
C	-1.964531	-1.652609	-3.405480	H	-6.224208	-0.601901	-1.882424
H	-1.921742	-1.969416	-4.457667	Cl	-3.765026	-1.717605	4.217040
C	-3.154027	-1.108418	-2.901221	Cl	-4.500780	-0.853972	-3.993571
C	-3.245987	-0.709803	-1.548672	C	2.697910	1.999778	-0.790938
C	-2.094903	-0.789701	-0.723415	C	3.149030	0.746875	-0.580506
C	-2.224199	-0.304526	0.687252	C	4.275218	-0.116996	-0.797791
C	-2.961302	-1.128793	1.591190	C	4.453634	-1.280932	-0.004375
C	-3.025188	-0.739690	2.951575	H	3.743764	-1.459464	0.813762
C	-2.436039	0.465229	3.372948	C	5.523645	-2.144779	-0.254601
H	-2.505957	0.736679	4.436250	C	6.415983	-1.876571	-1.310940
C	-1.761917	1.291802	2.473347	H	7.245983	-2.570306	-1.518219
H	-1.306021	2.224850	2.830128	C	6.251926	-0.723794	-2.103310
C	-1.643206	0.910548	1.121809	H	6.953077	-0.516565	-2.926901
C	-1.365012	1.988027	-1.591143	C	5.199617	0.161679	-1.840555
C	-2.736895	2.306138	-1.692362	H	5.052871	1.061686	-2.457100
H	-3.339159	2.431905	-0.780126	C	2.029108	4.396265	-1.344848
C	-3.343437	2.404527	-2.952639	H	2.343376	5.122095	-2.122100
H	-4.418559	2.628240	-3.025247	H	1.957015	4.955491	-0.382394
C	-2.587387	2.184087	-4.118381	H	1.003275	4.043369	-1.569739
H	-3.070229	2.245471	-5.105860	H	5.656274	-3.045712	0.363453
C	-1.223281	1.862032	-4.021447	O	2.806663	2.229279	3.488464
H	-0.633432	1.673824	-4.932102	C	2.583452	1.308641	2.696490
C	-0.611584	1.763697	-2.760536	O	1.472112	1.070622	2.081265
H	0.452724	1.492770	-2.664636	O	3.567689	0.370866	2.406459
C	-0.516584	3.577549	0.682014	C	4.841527	0.611231	2.999658
C	0.332708	3.889969	1.768846	H	5.511478	-0.188116	2.626836
H	0.944431	3.102563	2.234778	H	5.244315	1.602887	2.703881
C	0.407932	5.208051	2.247975	H	4.788234	0.576511	4.108630
H	1.076194	5.428482	3.095066	C	2.988340	3.254059	-1.239135
C	-0.344281	6.231492	1.645779	H	4.040094	3.447001	-1.535576
H	-0.274922	7.266050	2.017786				
C	-1.179846	5.926592	0.557469	(R)-IM2B			
H	-1.767389	6.720750	0.069978	Ni	1.047564	1.021182	-1.088023

P	0.913532	-1.038694	-0.419092	H	-5.732816	0.300137	-1.826275
P	-1.014896	1.569021	-0.753970	C	-4.331695	-0.406925	-3.337666
C	1.962260	-2.152230	-1.442419	H	-5.112720	-0.880118	-3.952353
C	1.894670	-2.002735	-2.846006	C	-2.984773	-0.487944	-3.728548
H	1.247374	-1.221853	-3.276835	H	-2.706932	-1.023438	-4.649580
C	2.655236	-2.830719	-3.684452	C	-1.986237	0.099805	-2.934709
H	2.588083	-2.712790	-4.777388	H	-0.922538	0.023573	-3.208569
C	3.515591	-3.795031	-3.127987	C	-1.452265	3.362113	-0.899141
H	4.123419	-4.436902	-3.784680	C	-0.638936	4.333508	-0.268813
C	3.614086	-3.919364	-1.732710	H	0.240294	4.004899	0.309102
H	4.308032	-4.650749	-1.290337	C	-0.923853	5.699520	-0.422163
C	2.837451	-3.105756	-0.889960	H	-0.283551	6.438394	0.084940
H	2.928211	-3.201077	0.201552	C	-2.000252	6.121515	-1.221531
C	1.287088	-1.478452	1.323046	H	-2.216536	7.194677	-1.343604
C	1.838593	-0.490295	2.155340	C	-2.790157	5.162498	-1.876577
H	2.060511	0.505434	1.752840	H	-3.626555	5.477769	-2.520246
C	2.091852	-0.770439	3.506420	C	-2.520601	3.792064	-1.719811
H	2.513366	0.022395	4.142364	H	-3.147894	3.061137	-2.247730
C	1.797678	-2.041023	4.028159	O	-1.895443	-2.087044	2.752730
H	1.987703	-2.260281	5.090576	C	-2.196203	-2.751379	3.976932
C	1.249028	-3.034262	3.194277	H	-2.597932	-3.738655	3.676953
H	1.015326	-4.030686	3.601702	H	-2.961224	-2.205966	4.565596
C	0.981648	-2.754666	1.845086	H	-1.289094	-2.898148	4.595611
H	0.517707	-3.519268	1.202953	O	-4.098714	-1.289046	0.836063
C	-0.762236	-1.806865	-0.599944	C	-4.929044	-2.144775	1.631104
C	-1.024484	-2.805873	-1.557301	H	-5.111249	-1.611857	2.585472
H	-0.212401	-3.198135	-2.184313	H	-4.421355	-3.107194	1.845369
C	-2.324297	-3.291776	-1.740525	H	-5.897415	-2.346982	1.129700
H	-2.542636	-4.042262	-2.513989	Cl	-1.082230	-0.294485	5.357891
C	-3.373400	-2.792172	-0.955826	Cl	-5.012624	-3.297679	-1.310839
C	-3.127148	-1.837738	0.058321	C	1.301987	2.555751	-2.515249
C	-1.813125	-1.334579	0.225063	C	2.429709	1.760968	-2.320520
C	-1.584284	-0.305521	1.288673	C	3.045028	0.892949	-1.615642
C	-1.601770	-0.766108	2.641100	C	4.172645	0.102246	-1.203575
C	-1.265924	0.153169	3.665125	C	4.535232	0.057248	0.166842
C	-0.999449	1.497522	3.352213	H	4.009279	0.706307	0.888344
H	-0.734179	2.183758	4.169052	C	5.585247	-0.776124	0.576993
C	-1.034522	1.953925	2.034410	C	6.286981	-1.558213	-0.358941
H	-0.784083	3.001282	1.829158	H	7.104017	-2.218209	-0.026747
C	-1.315441	1.051725	0.989783	C	5.947688	-1.490406	-1.722801
C	-2.332977	0.769615	-1.747481	H	6.496039	-2.096456	-2.460754
C	-3.687256	0.847136	-1.354466	C	4.898224	-0.665964	-2.147424
H	-3.956519	1.343321	-0.409762	H	4.608643	-0.625959	-3.207146
C	-4.681293	0.258519	-2.148184	H	5.859247	-0.810923	1.643131

O	1.583330	2.511760	0.521973	H	0.490455	-1.327850	4.532890
C	2.180573	2.815679	1.598862	C	2.150386	-0.391312	3.516311
O	3.168163	2.291658	2.148684	C	2.767009	-0.091754	2.277947
O	1.572843	3.923809	2.229380	C	2.112343	-0.491014	1.074644
C	2.163476	4.335126	3.457355	C	2.702179	0.000550	-0.212004
H	1.596062	5.224056	3.798129	C	3.884514	-0.622910	-0.684156
H	2.103299	3.537207	4.229515	C	4.445795	-0.187097	-1.907699
H	3.234968	4.600432	3.330726	C	3.887949	0.894500	-2.605705
C	0.517433	2.578808	-3.806452	H	4.352149	1.216789	-3.549124
H	0.540921	1.599175	-4.322406	C	2.733705	1.520951	-2.122066
H	-0.538891	2.859457	-3.618613	H	2.293955	2.353881	-2.689193
H	0.936514	3.341962	-4.499158	C	2.113856	1.066515	-0.941180
H	1.290575	3.497734	-1.931922	C	0.774719	2.318849	1.263254
				C	1.982527	2.966632	1.599977
(R)-IM2D				H	2.758820	3.112208	0.833164
Ni	-1.182312	0.289427	-0.494512	C	2.215028	3.377557	2.921548
P	-0.071538	-1.537342	-0.410423	H	3.164262	3.871820	3.181390
P	0.444269	1.694035	-0.439696	C	1.250879	3.135590	3.916108
C	-0.941523	-3.143056	-0.173738	H	1.443933	3.441831	4.955724
C	-2.067000	-3.351634	-1.000223	C	0.050991	2.482438	3.586481
H	-2.385372	-2.550130	-1.684635	H	-0.696504	2.272634	4.367395
C	-2.786005	-4.552858	-0.932992	C	-0.187404	2.073846	2.264822
H	-3.670885	-4.694671	-1.571498	H	-1.107426	1.529429	1.996474
C	-2.395004	-5.555213	-0.027880	C	0.243772	3.194805	-1.489243
H	-2.970524	-6.491672	0.041085	C	-0.394076	3.002762	-2.735304
C	-1.268854	-5.359415	0.790363	H	-0.740851	1.992816	-3.010212
H	-0.953345	-6.146341	1.493780	C	-0.620478	4.089388	-3.592861
C	-0.536590	-4.161563	0.713253	H	-1.119820	3.928406	-4.560984
H	0.349358	-4.022364	1.351340	C	-0.237028	5.385140	-3.200602
C	1.134369	-2.020259	-1.720599	H	-0.430546	6.242435	-3.864281
C	1.113342	-1.310272	-2.935851	C	0.379797	5.585348	-1.953357
H	0.410002	-0.469103	-3.046602	H	0.669116	6.600083	-1.637408
C	1.999557	-1.657375	-3.968495	C	0.625453	4.494507	-1.100684
H	1.989325	-1.090984	-4.912805	H	1.099555	4.659835	-0.121712
C	2.906128	-2.715591	-3.789490	O	4.345089	-1.671207	0.050591
H	3.610832	-2.978791	-4.593239	C	5.728803	-1.745533	0.407242
C	2.921897	-3.432456	-2.578606	H	5.768308	-2.183663	1.424541
H	3.639652	-4.254704	-2.433711	H	6.194893	-0.738866	0.426975
C	2.033620	-3.092551	-1.548562	H	6.295372	-2.391538	-0.293448
H	2.054034	-3.645891	-0.597570	O	3.903155	0.629825	2.089851
C	0.919216	-1.251180	1.121373	C	4.998604	0.598344	3.004775
C	0.342277	-1.553752	2.375566	H	5.895454	0.852467	2.406411
H	-0.606501	-2.106565	2.428310	H	5.129579	-0.409086	3.450665
C	0.950611	-1.123099	3.555362	H	4.877545	1.342098	3.817023

Cl	5.794845	-1.042427	-2.631489	H	0.028707	0.780968	4.608095
Cl	2.767683	0.203080	5.051763	C	0.396476	1.694045	2.283670
C	-2.800552	1.219162	-0.154300	C	-0.686424	2.584300	2.397093
C	-3.018635	-0.065988	-0.078387	H	-1.702752	2.231717	2.164576
C	-3.924389	-1.158079	0.207117	C	-0.458120	3.911939	2.802301
C	-3.731750	-1.954573	1.365296	H	-1.304409	4.610479	2.895272
H	-2.892948	-1.712694	2.035450	C	0.844448	4.347657	3.098325
C	-4.579123	-3.034566	1.642320	H	1.019358	5.389763	3.408029
C	-5.632420	-3.350922	0.764264	C	1.924846	3.450869	3.000854
H	-6.292326	-4.206836	0.975752	H	2.947225	3.788469	3.229728
C	-5.832498	-2.569647	-0.388440	C	1.705742	2.129749	2.589920
H	-6.657114	-2.807656	-1.079231	H	2.544935	1.422226	2.492294
C	-4.990622	-1.483113	-0.669677	C	-1.596610	-0.297820	1.423809
H	-5.144292	-0.869819	-1.569842	C	-2.337132	-1.067206	2.349533
H	-4.408485	-3.644835	2.543147	H	-1.882976	-1.351596	3.307477
O	-4.912141	2.235472	0.437914	C	-3.623515	-1.527869	2.055116
C	-5.657991	1.730364	-0.568927	H	-4.170858	-2.163951	2.765619
O	-5.388896	1.733693	-1.754446	C	-4.199969	-1.221716	0.816437
O	-6.815455	1.203124	-0.112234	C	-3.527051	-0.386700	-0.103246
C	-6.964812	0.947609	1.294860	C	-2.216660	0.080537	0.202957
H	-7.950954	0.460107	1.405727	C	-1.606576	0.950653	-0.857500
H	-6.167203	0.264704	1.652839	C	-2.155917	2.261042	-0.993485
H	-6.938312	1.886871	1.882709	C	-1.763995	3.060014	-2.095228
C	-3.483008	2.496988	0.172480	C	-0.827770	2.582131	-3.023974
H	-3.132036	2.815950	1.178109	H	-0.545117	3.222242	-3.871795
C	-3.269707	3.651978	-0.803095	C	-0.272431	1.309290	-2.874630
H	-2.201825	3.942415	-0.785602	H	0.456428	0.956257	-3.615476
H	-3.543177	3.356318	-1.831231	C	-0.652922	0.481512	-1.799521
H	-3.878510	4.526028	-0.495951	C	-1.111909	-2.317021	-1.245453
				C	-2.161522	-2.412901	-2.184547
				H	-2.171312	-1.755881	-3.067403
(R)-IM3E				C	-3.208498	-3.320770	-1.969689
Ni	1.674545	-0.646590	0.117200	H	-4.037425	-3.379499	-2.691271
P	0.218115	-0.045048	1.734994	C	-3.214048	-4.131124	-0.820084
P	0.237119	-1.095877	-1.466611	H	-4.046766	-4.829319	-0.644954
C	0.433413	-0.941511	3.334147	C	-2.170482	-4.034339	0.116098
C	0.734319	-2.319844	3.305545	H	-2.180806	-4.655153	1.025055
H	0.931626	-2.807742	2.339288	C	-1.118044	-3.130016	-0.095677
C	0.841129	-3.043520	4.502609	H	-0.308610	-3.023717	0.641236
H	1.088888	-4.115987	4.468769	C	1.077117	-1.599086	-3.012635
C	0.658282	-2.398235	5.738933	C	2.141081	-0.807906	-3.514412
H	0.750364	-2.965929	6.678306	H	2.398026	0.143892	-3.030999
C	0.370993	-1.022670	5.772162	C	2.879428	-1.234996	-4.629880
H	0.234489	-0.508838	6.736889	H	3.690884	-0.599531	-5.017343
C	0.258139	-0.294624	4.575339				

C	2.600643	-2.473268	-5.232104	H	4.614720	-1.850216	-1.024421
H	3.191692	-2.814292	-6.096285				
C	1.569987	-3.280866	-4.717285	IM1F			
H	1.350012	-4.256696	-5.177927	Ni	0.786206	-0.718454	-1.085449
C	0.812768	-2.850334	-3.617312	P	0.477511	0.973651	0.203508
H	0.010779	-3.491203	-3.223064	P	-1.105721	-1.634927	-1.031091
O	-3.095277	2.604137	-0.067165	C	2.017842	1.459884	1.063937
C	-3.166036	3.922956	0.492213	C	2.726003	0.448202	1.758222
H	-2.163177	4.391402	0.543599	H	2.292095	-0.561425	1.844975
H	-3.559180	3.793226	1.519549	C	3.980818	0.714127	2.325868
H	-3.850834	4.573820	-0.084969	H	4.516990	-0.083461	2.861108
O	-4.028424	-0.111932	-1.341831	C	4.567469	1.981787	2.172212
C	-5.211628	0.696883	-1.447139	H	5.566258	2.181800	2.588595
H	-5.448954	0.743723	-2.526238	C	3.877701	2.988716	1.472509
H	-5.010121	1.717010	-1.062984	H	4.329620	3.986918	1.357541
H	-6.068127	0.247735	-0.904284	C	2.611936	2.733609	0.920648
Cl	-2.468835	4.639299	-2.396976	H	2.080417	3.526050	0.372192
Cl	-5.726003	-1.961266	0.381747	C	-0.138981	2.500214	-0.606604
C	4.472678	-0.771585	-1.216206	C	-0.168768	2.524350	-2.015929
C	3.378000	-0.155163	-0.705236	H	0.192309	1.643009	-2.570547
C	2.566936	0.867937	-0.411650	C	-0.690307	3.638439	-2.691220
C	2.488150	2.301477	-0.438982	H	-0.732024	3.644014	-3.791350
C	1.241554	2.974754	-0.388025	C	-1.179606	4.734804	-1.960242
H	0.327086	2.377090	-0.333983	H	-1.601954	5.603183	-2.488716
C	1.180647	4.370570	-0.406230	C	-1.144029	4.717757	-0.553781
C	2.365862	5.128705	-0.430223	H	-1.531406	5.576048	0.017659
H	2.319221	6.228930	-0.422711	C	-0.629949	3.602046	0.124922
C	3.614984	4.476199	-0.465684	H	-0.629468	3.571766	1.225443
H	4.544590	5.066672	-0.482008	C	-0.767262	0.678284	1.528386
C	3.680170	3.078390	-0.494586	C	-0.397107	0.518873	2.878976
H	4.651723	2.562505	-0.525263	H	0.640533	0.702183	3.191657
H	0.201223	4.872459	-0.393180	C	-1.334869	0.101377	3.830175
O	3.382995	-1.188384	2.181991	H	-1.041538	-0.063864	4.877051
C	3.517552	-2.296546	1.683603	C	-2.662660	-0.138974	3.445745
O	4.245232	-3.271980	1.691086	C	-3.078628	0.080009	2.111793
O	2.220217	-2.516091	0.638158	C	-2.118886	0.469341	1.145257
C	2.371275	-3.543781	-0.328385	C	-2.589595	0.666399	-0.264763
H	3.035194	-4.328019	0.091061	C	-3.330573	1.858448	-0.531479
H	1.381057	-3.989046	-0.566149	C	-3.703347	2.135940	-1.870104
H	2.816703	-3.163344	-1.275314	C	-3.398370	1.223958	-2.895626
C	5.533213	-0.078123	-2.024154	H	-3.700513	1.472679	-3.923383
H	6.515186	-0.094928	-1.498453	C	-2.706827	0.042915	-2.621646
H	5.693673	-0.599770	-2.994419	H	-2.467759	-0.648523	-3.442579
H	5.270694	0.977482	-2.235311	C	-2.293626	-0.249072	-1.303590

C	-1.645685	-2.435822	0.536920	H	4.848406	1.437523	-1.485457
C	-2.987950	-2.787230	0.788124	C	6.629793	1.018993	-0.250492
H	-3.767661	-2.561487	0.046353	C	7.274774	0.076476	0.598580
C	-3.342953	-3.372538	2.011853	H	8.245239	0.359104	1.032496
H	-4.396098	-3.621902	2.212849	C	6.678530	-1.157448	0.888491
C	-2.361769	-3.613680	2.990593	H	7.165019	-1.874232	1.567869
H	-2.645988	-4.060928	3.955492	C	5.438517	-1.459004	0.307694
C	-1.022969	-3.267628	2.743055	C	6.685785	3.187683	-1.247372
H	-0.251795	-3.446883	3.508060	H	5.689890	3.493044	-0.857770
C	-0.665841	-2.679444	1.519596	H	6.568706	2.829873	-2.294513
H	0.377551	-2.392837	1.315207	H	7.366249	4.059151	-1.235389
C	-1.543763	-2.873237	-2.327119				
C	-0.459411	-3.483020	-2.991506	TS1F			
H	0.564492	-3.170330	-2.724058	Ni	0.775699	-0.835193	-1.057791
C	-0.684979	-4.470813	-3.964815	P	0.461801	0.970557	0.161459
H	0.169518	-4.945319	-4.472098	P	-1.134844	-1.646036	-1.033189
C	-1.999804	-4.845066	-4.290609	C	2.024135	1.379962	1.030624
H	-2.180761	-5.615295	-5.056842	C	2.685972	0.322565	1.700666
C	-3.087320	-4.231913	-3.639891	H	2.229839	-0.680875	1.724293
H	-4.118432	-4.520595	-3.898354	C	3.923255	0.540841	2.325373
C	-2.862714	-3.251891	-2.660183	H	4.423909	-0.288118	2.847252
H	-3.719507	-2.770370	-2.164716	C	4.533821	1.804896	2.255290
O	-3.529875	2.629742	0.567762	H	5.516363	1.968900	2.722866
C	-4.510331	3.660835	0.661679	C	3.892747	2.852393	1.571250
H	-4.615837	3.862980	1.745292	H	4.368915	3.844062	1.513565
H	-5.488502	3.337973	0.251201	C	2.642025	2.645760	0.963402
H	-4.184020	4.585908	0.146630	H	2.143232	3.471029	0.432620
O	-4.346437	-0.137599	1.663810	C	-0.159215	2.539119	-0.555645
C	-5.435709	0.547140	2.292620	C	-0.262447	2.609708	-1.960367
H	-6.165839	0.782940	1.492774	H	0.053922	1.742124	-2.562003
H	-5.095813	1.492750	2.762893	C	-0.802845	3.752524	-2.569465
H	-5.923055	-0.085462	3.062310	H	-0.905109	3.795113	-3.664733
Cl	-4.483083	3.632940	-2.372329	C	-1.234194	4.831193	-1.777732
Cl	-3.781023	-0.791717	4.626820	H	-1.669363	5.722901	-2.254601
H	1.515445	-2.480434	-0.572706	C	-1.122908	4.768000	-0.376487
O	2.318677	-3.114445	-0.403574	H	-1.462282	5.613724	0.242205
O	4.651905	-3.623964	1.211024	C	-0.594187	3.621653	0.237307
O	2.579133	-0.549102	-1.624453	H	-0.537420	3.554088	1.334851
O	7.287413	2.198345	-0.420286	C	-0.744664	0.624802	1.519927
N	3.384983	-2.271423	-0.247927	C	-0.338224	0.418517	2.853042
C	4.529749	-2.609437	0.534132	H	0.710402	0.570931	3.142500
C	3.505361	-1.057702	-0.924484	C	-1.255865	-0.008642	3.820118
C	4.810538	-0.521519	-0.557828	H	-0.932544	-0.216714	4.850312
C	5.384274	0.722440	-0.848699	C	-2.601083	-0.198482	3.472538

C	-3.052086	0.073625	2.160516	H	1.085342	-2.292789	-1.189925
C	-2.109506	0.456198	1.174861	O	2.383278	-3.076349	-0.366937
C	-2.604978	0.665961	-0.222248	O	4.743201	-3.557557	1.162484
C	-3.344782	1.861738	-0.474202	O	2.608158	-0.467160	-1.586864
C	-3.753395	2.130903	-1.804301	O	7.232676	2.311064	-0.481275
C	-3.484283	1.206972	-2.829149	N	3.416533	-2.266940	-0.306858
H	-3.818415	1.446802	-3.849074	C	4.605762	-2.559161	0.477196
C	-2.789940	0.024503	-2.567644	C	3.526612	-1.041713	-0.930678
H	-2.581738	-0.675774	-3.389085	C	4.849671	-0.482659	-0.595059
C	-2.335406	-0.256333	-1.261030	C	5.371681	0.773199	-0.888726
C	-1.611341	-2.524937	0.503310	H	4.800296	1.472825	-1.511546
C	-2.955487	-2.691616	0.895824	C	6.622863	1.109437	-0.302571
H	-3.767745	-2.255545	0.295059	C	7.302184	0.188399	0.531087
C	-3.257399	-3.344326	2.099668	H	8.268076	0.496424	0.957678
H	-4.306256	-3.444536	2.417540	C	6.742758	-1.070398	0.821966
C	-2.220312	-3.832758	2.914537	H	7.255075	-1.772288	1.497749
H	-2.459330	-4.329293	3.867972	C	5.511570	-1.400342	0.250031
C	-0.880917	-3.674381	2.519253	C	6.580885	3.285417	-1.289747
H	-0.066926	-4.057528	3.154441	H	5.584510	3.556294	-0.876874
C	-0.568665	-3.020209	1.315455	H	6.454403	2.930920	-2.336520
H	0.480726	-2.902894	0.990988	H	7.233293	4.178057	-1.285313
C	-1.577082	-2.797652	-2.400854				
C	-0.586389	-3.102055	-3.354922	IM2F			
H	0.415522	-2.657618	-3.233232	Ni	-0.260409	-1.790905	1.042807
C	-0.874872	-3.967200	-4.424265	P	-0.579192	-0.585876	-0.775038
H	-0.093374	-4.202581	-5.163515	P	1.508117	-0.881955	1.684504
C	-2.155136	-4.533667	-4.542599	C	-1.703475	-1.424614	-1.958169
H	-2.382299	-5.214988	-5.377655	C	-1.514405	-2.812498	-2.158651
C	-3.147648	-4.234338	-3.589830	H	-0.734235	-3.343845	-1.593709
H	-4.150496	-4.680958	-3.678279	C	-2.345347	-3.517504	-3.040731
C	-2.861982	-3.369501	-2.522385	H	-2.191741	-4.597599	-3.185537
H	-3.642958	-3.139749	-1.782137	C	-3.398889	-2.859129	-3.697662
O	-3.512215	2.631227	0.630260	H	-4.062616	-3.419579	-4.374129
C	-4.419106	3.727454	0.726912	C	-3.624989	-1.493260	-3.459244
H	-4.474342	3.960667	1.807802	H	-4.469495	-0.978000	-3.942862
H	-5.429184	3.460782	0.355870	C	-2.781627	-0.774914	-2.595905
H	-4.047234	4.615492	0.178939	H	-2.973090	0.291401	-2.408312
O	-4.341304	-0.095434	1.750741	C	-1.088717	1.181902	-0.826629
C	-5.379061	0.633672	2.417722	C	-1.541228	1.809528	0.350950
H	-6.151778	0.850401	1.653952	H	-1.590176	1.233550	1.286915
H	-4.993342	1.590703	2.825240	C	-1.912016	3.163887	0.322623
H	-5.828445	0.042095	3.241208	H	-2.237329	3.657534	1.251797
Cl	-4.544721	3.623250	-2.300823	C	-1.847943	3.892530	-0.876625
Cl	-3.699777	-0.863634	4.663564	H	-2.134312	4.955411	-0.893386

C	-1.402552	3.265041	-2.055126	H	2.303944	3.976226	-3.437611
H	-1.351370	3.832282	-2.997834	H	2.805081	4.829098	-1.923851
C	-1.012190	1.917889	-2.030219	H	1.053890	4.724657	-2.369286
H	-0.632658	1.435639	-2.944348	O	4.293093	1.149765	-1.178848
C	1.064059	-0.545223	-1.639398	C	5.000107	2.037229	-2.054041
C	1.378221	-1.451443	-2.671426	H	5.169423	2.972193	-1.484137
H	0.604767	-2.119085	-3.075028	H	4.399314	2.267945	-2.957524
C	2.678648	-1.528115	-3.184369	H	5.975952	1.610480	-2.363174
H	2.934221	-2.262432	-3.962005	Cl	1.197410	5.369344	0.278471
C	3.678169	-0.676649	-2.691488	Cl	5.321803	-0.875783	-3.264508
C	3.376828	0.291473	-1.706680	H	0.374235	-2.744582	2.004837
C	2.068071	0.335424	-1.161844	O	-1.817593	-2.978171	0.966528
C	1.805301	1.327125	-0.072340	O	-4.135896	-3.654320	-0.628167
C	1.732527	2.705837	-0.437805	O	-2.319644	-0.510762	2.258004
C	1.421372	3.648070	0.574844	O	-6.681210	2.350914	0.281791
C	1.230768	3.228220	1.903015	N	-2.908720	-2.228661	0.792747
H	0.990273	3.988856	2.659826	C	-4.008323	-2.589304	-0.048901
C	1.324841	1.880608	2.254706	C	-3.100768	-1.004718	1.431277
H	1.160125	1.576652	3.297553	C	-4.347048	-0.433562	0.844231
C	1.611468	0.917565	1.266148	C	-4.900223	0.834018	1.010398
C	3.046398	-1.599618	0.998500	H	-4.429968	1.554507	1.691691
C	4.283858	-0.923756	1.044264	C	-6.058418	1.143200	0.246062
H	4.353142	0.074785	1.501435	C	-6.628498	0.177063	-0.619725
C	5.412306	-1.491645	0.434530	H	-7.526498	0.464172	-1.186704
H	6.370924	-0.951207	0.450900	C	-6.052044	-1.098412	-0.763238
C	5.309375	-2.726448	-0.229896	H	-6.482611	-1.841266	-1.451373
H	6.192217	-3.158211	-0.725811	C	-4.898404	-1.389232	-0.031911
C	4.075138	-3.397129	-0.283671	C	-6.104969	3.382375	1.076273
H	3.988570	-4.355619	-0.818551	H	-5.064868	3.610043	0.753191
C	2.944247	-2.836127	0.328628	H	-6.099013	3.115058	2.156219
H	1.958806	-3.326865	0.279797	H	-6.737713	4.277047	0.929153
C	1.663123	-0.860123	3.516154				
C	0.468751	-0.994545	4.256861	IM3F			
H	-0.483153	-1.152051	3.722534	Ni	0.791294	-1.040202	-0.003875
C	0.504388	-0.921290	5.658914	P	0.289352	0.104038	-1.762881
H	-0.430087	-1.021589	6.232869	P	0.319642	0.574443	1.458226
C	1.728294	-0.734345	6.326014	C	0.913394	-0.486843	-3.385919
H	1.755734	-0.687959	7.426150	C	2.290872	-0.390247	-3.688791
C	2.919755	-0.615468	5.588014	H	2.989091	0.030516	-2.951415
H	3.881244	-0.480495	6.107921	C	2.784902	-0.858498	-4.914118
C	2.889295	-0.672513	4.184538	H	3.858351	-0.767886	-5.136189
H	3.825094	-0.582242	3.613506	C	1.922176	-1.478725	-5.832926
O	1.938071	2.915671	-1.761115	H	2.315215	-1.860196	-6.787956
C	2.025328	4.193134	-2.388561	C	0.564950	-1.640041	-5.511403

H	-0.112567	-2.156285	-6.209298	C	1.114737	-1.146737	5.097119
C	0.061464	-1.150005	-4.296197	H	1.645399	-2.046267	5.440983
H	-1.000495	-1.292321	-4.053411	C	0.604286	-0.221750	6.023199
C	-1.538978	0.088744	-2.006641	H	0.726225	-0.398655	7.103447
C	-2.366520	-0.630877	-1.131082	C	-0.072912	0.925419	5.570335
H	-1.902802	-1.145346	-0.281197	H	-0.489199	1.644952	6.293136
C	-3.757889	-0.640380	-1.310584	C	-0.215903	1.161405	4.193846
H	-4.393663	-1.191646	-0.602884	H	-0.752636	2.057734	3.847194
C	-4.326854	0.058703	-2.386648	O	-2.479707	3.597705	-1.581839
H	-5.417647	0.051417	-2.532984	C	-3.577008	4.133444	-2.320859
C	-3.501287	0.778293	-3.271789	H	-3.109837	4.681404	-3.161377
H	-3.944590	1.321486	-4.121127	H	-4.181825	4.835002	-1.712469
C	-2.112490	0.809652	-3.077644	H	-4.229205	3.332658	-2.718975
H	-1.470642	1.391089	-3.756863	O	-0.327035	4.798775	0.385238
C	0.606475	1.933841	-1.728837	C	-1.015458	6.003015	0.018458
C	1.655680	2.499696	-2.480763	H	-1.553101	6.332698	0.927042
H	2.176078	1.901290	-3.238747	H	-1.747180	5.795497	-0.788123
C	2.075033	3.815723	-2.263142	H	-0.315278	6.800505	-0.304190
H	2.924856	4.236213	-2.819905	Cl	-5.384585	2.811346	-0.283927
C	1.438685	4.593240	-1.286603	Cl	2.109946	6.157950	-0.878999
C	0.316013	4.093356	-0.588881	O	0.351504	-2.701249	1.141030
C	-0.105046	2.754776	-0.809797	O	-0.854015	-4.091916	-1.057680
C	-1.313717	2.306861	-0.039217	O	-1.777774	-1.896887	2.944146
C	-2.581291	2.785851	-0.497727	O	-6.916326	-3.145569	1.283400
C	-3.746998	2.362528	0.187716	N	-0.950657	-2.935438	0.995846
C	-3.647930	1.509457	1.302449	C	-1.497345	-3.655046	-0.115006
H	-4.576150	1.194010	1.800502	C	-1.952221	-2.526481	1.907739
C	-2.410664	1.054295	1.754067	C	-3.243583	-2.995952	1.311389
H	-2.356314	0.348135	2.595114	C	-4.542031	-2.778502	1.768487
C	-1.232464	1.460074	1.088343	H	-4.708883	-2.227255	2.703603
C	1.672468	1.841045	1.362319	C	-5.603534	-3.288117	0.971625
C	1.598491	3.037080	2.106677	C	-5.327857	-3.987830	-0.232171
H	0.715065	3.250856	2.723720	H	-6.184380	-4.359959	-0.813548
C	2.632955	3.980413	2.032049	C	-4.008636	-4.188218	-0.670490
H	2.554068	4.921225	2.597695	H	-3.798626	-4.716093	-1.612744
C	3.754372	3.735872	1.218476	C	-2.967454	-3.684046	0.116533
H	4.560100	4.482968	1.151258	C	-7.258563	-2.439681	2.472790
C	3.835287	2.541732	0.483414	H	-6.897311	-1.387992	2.440740
H	4.709278	2.342679	-0.156044	H	-6.845603	-2.937789	3.377144
C	2.800807	1.594656	0.556307	H	-8.362550	-2.443082	2.527466
H	2.862877	0.659202	-0.019039	C	4.371415	-2.515465	1.182601
C	0.313073	0.242024	3.262405	H	5.236623	-1.842801	0.982825
C	0.957935	-0.925028	3.719955	C	3.090866	-1.885243	0.656132
H	1.290926	-1.680192	2.993228	C	2.423467	-2.004391	-0.515033

C	2.867415	-2.651204	-1.744126	H	3.797568	-1.952067	0.164150
C	1.996570	-3.479288	-2.493095	C	3.409284	-2.503114	-1.906797
H	0.967763	-3.621636	-2.130107	H	4.276152	-3.178311	-1.973063
C	2.452521	-4.119635	-3.652750	C	2.562152	-2.332363	-3.017972
C	3.776244	-3.941846	-4.097511	H	2.774162	-2.864773	-3.958860
H	4.126217	-4.445306	-5.012455	C	1.447999	-1.481398	-2.933923
C	4.644022	-3.100993	-3.377575	H	0.771588	-1.366510	-3.795091
H	5.676487	-2.940713	-3.727557	C	-1.681486	-0.683113	-1.951065
C	4.190311	-2.451217	-2.221990	C	-2.731618	-0.233330	-2.778347
H	4.858456	-1.770052	-1.671094	H	-2.611521	0.681430	-3.371902
C	4.652291	-3.932425	0.696892	C	-3.946487	-0.923258	-2.853750
H	5.538120	-4.338447	1.223839	H	-4.773058	-0.542286	-3.471193
H	4.843985	-3.947286	-0.390771	C	-4.126013	-2.099538	-2.113581
H	3.777302	-4.579061	0.904821	C	-3.066054	-2.631298	-1.346787
H	1.764026	-4.763905	-4.221821	C	-1.844438	-1.910531	-1.254648
C	4.271806	-1.601345	3.478165	C	-0.776505	-2.520282	-0.400057
O	4.237566	-1.736251	4.685855	C	-0.090950	-3.655097	-0.930875
O	4.315639	-0.412613	2.826864	C	0.899604	-4.275206	-0.130859
C	4.203718	0.750112	3.670278	C	1.190772	-3.779161	1.150937
H	4.314855	1.618549	2.998356	H	1.965596	-4.285225	1.744694
H	3.208594	0.771449	4.157129	C	0.522991	-2.664130	1.657882
H	4.992387	0.744330	4.448173	H	0.788897	-2.281995	2.652210
O	4.269472	-2.653845	2.643615	C	-0.464382	-2.021692	0.883379
H	2.615438	-1.263923	1.444256	C	-2.991334	-0.647925	1.278027
				C	-3.651266	-1.833529	1.661095
TS2F				H	-3.074847	-2.677182	2.068114
Ni	-0.526672	1.348418	0.352797	C	-5.032786	-1.966110	1.455442
P	-0.209151	0.400484	-1.570024	H	-5.538767	-2.901803	1.737809
P	-1.172756	-0.407974	1.453557	C	-5.760853	-0.927645	0.849033
C	-0.050745	1.500897	-3.038632	H	-6.839302	-1.047892	0.663975
C	-1.087856	2.418971	-3.327127	C	-5.103012	0.247384	0.444564
H	-1.958983	2.486182	-2.658946	H	-5.662103	1.045652	-0.068986
C	-0.997259	3.282380	-4.427584	C	-3.723418	0.389692	0.662493
H	-1.816222	3.987587	-4.634713	H	-3.178683	1.286757	0.319651
C	0.157577	3.282078	-5.227832	C	-0.786820	-0.509136	3.258223
H	0.238625	3.972601	-6.081699	C	0.440205	0.081875	3.637181
C	1.224135	2.428090	-4.903947	H	1.056303	0.622148	2.887072
H	2.152433	2.453373	-5.496171	C	0.877104	-0.007593	4.969031
C	1.124743	1.543733	-3.816854	H	1.851313	0.431853	5.230853
H	1.979698	0.907104	-3.552977	C	0.081383	-0.653592	5.930790
C	1.201526	-0.769231	-1.741803	H	0.418419	-0.715964	6.978072
C	2.049268	-0.942837	-0.632984	C	-1.153172	-1.218016	5.557016
H	1.811246	-0.394033	0.289275	H	-1.785679	-1.712561	6.311316
C	3.144039	-1.816198	-0.710501	C	-1.586148	-1.155203	4.222976

H	-2.555314	-1.591185	3.943716	H	-1.754275	6.974426	-2.752153
O	-0.508662	-4.005481	-2.175362	C	-1.262885	5.274858	-1.493355
C	0.210537	-4.853500	-3.072734	H	-2.244424	5.250355	-0.993992
H	-0.256489	-4.683256	-4.061990	C	0.128161	3.974964	3.155445
H	0.111888	-5.922326	-2.796323	H	-0.042830	4.122911	4.240027
H	1.281154	-4.578574	-3.118385	H	0.504413	4.926454	2.724333
O	-3.194284	-3.764005	-0.594269	H	0.894295	3.195794	2.952510
C	-3.390341	-5.012903	-1.273078	H	2.221511	5.296481	-3.264911
H	-3.394784	-5.788144	-0.484018	C	-3.178040	2.155876	3.389828
H	-2.552098	-5.202570	-1.973153	O	-3.578704	1.199520	3.988823
H	-4.355483	-5.040531	-1.819538	O	-3.846526	3.142167	2.815697
Cl	1.814926	-5.690194	-0.639630	C	-5.292067	3.037337	2.911508
Cl	-5.704582	-2.863280	-2.097268	H	-5.684414	3.916645	2.373817
O	1.787547	1.833187	1.435092	H	-5.622612	2.095599	2.432059
O	3.025553	2.028434	-1.162775	H	-5.601228	3.051987	3.974225
O	3.630101	0.558205	3.209961	O	-1.770557	2.371744	3.218515
O	8.368406	-1.210860	0.879194	H	-1.373678	1.645726	2.531767
N	3.008895	1.455555	1.125781				
C	3.573776	1.542993	-0.172242	IM4F			
C	3.877095	0.800951	2.028795	Ni	0.095590	1.169898	0.921609
C	5.095610	0.440559	1.235008	P	0.758361	1.132591	-1.183864
C	6.227388	-0.268565	1.629643	P	-1.363615	-0.456121	1.173843
H	6.325235	-0.610771	2.668851	C	0.990763	2.749351	-2.018262
C	7.214849	-0.526807	0.635502	C	-0.133282	3.540343	-2.362067
C	7.032651	-0.074791	-0.691809	H	-1.149247	3.161039	-2.185587
H	7.820972	-0.303916	-1.424401	C	0.029872	4.823270	-2.901864
C	5.874665	0.639984	-1.063016	H	-0.859070	5.415730	-3.165263
H	5.726214	0.977818	-2.099794	C	1.316566	5.362204	-3.069162
C	4.913119	0.894484	-0.084371	H	1.444075	6.372718	-3.487270
C	8.603951	-1.689172	2.197267	C	2.434166	4.620099	-2.653381
H	7.822604	-2.413498	2.519126	H	3.444818	5.051033	-2.730473
H	8.648097	-0.857988	2.935868	C	2.275305	3.331210	-2.121719
H	9.583385	-2.202194	2.171426	H	3.154464	2.788722	-1.750156
C	-1.158305	3.652966	2.426778	C	2.317798	0.193436	-1.534525
H	-1.963770	4.400521	2.549602	C	2.692259	-0.823725	-0.634124
C	-0.983206	3.108159	1.091096	H	2.053452	-1.031675	0.233484
C	-0.572518	3.337387	-0.111873	C	3.865099	-1.569016	-0.840639
C	-0.283941	4.311488	-1.135176	H	4.131834	-2.365426	-0.131302
C	0.974451	4.326874	-1.786096	C	4.686087	-1.296733	-1.944681
H	1.720732	3.564706	-1.513866	H	5.616215	-1.865672	-2.096462
C	1.241724	5.295142	-2.762230	C	4.300141	-0.309087	-2.871152
C	0.267813	6.247081	-3.116587	H	4.921283	-0.111716	-3.759059
H	0.482561	6.997170	-3.894227	C	3.116307	0.420388	-2.678408
C	-0.986368	6.233026	-2.478397	H	2.812661	1.168516	-3.425225

C	-0.466975	0.183945	-2.244752	C	-2.206443	-4.148728	-3.176770
C	-1.046878	0.793022	-3.378851	H	-2.541124	-5.026671	-2.593320
H	-0.702632	1.779905	-3.710195	H	-1.161014	-4.301711	-3.509494
C	-2.071125	0.173517	-4.101759	H	-2.878706	-4.009309	-4.046665
H	-2.544898	0.684055	-4.952905	Cl	2.496451	-5.015076	-1.098368
C	-2.522350	-1.097482	-3.723783	Cl	-3.930573	-1.762958	-4.525905
C	-1.882849	-1.799892	-2.677861	O	1.458460	0.500763	2.176071
C	-0.863663	-1.148391	-1.922173	O	3.112780	2.409525	0.782588
C	-0.196287	-2.003180	-0.888866	O	3.086500	-1.651396	3.035376
C	0.638846	-3.042892	-1.377824	O	8.389430	-1.467217	1.357574
C	1.371351	-3.834312	-0.468412	N	2.772919	0.438550	2.011576
C	1.239959	-3.653013	0.916699	C	3.546134	1.376772	1.283156
H	1.832976	-4.266144	1.609419	C	3.529851	-0.678809	2.440583
C	0.359847	-2.679996	1.399340	C	4.919497	-0.410286	1.949547
H	0.264237	-2.542305	2.484271	C	6.047280	-1.222698	2.037023
C	-0.371751	-1.858251	0.514256	H	5.999137	-2.171934	2.587462
C	-2.904384	-0.525942	0.174692	C	7.220971	-0.777633	1.369861
C	-3.595193	-1.745938	0.015806	C	7.220761	0.446498	0.652768
H	-3.210827	-2.664095	0.483353	H	8.152124	0.741941	0.147398
C	-4.746113	-1.806697	-0.785006	C	6.070183	1.248824	0.585172
H	-5.266971	-2.767280	-0.911727	H	6.070416	2.191950	0.018623
C	-5.211777	-0.654285	-1.436194	C	4.917985	0.806773	1.242248
H	-6.107916	-0.704413	-2.073156	C	8.453685	-2.708894	2.053549
C	-4.515283	0.559547	-1.296639	H	7.732925	-3.447556	1.638677
H	-4.866534	1.461215	-1.821500	H	8.255265	-2.578870	3.140064
C	-3.367609	0.625897	-0.496110	H	9.482666	-3.088054	1.914700
H	-2.810709	1.567400	-0.390597	C	-3.067033	2.257121	2.793283
C	-1.845013	-0.975557	2.871403	H	-4.109598	2.228015	2.420537
C	-0.899607	-0.735296	3.895978	C	-2.100406	2.445912	1.900189
H	0.088346	-0.317846	3.635674	C	-1.116591	2.653724	1.044427
C	-1.220640	-1.032771	5.230380	C	-0.757497	4.012553	0.588207
H	-0.474388	-0.850081	6.019415	C	0.589104	4.448278	0.583128
C	-2.491283	-1.536649	5.564646	H	1.385129	3.736392	0.848079
H	-2.744441	-1.747473	6.615462	C	0.902236	5.768555	0.235251
C	-3.434603	-1.772804	4.549565	C	-0.114170	6.672166	-0.124381
H	-4.431454	-2.176014	4.787289	H	0.138433	7.707660	-0.402305
C	-3.109676	-1.506880	3.207192	C	-1.454489	6.245008	-0.137153
H	-3.847512	-1.758212	2.430418	H	-2.255609	6.946060	-0.421449
O	0.711930	-3.324598	-2.714441	C	-1.774208	4.925531	0.212404
C	1.572536	-2.518144	-3.531936	H	-2.820953	4.582748	0.211789
H	1.221710	-1.467093	-3.573804	C	-2.861539	2.097088	4.278483
H	1.532201	-2.959719	-4.545202	H	-3.273873	1.129224	4.638533
H	2.614761	-2.543462	-3.155634	H	-3.392664	2.898734	4.837618
O	-2.266797	-3.038485	-2.265422	H	-1.787901	2.131055	4.543511

H	1.954362	6.092568	0.236504	C	-0.274300	-2.430228	-2.259932
C	-6.350903	-0.675704	1.849410	C	0.976081	-3.071219	-2.089585
O	-6.205115	-1.847891	2.159043	C	1.549688	-3.175761	-0.811338
O	-7.369435	-0.176588	1.128343	H	2.528221	-3.666354	-0.709163
C	-8.318251	-1.150274	0.667626	C	0.907648	-2.652766	0.309850
H	-9.106448	-0.579467	0.144907	H	1.405420	-2.733442	1.283100
H	-7.835720	-1.863796	-0.030886	C	-0.334325	-1.998840	0.177473
H	-8.750143	-1.717244	1.516660	C	-2.831717	-1.345547	1.525903
O	-5.529251	0.335467	2.180851	C	-3.373448	-2.637533	1.362634
H	-4.749560	-0.063970	2.635885	H	-2.702635	-3.503060	1.251770
				C	-4.761293	-2.817055	1.309162
(S)-L2-TS3A				H	-5.171675	-3.828496	1.160100
Ni	-0.462164	1.063140	1.337283	C	-5.644322	-1.719080	1.418095
P	-0.965789	1.271880	-0.753147	C	-5.089886	-0.432746	1.589012
P	-1.021619	-1.045960	1.608059	H	-5.759540	0.439001	1.669879
C	-1.446113	2.968323	-1.271269	C	-3.701525	-0.245155	1.641331
C	-2.396799	3.638344	-0.465944	H	-3.268512	0.763275	1.751899
H	-2.812821	3.126897	0.417011	C	-0.558851	-1.968713	3.146863
C	-2.783190	4.949676	-0.756575	C	0.796519	-2.100355	3.533427
H	-3.517902	5.454061	-0.109168	H	1.589761	-1.647741	2.919322
C	-2.209269	5.654036	-1.839195	C	1.138659	-2.755396	4.724083
C	-1.244309	4.989842	-2.621191	H	2.205216	-2.851517	4.986975
H	-0.767851	5.524099	-3.459531	C	0.153710	-3.275362	5.592501
C	-0.864718	3.664996	-2.346297	C	-1.195288	-3.104730	5.221233
H	-0.094298	3.182565	-2.965127	H	-1.992040	-3.479791	5.884780
C	0.367827	0.753003	-1.905975	C	-1.550289	-2.467703	4.020840
C	1.583520	0.320770	-1.342413	H	-2.614959	-2.357561	3.771672
H	1.659777	0.302765	-0.246552	O	-0.977683	-2.231609	-3.405395
C	2.624071	-0.129242	-2.162733	C	-0.577336	-2.656924	-4.704187
H	3.562405	-0.485956	-1.710346	H	-1.393427	-2.325525	-5.375018
C	2.486755	-0.143605	-3.567765	H	-0.474223	-3.758932	-4.766647
C	1.258713	0.280394	-4.121781	H	0.371081	-2.178133	-5.017332
H	1.128971	0.269190	-5.216602	O	-3.145452	-3.351077	-1.629547
C	0.199983	0.708316	-3.304878	C	-3.437028	-4.139483	-2.789577
H	-0.763107	0.992428	-3.756490	H	-2.648742	-4.916249	-2.853800
C	-2.376797	0.228527	-1.341870	H	-3.409109	-3.521674	-3.710053
C	-3.626007	0.799056	-1.658551	H	-4.430090	-4.626848	-2.705336
H	-3.744292	1.891759	-1.664255	Cl	1.923737	-3.760613	-3.410471
C	-4.731380	-0.009157	-1.946799	Cl	-6.010461	-2.408422	-2.171150
H	-5.715161	0.432517	-2.162230	C	1.368263	1.295307	3.689672
C	-4.591289	-1.403905	-1.932332	H	1.091819	0.380503	4.242233
C	-3.338250	-2.004062	-1.675758	C	0.387892	1.938858	2.952114
C	-2.225522	-1.181705	-1.362259	C	-0.042071	2.771377	2.034220
C	-0.919182	-1.876576	-1.107197	C	-0.224185	4.177018	1.724414

C	0.479554	4.741405	0.631933	H	0.935688	-5.007298	6.644146
H	1.159801	4.099027	0.054809	H	1.335606	-3.448509	7.412311
C	0.314698	6.094897	0.313020	C	-7.136591	-1.907642	1.300699
C	-0.557711	6.905033	1.063702	H	-7.453059	-2.907292	1.660659
H	-0.684034	7.968978	0.808437	H	-7.694105	-1.136324	1.869222
C	-1.264852	6.348404	2.144002	H	-7.447146	-1.830357	0.235850
H	-1.951143	6.974753	2.736273				
C	-1.100459	4.995102	2.477045	(S)-L2-TS3B			
H	-1.655071	4.552684	3.318851	Ni	-0.412095	0.949347	1.436951
C	2.666739	1.952567	4.054258	P	-1.004231	1.406331	-0.585231
H	3.496405	1.214745	4.056622	P	-0.898777	-1.197719	1.432956
H	2.600164	2.367924	5.085616	C	-1.542215	3.137022	-0.890343
H	2.909275	2.772998	3.353589	C	-2.415496	3.717418	0.057490
H	0.867885	6.521138	-0.538288	H	-2.737230	3.123113	0.927900
O	1.996900	0.161349	1.975671	C	-2.838046	5.042922	-0.078576
O	3.165462	2.457947	0.749620	H	-3.507210	5.479126	0.679965
O	3.840396	-2.020349	1.807431	C	-2.380645	5.845416	-1.148104
O	8.305253	-1.060370	-1.375675	C	-1.502061	5.263021	-2.082882
N	3.217996	0.221477	1.480819	H	-1.121601	5.872451	-2.918947
C	3.724963	1.372023	0.796019	C	-1.085772	3.926861	-1.960926
C	4.062041	-0.905912	1.346606	H	-0.381422	3.508588	-2.694580
C	5.206758	-0.435312	0.502274	C	0.339765	1.081246	-1.790887
C	6.292280	-1.163493	0.018516	C	1.603048	0.737012	-1.270701
H	6.404128	-2.223311	0.284063	H	1.711897	0.674568	-0.177891
C	7.210052	-0.479839	-0.824908	C	2.662840	0.437898	-2.134649
C	7.011512	0.888574	-1.144559	H	3.643757	0.158151	-1.720018
H	7.748157	1.370455	-1.804440	C	2.492840	0.478114	-3.535524
C	5.909608	1.599743	-0.641956	C	1.217679	0.805890	-4.044407
H	5.751197	2.657238	-0.901678	H	1.056498	0.811051	-5.134445
C	5.005980	0.923159	0.184737	C	0.146707	1.099267	-3.187087
C	8.555311	-2.436778	-1.103892	H	-0.850095	1.306406	-3.605308
H	7.726488	-3.081983	-1.469664	C	-2.416289	0.425315	-1.268282
H	8.704351	-2.618130	-0.016855	C	-3.680812	1.020150	-1.453431
H	9.483380	-2.694833	-1.646063	H	-3.808515	2.103034	-1.318809
C	-2.592291	7.088133	-2.106781	C	-4.786309	0.234691	-1.785629
H	-2.266700	7.739080	-1.266872	H	-5.783194	0.684795	-1.899811
H	-2.126462	7.472200	-3.035638	C	-4.652245	-1.154201	-1.943439
H	-3.692685	7.205725	-2.196554	C	-3.383092	-1.771853	-1.831428
C	3.619029	-0.632626	-4.436964	C	-2.263348	-0.965753	-1.472839
H	3.426634	-0.442310	-5.511428	C	-0.931695	-1.647937	-1.373387
H	4.577002	-0.144503	-4.161385	C	-0.332687	-2.012498	-2.612082
H	3.758667	-1.726692	-4.304054	C	0.954445	-2.591989	-2.613796
C	0.538182	-3.992353	6.864543	C	1.614237	-2.862257	-1.407202
H	-0.328377	-4.114215	7.544434	H	2.620422	-3.304876	-1.423257

C	1.009576	-2.531719	-0.191821	C	-0.959645	6.199747	2.703539
H	1.569894	-2.731501	0.727065	H	-1.560653	6.797501	3.407478
C	-0.256958	-1.913021	-0.152284	C	-0.820866	4.818707	2.909442
C	-2.706970	-1.533080	1.361309	H	-1.312808	4.325408	3.761887
C	-3.217272	-2.821722	1.102621	H	0.918014	6.522639	-0.150249
H	-2.525411	-3.652225	0.895299	O	2.071150	-0.112424	1.997360
C	-4.600942	-3.041921	1.096347	O	3.359839	2.311750	1.240291
H	-4.989827	-4.051310	0.885176	O	3.833012	-2.310647	1.410636
C	-5.509460	-1.990223	1.350475	O	8.378573	-0.960082	-1.492567
C	-4.985065	-0.705787	1.611979	N	3.291062	-0.024197	1.493779
H	-5.674863	0.131775	1.805780	C	3.865259	1.213023	1.060128
C	-3.602423	-0.478087	1.619262	C	4.093926	-1.135321	1.164313
H	-3.192570	0.528597	1.806641	C	5.268754	-0.565833	0.428663
C	-0.406869	-2.340298	2.809448	C	6.331239	-1.236462	-0.173644
C	0.938728	-2.689081	3.064172	H	6.391864	-2.331553	-0.116525
H	1.752266	-2.252915	2.470136	C	7.297082	-0.445659	-0.854830
C	1.270849	-3.524044	4.140169	C	7.166579	0.966203	-0.903168
H	2.330781	-3.784688	4.296617	H	7.938288	1.532030	-1.445896
C	0.293044	-4.002050	5.037444	C	6.086429	1.617529	-0.284178
C	-1.040733	-3.600197	4.815865	H	5.981623	2.711901	-0.331971
H	-1.830467	-3.930428	5.510920	C	5.136255	0.836111	0.381810
C	-1.389276	-2.793890	3.721419	C	8.563116	-2.372891	-1.487280
H	-2.443040	-2.514158	3.583950	H	7.715260	-2.897574	-1.980289
O	-1.025355	-1.688821	-3.740526	H	8.681207	-2.765730	-0.453527
C	-1.259375	-2.680507	-4.743145	H	9.490444	-2.565317	-2.057341
H	-2.276126	-2.492752	-5.143680	C	1.266142	0.013274	4.797274
H	-1.219973	-3.704087	-4.316650	H	0.280958	-0.470754	4.666512
H	-0.521612	-2.606019	-5.567898	H	2.048937	-0.768957	4.812667
O	-3.099618	-3.094486	-1.948100	H	1.283856	0.516664	5.791871
C	-3.852642	-3.998532	-2.755417	H	2.540215	1.487335	3.720174
H	-3.164046	-4.835776	-2.982503	C	-2.789069	7.294072	-1.244900
H	-4.181885	-3.527044	-3.703664	H	-2.343122	7.877089	-0.410049
H	-4.738777	-4.389653	-2.217404	H	-2.455485	7.753614	-2.196125
Cl	1.791276	-2.915232	-4.123700	H	-3.890054	7.413596	-1.168290
Cl	-6.133795	-2.068198	-2.209560	C	-7.000708	-2.215989	1.307847
C	1.532391	1.031341	3.736854	H	-7.255397	-3.290197	1.403792
C	0.551764	1.726210	3.052548	H	-7.521392	-1.659163	2.113648
C	0.091797	2.603057	2.197443	H	-7.414889	-1.862921	0.338792
C	-0.054824	4.035981	2.013082	C	0.660119	-4.913752	6.183566
C	0.569302	4.666709	0.909844	H	-0.089211	-4.868824	6.999268
H	1.164457	4.054344	0.217585	H	0.716673	-5.972256	5.845992
C	0.429470	6.046213	0.713848	H	1.652672	-4.657110	6.606917
C	-0.336315	6.819613	1.606150	C	3.647277	0.143687	-4.447800
H	-0.444060	7.904208	1.447583	H	3.394535	0.317546	-5.512299

H	4.544471	0.748149	-4.198336	H	-1.583974	7.793441	-2.070927
H	3.931059	-0.924399	-4.337858	C	-2.259248	6.285377	-0.648951
				H	-3.279287	6.695381	-0.577985
(S)-L3-TS3A				C	-1.915413	5.143081	0.088653
Ni	-0.650453	1.576550	0.807821	H	-2.654445	4.645486	0.735777
P	-1.613768	1.087825	-1.053607	C	2.964113	3.161090	2.348815
P	-0.856602	-0.297614	1.953329	H	3.751415	2.392660	2.499675
C	-2.986143	-0.142590	-0.896650	H	3.110145	3.931404	3.139805
C	-4.323283	0.262858	-1.103019	H	3.107731	3.632644	1.359352
H	-4.539573	1.255676	-1.518921	H	0.741132	6.853559	-2.219918
C	-5.389671	-0.573230	-0.757019	O	1.899189	0.796547	1.252207
H	-6.431189	-0.243336	-0.884264	O	3.219478	2.188176	-0.867883
C	-5.136807	-1.831375	-0.189691	O	3.592018	-1.328418	2.153696
C	-3.809486	-2.295318	-0.032321	O	8.254831	-2.053942	-0.803363
C	-2.732836	-1.444518	-0.399929	N	3.070872	0.481544	0.749454
C	-1.354277	-2.012193	-0.258769	C	3.678787	1.184952	-0.339603
C	-0.927792	-2.897214	-1.285327	C	3.866912	-0.590445	1.210753
C	0.361894	-3.471060	-1.203210	C	5.060411	-0.609752	0.306556
C	1.186471	-3.220137	-0.096110	C	6.143485	-1.486706	0.305086
H	2.186395	-3.676384	-0.054909	H	6.194740	-2.296621	1.045155
C	0.761162	-2.347237	0.909404	C	7.147761	-1.279159	-0.679696
H	1.450230	-2.122000	1.733532	C	7.033853	-0.214044	-1.609741
C	-0.497127	-1.711456	0.825843	H	7.837746	-0.095666	-2.351378
O	-1.778895	-3.050423	-2.340618	C	5.932700	0.657920	-1.584244
C	-2.070979	-4.353808	-2.853429	H	5.847717	1.482741	-2.307887
H	-3.135379	-4.338510	-3.163526	C	4.942627	0.448022	-0.617828
H	-1.928296	-5.135762	-2.079044	C	8.427239	-3.143234	0.098681
H	-1.437886	-4.598472	-3.730200	H	7.599909	-3.881380	0.010784
O	-3.467826	-3.486170	0.535068	H	8.492260	-2.794676	1.152870
C	-4.088090	-4.703055	0.106526	H	9.379335	-3.629433	-0.182523
H	-3.304626	-5.486049	0.149528	C	-0.498299	0.389689	-2.331641
H	-4.464957	-4.621166	-0.933767	C	0.810827	1.116915	-2.621129
H	-4.928101	-4.987986	0.771678	C	0.837416	-0.209501	-1.923740
Cl	1.024794	-4.394535	-2.544592	H	-1.017982	-0.090557	-3.178236
Cl	-6.498244	-2.759749	0.419517	H	1.063260	1.996194	-2.007345
C	1.594940	2.558990	2.474521	H	1.126673	1.180184	-3.674723
H	1.390314	1.960524	3.378986	H	1.164772	-1.104202	-2.474055
C	0.515621	2.970822	1.722541	H	1.070624	-0.203625	-0.847650
C	-0.234589	3.406613	0.739864	C	-2.447915	2.478886	-1.912840
C	-0.605013	4.612774	0.019337	C	-1.733266	3.343499	-2.929262
C	0.349103	5.245738	-0.816209	C	-2.865109	2.448425	-3.373516
H	1.362771	4.820465	-0.879162	H	-3.106864	3.032055	-1.222509
C	-0.006175	6.376422	-1.566213	H	-0.711066	3.063120	-3.220163
C	-1.308981	6.902888	-1.484395	H	-1.905489	4.428543	-2.857055

H	-3.832719	2.905393	-3.638205	O	-3.622386	-3.343855	0.310804
H	-2.614162	1.550642	-3.961703	C	-4.289299	-4.508311	-0.187533
C	-2.521249	-0.599954	2.668362	H	-3.548770	-5.332280	-0.151185
C	-3.073164	0.465457	3.614534	H	-4.624753	-4.365469	-1.235301
C	-3.684461	0.282072	2.256863	H	-5.165249	-4.774875	0.437570
H	-2.755542	-1.652906	2.899149	Cl	0.969895	-4.348399	-2.567078
H	-2.463077	1.371072	3.771288	Cl	-6.612222	-2.462995	0.114097
H	-3.616421	0.117189	4.507396	C	1.694088	2.576450	2.566389
H	-4.670522	-0.198089	2.165384	C	0.662650	2.994400	1.758051
H	-3.469873	1.054831	1.501610	C	-0.026091	3.398680	0.722840
C	0.287552	-0.636195	3.349372	C	-0.208771	4.588274	-0.094895
C	-0.014989	-0.294663	4.794937	C	0.849961	5.006131	-0.939547
C	0.059031	-1.740990	4.360738	H	1.787024	4.427780	-0.932442
H	1.324909	-0.464404	3.016605	C	0.690729	6.126158	-1.768698
H	-1.005530	0.108084	5.051398	C	-0.514550	6.853296	-1.758002
H	0.813671	0.120265	5.391666	H	-0.634869	7.735010	-2.406833
H	0.933338	-2.344386	4.653735	C	-1.565418	6.449698	-0.912660
H	-0.886971	-2.304615	4.311685	H	-2.508593	7.018746	-0.896160
				C	-1.419136	5.319668	-0.093854
(S)-L3-TS3B				H	-2.238047	4.991813	0.565329
Ni	-0.580223	1.614447	0.898028	H	1.516833	6.438640	-2.427122
P	-1.487915	1.195798	-1.006262	O	1.912817	0.681738	1.543431
P	-0.942756	-0.289498	1.967787	O	3.235099	2.224544	-0.448099
C	-2.926468	0.033722	-0.938986	O	3.538628	-1.600016	2.175891
C	-4.233814	0.518765	-1.165085	O	8.055388	-2.230639	-1.021362
H	-4.386621	1.541896	-1.531963	N	3.064201	0.369287	0.984980
C	-5.351380	-0.278304	-0.899920	C	3.665260	1.149528	-0.048546
H	-6.369930	0.110849	-1.044379	C	3.818990	-0.778482	1.306521
C	-5.182890	-1.575806	-0.391810	C	4.977437	-0.761933	0.354974
C	-3.886931	-2.113325	-0.210961	C	6.014042	-1.683220	0.221279
C	-2.757732	-1.300246	-0.497876	H	6.050244	-2.566903	0.872561
C	-1.411338	-1.927463	-0.321733	C	6.993394	-1.421495	-0.776088
C	-0.979208	-2.809016	-1.349880	C	6.901902	-0.261686	-1.587022
C	0.288637	-3.423385	-1.235557	H	7.684366	-0.104870	-2.344311
C	1.084610	-3.211911	-0.099100	C	5.847943	0.654192	-1.428218
H	2.070314	-3.695236	-0.033214	H	5.780022	1.553143	-2.059492
C	0.653395	-2.342549	0.905968	C	4.882548	0.391025	-0.450583
H	1.323759	-2.150883	1.753368	C	8.201950	-3.415154	-0.243794
C	-0.584190	-1.670484	0.795023	H	7.335657	-4.100348	-0.375299
O	-1.802070	-2.916175	-2.433158	H	8.319868	-3.182961	0.837597
C	-2.105213	-4.197765	-2.992084	H	9.118130	-3.913778	-0.609924
H	-3.154772	-4.145517	-3.345447	C	1.539545	2.183575	4.003155
H	-2.015672	-5.002386	-2.233139	H	0.508710	1.849044	4.220947
H	-1.442611	-4.437328	-3.848122	H	2.246248	1.374618	4.274388

H	1.774864	3.057444	4.653260	C	-4.573935	-1.650047	-1.362170
H	2.714018	2.838368	2.227572	C	-3.315481	-2.209288	-1.037259
C	-0.326901	0.457040	-2.220697	C	-2.174247	-1.361925	-0.983054
C	1.001111	1.168549	-2.459698	C	-0.876286	-1.991578	-0.578970
C	0.981798	-0.142851	-1.735344	C	-0.229311	-2.838683	-1.524456
H	-0.811667	-0.032348	-3.082699	C	1.030299	-3.391433	-1.187639
H	1.226489	2.061135	-1.854888	C	1.598940	-3.154937	0.075940
H	1.368830	1.206167	-3.497626	H	2.583235	-3.586729	0.307674
H	1.332164	-1.050668	-2.248387	C	0.947509	-2.350387	1.012386
H	1.153900	-0.115938	-0.648396	H	1.416064	-2.164928	1.985957
C	-2.212286	2.621496	-1.909512	C	-0.290262	-1.761731	0.690716
C	-1.463004	3.379371	-2.985010	O	-0.866017	-2.953340	-2.722585
C	-2.663282	2.546388	-3.359425	C	-0.849968	-4.165462	-3.481017
H	-2.817078	3.252930	-1.237076	H	-1.799213	-4.177789	-4.052141
H	-0.470441	3.012877	-3.280923	H	-0.806075	-5.057154	-2.822876
H	-1.556633	4.476027	-2.965202	H	0.003531	-4.194602	-4.186780
H	-3.603337	3.055048	-3.629117	O	-3.117007	-3.498260	-0.656109
H	-2.490766	1.601938	-3.901426	C	-3.662920	-4.583136	-1.415847
C	-2.670576	-0.516342	2.553122	H	-2.922767	-5.405307	-1.357605
C	-3.192039	0.517268	3.549666	H	-3.809838	-4.297441	-2.477252
C	-3.726813	0.493701	2.148231	H	-4.628918	-4.926796	-0.995686
H	-3.002717	-1.560015	2.684986	Cl	1.990023	-4.301633	-2.342571
H	-2.518648	1.348911	3.818669	Cl	-6.040141	-2.601311	-1.254314
H	-3.822236	0.152187	4.376355	C	1.297713	2.281435	3.360640
H	-4.742371	0.113740	1.960486	H	0.918143	1.640373	4.172773
H	-3.396715	1.299211	1.472326	C	0.402943	2.824706	2.451984
C	0.069063	-0.807919	3.413630	C	0.051320	3.330490	1.300777
C	-0.389312	-0.747052	4.856163	C	-0.090985	4.561326	0.545116
C	-0.221061	-2.085630	4.177979	C	0.662429	4.734438	-0.643841
H	1.126874	-0.568835	3.216074	H	1.361593	3.939288	-0.939958
H	-1.414008	-0.413041	5.074463	C	0.516801	5.901161	-1.404649
H	0.360374	-0.434537	5.600990	C	-0.392239	6.901452	-1.011779
H	0.640082	-2.718695	4.446175	H	-0.518998	7.806189	-1.625843
H	-1.133752	-2.647993	3.919799	C	-1.144569	6.732604	0.164021
				H	-1.858230	7.510782	0.478480
(S)-L4-TS3A				C	-0.994890	5.574308	0.943455
Ni	-0.414091	1.502441	1.054632	H	-1.586889	5.433093	1.860710
P	-0.848467	1.142922	-0.990673	C	2.686405	2.829032	3.523699
P	-0.991370	-0.457821	1.770477	H	3.405155	2.011272	3.739290
C	-2.299811	0.020049	-1.282374	H	2.718195	3.527639	4.390022
C	-3.555440	0.533315	-1.664540	H	3.008763	3.372049	2.616219
H	-3.671070	1.596016	-1.916316	H	1.108376	6.025924	-2.325010
C	-4.683061	-0.292115	-1.700953	O	1.661700	0.535200	2.192925
H	-5.670795	0.115017	-1.961310	O	2.704624	2.347756	0.242395

O	3.567683	-1.597262	2.555002	H	-5.072613	-3.364508	2.365273
O	7.643690	-1.734730	-1.223502	C	-0.646401	-0.950804	3.527677
N	2.805883	0.394367	1.554417	N	-0.165632	-2.165901	3.835874
C	3.234738	1.281556	0.515329	C	-0.966335	-0.006062	4.524827
C	3.681505	-0.704602	1.723306	C	0.033786	-2.419954	5.142256
C	4.715557	-0.539957	0.651503	C	-0.745218	-0.397252	5.851542
C	5.770340	-1.388487	0.317900	H	-1.373304	0.983112	4.261675
H	5.935512	-2.310703	0.891168	N	-0.231332	-1.601876	6.173231
C	6.590469	-1.005833	-0.778114	H	0.454243	-3.412419	5.388556
C	6.336053	0.201243	-1.480939	H	-0.983713	0.283373	6.689002
H	6.999427	0.451095	-2.322091				
C	5.269595	1.039917	-1.120887	(S)-L4-TS3B			
H	5.065243	1.967682	-1.676080	Ni	-0.220306	1.291405	1.197845
C	4.454999	0.651476	-0.051387	P	-0.725391	1.174803	-0.866913
C	7.938776	-2.969233	-0.575920	P	-0.916736	-0.723088	1.702408
H	7.087695	-3.681396	-0.649720	C	-2.361836	0.407891	-1.177009
H	8.194375	-2.817655	0.495808	C	-3.505883	1.218515	-1.332503
H	8.814079	-3.392310	-1.101908	H	-3.388724	2.297382	-1.494573
C	0.419176	0.292989	-2.062984	C	-4.780463	0.645888	-1.312031
N	1.600700	-0.023517	-1.504219	H	-5.679593	1.271871	-1.408210
C	0.108967	-0.060161	-3.389314	C	-4.935898	-0.739844	-1.140224
C	2.456550	-0.725384	-2.268326	C	-3.804486	-1.582376	-1.025279
C	1.093725	-0.763452	-4.096069	C	-2.508254	-0.992904	-1.013635
H	-0.860765	0.187617	-3.840035	C	-1.340807	-1.910482	-0.818883
N	2.269546	-1.109797	-3.542135	C	-0.964460	-2.717527	-1.930856
H	3.408563	-1.020757	-1.794850	C	0.170424	-3.554825	-1.812430
H	0.925065	-1.069927	-5.144308	C	0.874213	-3.635036	-0.599548
C	-1.315326	2.626468	-2.008713	H	1.755486	-4.290467	-0.540542
N	-0.752562	2.828739	-3.211656	C	0.495837	-2.854141	0.496511
C	-2.215595	3.555698	-1.447914	H	1.079578	-2.872384	1.429140
C	-1.105787	3.955189	-3.858348	C	-0.606754	-1.982362	0.393201
C	-2.532305	4.673768	-2.230580	O	-1.691661	-2.526682	-3.060844
H	-2.632356	3.407902	-0.440567	C	-2.066868	-3.620246	-3.904693
N	-1.980422	4.883945	-3.442130	H	-3.043924	-3.342861	-4.346607
H	-0.626932	4.126118	-4.840373	H	-2.178927	-4.559609	-3.325265
H	-3.243907	5.434481	-1.865145	H	-1.330303	-3.780365	-4.716466
C	-2.813265	-0.869308	1.834744	O	-3.842786	-2.923558	-0.821903
N	-3.669974	0.153796	1.658778	C	-4.720841	-3.766094	-1.576671
C	-3.257426	-2.176003	2.116008	H	-4.188461	-4.729505	-1.700831
C	-4.979302	-0.149900	1.734322	H	-4.937034	-3.334571	-2.575366
C	-4.644585	-2.365328	2.168453	H	-5.675637	-3.940752	-1.042547
H	-2.545966	-3.001124	2.266047	Cl	0.822702	-4.413926	-3.194733
N	-5.516903	-1.356200	1.976660	Cl	-6.562226	-1.367875	-0.964537
H	-5.685182	0.686819	1.579367	C	1.564007	2.017490	3.426076

C	0.656246	2.636744	2.601614	N	0.528585	-2.409304	5.748429
C	0.043591	3.131724	1.565036	H	2.186768	-3.002291	4.610169
C	-0.298024	4.398384	0.946955	H	-1.248365	-1.726140	6.617370
C	0.666160	5.435086	0.888785	C	-2.767233	-0.779037	1.902929
H	1.645856	5.273913	1.363303	N	-3.337468	-1.982612	2.105905
C	0.386467	6.624085	0.200884	C	-3.513824	0.410445	1.885976
C	-0.861630	6.804359	-0.423480	C	-4.670406	-1.987092	2.266613
H	-1.074729	7.733572	-0.973786	C	-4.898940	0.277557	2.072799
C	-1.833439	5.789083	-0.353239	H	-3.021194	1.380482	1.716636
H	-2.809498	5.925230	-0.843882	N	-5.487116	-0.917123	2.265193
C	-1.550938	4.592939	0.318084	H	-5.145569	-2.973672	2.416744
H	-2.290977	3.778615	0.352804	H	-5.558335	1.164004	2.065772
H	1.149867	7.415834	0.143786	C	-0.596489	2.700118	-1.922913
O	1.966153	0.398734	2.061134	N	-1.619798	3.138687	-2.670617
O	2.958237	2.234369	0.139554	C	0.635670	3.384331	-1.870680
O	3.867591	-1.759423	2.346611	C	-1.409930	4.264639	-3.376648
O	8.011913	-1.706289	-1.359120	C	0.728530	4.548537	-2.643384
N	3.129913	0.291948	1.445304	H	1.469326	3.033844	-1.239523
C	3.552232	1.201815	0.433689	N	-0.288711	4.999456	-3.405780
C	3.998707	-0.826451	1.568500	H	-2.256191	4.619664	-3.993645
C	5.049973	-0.607006	0.519502	H	1.655692	5.148665	-2.642748
C	6.116876	-1.431890	0.169811	C	0.460210	0.145103	-1.881155
H	6.285641	-2.370786	0.714249	N	0.234499	0.066625	-3.204733
C	6.943735	-1.005969	-0.906222	C	1.571489	-0.450106	-1.270248
C	6.675139	0.213557	-1.580685	C	1.136040	-0.633041	-3.913962
H	7.340101	0.494782	-2.410585	C	2.456803	-1.133160	-2.117782
C	5.594479	1.027930	-1.206505	H	1.692549	-0.395550	-0.182611
H	5.384165	1.968028	-1.738222	N	2.247893	-1.228571	-3.443944
C	4.781935	0.604666	-0.148228	H	0.945972	-0.723165	-4.999222
C	8.330314	-2.946316	-0.732175	H	3.363149	-1.618937	-1.714124
H	7.497813	-3.677279	-0.828654				
H	8.571451	-2.808818	0.344660	(S)-L5-TS3A			
H	9.220635	-3.337636	-1.257355	Ni	-0.316844	1.366830	1.055450
C	1.213929	1.225380	4.649121	P	-0.914336	1.193095	-0.990816
H	0.159599	0.896591	4.626679	P	-1.065164	-0.543083	1.824308
H	1.867351	0.335410	4.731611	C	-2.431033	0.177984	-1.309504
H	1.369766	1.844590	5.560695	C	-3.631657	0.789872	-1.718731
H	2.606749	2.384877	3.359599	H	-3.641943	1.860016	-1.969001
C	-0.431016	-1.511797	3.313209	C	-4.819907	0.055098	-1.768081
N	0.770524	-2.107124	3.380626	H	-5.770762	0.535038	-2.041948
C	-1.222697	-1.348243	4.469713	C	-4.818898	-1.301738	-1.410886
C	1.190351	-2.525854	4.583601	C	-3.612365	-1.960040	-1.074619
C	-0.682362	-1.824531	5.673116	C	-2.410767	-1.205692	-1.012156
H	-2.210769	-0.867704	4.442952	C	-1.153197	-1.937123	-0.647819

C	-0.579737	-2.758017	-1.662206	C	3.780096	-1.057127	1.547464
C	0.645336	-3.415540	-1.397572	C	4.912857	-0.900760	0.580744
C	1.240070	-3.332118	-0.129071	C	5.883433	-1.830506	0.211876
H	2.193442	-3.848155	0.054054	H	5.888623	-2.829372	0.668445
C	0.653947	-2.558251	0.875108	C	6.830750	-1.426696	-0.768160
H	1.161536	-2.481790	1.844032	C	6.776592	-0.123539	-1.328169
C	-0.529743	-1.839193	0.620816	H	7.530858	0.138216	-2.085035
O	-1.244606	-2.765543	-2.849685	C	5.793034	0.797197	-0.932177
C	-1.371695	-3.956313	-3.628085	H	5.749326	1.805294	-1.371060
H	-2.337322	-3.869853	-4.164837	C	4.857727	0.394127	0.027462
H	-1.389995	-4.861841	-2.986851	C	7.930667	-3.548929	-0.713234
H	-0.550319	-4.054042	-4.365655	H	7.016812	-4.146139	-0.926017
O	-3.516224	-3.264463	-0.701081	H	8.114144	-3.543558	0.383634
C	-4.154772	-4.293696	-1.462406	H	8.794713	-4.011752	-1.224130
H	-3.484218	-5.174991	-1.418925	C	0.264737	0.386903	-2.121462
H	-4.289365	-3.989582	-2.520725	C	0.075835	-0.061523	-3.426407
H	-5.142249	-4.562546	-1.036547	S	1.840685	-0.059732	-1.530420
Cl	1.527754	-4.275036	-2.652760	C	1.216802	-0.744567	-3.943658
Cl	-6.362908	-2.127997	-1.288897	H	-0.871004	0.068295	-3.968171
C	1.439625	1.913432	3.397533	C	2.254027	-0.819598	-3.025935
H	0.978698	1.205343	4.108593	H	1.267917	-1.185880	-4.949169
C	0.618317	2.547503	2.478436	H	3.234965	-1.297124	-3.142464
C	0.363032	3.129793	1.334723	C	-1.310346	2.753562	-1.834304
C	0.398846	4.390900	0.620644	C	-2.036366	3.801818	-1.278017
C	1.043639	4.454656	-0.639154	S	-0.782458	3.150571	-3.450698
H	1.522345	3.546429	-1.030960	C	-2.178584	4.913061	-2.161479
C	1.076909	5.657424	-1.353878	H	-2.423796	3.765144	-0.249995
C	0.453801	6.809964	-0.839005	C	-1.546064	4.706417	-3.376647
H	0.468362	7.750313	-1.412061	H	-2.698834	5.845070	-1.900317
C	-0.191793	6.752731	0.408330	H	-1.462191	5.397847	-4.225319
H	-0.681480	7.650468	0.818640	C	-2.875787	-0.713168	1.897672
C	-0.216307	5.554484	1.139861	C	-3.658984	-1.853357	2.051866
H	-0.724693	5.500927	2.114913	S	-3.863936	0.718598	1.780944
C	2.825177	2.396658	3.710706	C	-5.055361	-1.563505	2.069619
H	3.498531	1.542778	3.933573	H	-3.230926	-2.862710	2.114288
H	2.801691	3.037548	4.621297	C	-5.318977	-0.208678	1.935827
H	3.240741	2.984451	2.871527	H	-5.843002	-2.324781	2.157395
H	1.582798	5.692534	-2.331206	H	-6.295318	0.291906	1.906071
O	1.874774	0.342018	2.007346	C	-0.637291	-1.161215	3.494128
O	3.291461	2.251327	0.421196	C	0.609566	-1.396176	4.069970
O	3.479033	-2.023683	2.240884	S	-1.914374	-1.374569	4.684091
O	7.823338	-2.226000	-1.232233	C	0.527952	-1.761885	5.448734
N	3.070330	0.163748	1.484040	H	1.547617	-1.278400	3.509356
C	3.689267	1.111090	0.607238	C	-0.773143	-1.777399	5.923811

H	1.404278	-1.999049	6.069664	H	0.643502	7.730928	-1.275656
H	-1.127032	-2.009231	6.937285	C	-0.030275	6.739760	0.543427
				H	-0.468135	7.653899	0.975465
(S)-L5-TS3B				C	-0.102300	5.532413	1.256041
Ni	-0.348031	1.327328	1.151939	H	-0.598478	5.486875	2.237771
P	-0.928262	1.264298	-0.906491	C	0.912097	1.298141	4.773531
P	-1.035257	-0.663919	1.767016	H	0.876315	2.077461	5.569762
C	-2.390123	0.216345	-1.339749	H	1.586306	0.495527	5.127422
C	-3.607638	0.810318	-1.725811	H	-0.104289	0.882209	4.644476
H	-3.659127	1.895883	-1.889541	H	1.643322	5.636720	-2.242347
C	-4.761047	0.032441	-1.859513	O	1.853003	0.285715	2.260680
H	-5.726735	0.492371	-2.115117	O	3.310988	2.313004	0.861629
C	-4.708967	-1.347700	-1.609669	O	3.448516	-2.108943	2.287809
C	-3.482567	-1.980608	-1.297777	O	7.641773	-2.118332	-1.360874
C	-2.317156	-1.182917	-1.150747	N	3.054884	0.140293	1.723214
C	-1.034013	-1.878467	-0.812868	C	3.680206	1.150579	0.924619
C	-0.402610	-2.590198	-1.874306	C	3.745709	-1.087553	1.672508
C	0.852821	-3.198810	-1.640316	C	4.851206	-0.875581	0.684083
C	1.421531	-3.184482	-0.357879	C	5.777271	-1.795663	0.196565
H	2.396605	-3.664776	-0.192955	H	5.769092	-2.830735	0.563634
C	0.778459	-2.520928	0.688961	C	6.696599	-1.333927	-0.784930
H	1.265325	-2.502909	1.669644	C	6.662805	0.014735	-1.225423
C	-0.434798	-1.839906	0.470245	H	7.393411	0.320871	-1.988814
O	-1.044840	-2.543819	-3.073551	C	5.726371	0.924963	-0.707734
C	-1.121479	-3.693392	-3.918826	H	5.697344	1.968589	-1.055447
H	-2.088824	-3.618109	-4.454296	C	4.816180	0.463779	0.249534
H	-1.102611	-4.633384	-3.329355	C	7.717826	-3.487711	-0.973892
H	-0.295071	-3.715035	-4.657010	H	6.773005	-4.028860	-1.201210
O	-3.333805	-3.303356	-1.018325	H	7.946192	-3.594381	0.109294
C	-3.932193	-4.303658	-1.847853	H	8.541286	-3.929939	-1.563970
H	-3.232367	-5.162816	-1.851574	C	0.328720	0.597974	-2.042952
H	-4.068775	-3.939250	-2.886711	C	0.224777	0.214543	-3.377439
H	-4.913072	-4.631196	-1.448959	S	1.913570	0.246967	-1.412417
Cl	1.794039	-3.909026	-2.943943	C	1.436713	-0.345069	-3.882702
Cl	-6.220870	-2.239196	-1.580199	H	-0.708259	0.298448	-3.950987
C	1.415014	1.919854	3.511091	C	2.442814	-0.390391	-2.928950
H	2.474279	2.240277	3.493478	H	1.560208	-0.723219	-4.907452
C	0.593029	2.509802	2.559693	H	3.463422	-0.780723	-3.029556
C	0.356865	3.082023	1.410782	C	-1.376878	2.857210	-1.656525
C	0.446512	4.348247	0.710141	C	-2.090029	3.870545	-1.025977
C	1.076147	4.401562	-0.556840	S	-0.927007	3.326811	-3.277381
H	1.505015	3.478555	-0.972363	C	-2.278548	5.018125	-1.852968
C	1.152627	5.611186	-1.256962	H	-2.433158	3.783825	0.014669
C	0.594227	6.784256	-0.715088	C	-1.699906	4.869512	-3.102866

H	-2.794687	5.932829	-1.529646	O	-3.555936	-3.314163	-0.199674
H	-1.661665	5.596579	-3.924608	C	-4.364262	-4.361673	-0.743169
C	-2.846241	-0.860620	1.774368	H	-3.703436	-5.247163	-0.820904
C	-3.624777	-2.013041	1.821802	H	-4.746054	-4.099788	-1.751111
S	-3.841482	0.571286	1.762591	H	-5.220711	-4.600264	-0.082041
C	-5.023132	-1.732639	1.839792	Cl	1.180761	-3.965481	-2.978216
H	-3.191074	-3.021970	1.811754	Cl	-6.522332	-2.221740	-0.320343
C	-5.293277	-0.372526	1.816130	C	1.767191	2.597149	3.198200
H	-5.807173	-2.502603	1.851769	H	1.366714	2.174633	4.135983
H	-6.272162	0.124020	1.814453	C	0.920706	2.934257	2.186296
C	-0.660424	-1.446945	3.381255	C	0.544518	3.225244	0.964421
C	0.551837	-1.816060	3.956970	C	0.450997	4.399932	0.112442
S	-1.972538	-1.635363	4.540053	C	0.698352	4.305907	-1.276151
C	0.415178	-2.273727	5.303623	H	0.981500	3.335044	-1.705248
H	1.517570	-1.710601	3.443490	C	0.590489	5.439674	-2.090953
C	-0.889072	-2.212138	5.763566	C	0.233951	6.681956	-1.536567
H	1.259543	-2.622825	5.915993	H	0.135294	7.568009	-2.183027
H	-1.278827	-2.486959	6.752801	C	0.006922	6.788984	-0.152364
				H	-0.265600	7.760466	0.289804
(S)-L6-TS3A				C	0.120298	5.659978	0.669848
Ni	-0.150178	1.452303	1.052671	H	-0.069275	5.730287	1.752109
P	-1.201864	1.242021	-0.783070	C	3.240942	2.866683	3.152827
P	-0.783697	-0.453318	1.904469	H	3.804664	1.928164	3.344085
C	-2.692863	0.168427	-0.895302	H	3.526544	3.577241	3.961314
C	-3.954572	0.752876	-1.130837	H	3.545218	3.275701	2.172470
H	-4.040871	1.823481	-1.361898	H	0.777582	5.349343	-3.171927
C	-5.111104	-0.022900	-1.021398	O	1.920815	0.459554	1.830378
H	-6.104519	0.429193	-1.153589	O	3.180656	2.144834	-0.094595
C	-5.025513	-1.379052	-0.669689	O	3.526073	-1.923136	2.131579
C	-3.766554	-2.011338	-0.515159	O	7.796614	-2.352739	-1.394770
C	-2.593908	-1.216795	-0.620127	N	2.989439	0.148779	1.137900
C	-1.265807	-1.892882	-0.478023	C	3.593028	1.022912	0.181200
C	-0.829365	-2.691003	-1.574266	C	3.759207	-1.033763	1.322045
C	0.489985	-3.205216	-1.558772	C	4.865628	-0.944703	0.318423
C	1.309840	-3.049909	-0.429373	C	5.861845	-1.875206	0.031573
H	2.325826	-3.470255	-0.437967	H	5.912384	-2.816946	0.594525
C	0.852578	-2.328940	0.674974	C	6.779691	-1.545491	-1.003644
H	1.512208	-2.192463	1.542750	C	6.668974	-0.313183	-1.698625
C	-0.422727	-1.727303	0.647712	H	7.404573	-0.105767	-2.489880
O	-1.710024	-2.828367	-2.600839	C	5.657134	0.609479	-1.385557
C	-1.901096	-4.098700	-3.230659	H	5.572997	1.564532	-1.925679
H	-2.957454	-4.121477	-3.562712	C	4.753958	0.278784	-0.368961
H	-1.723174	-4.932220	-2.519645	C	7.963276	-3.606213	-0.737384
H	-1.237984	-4.224698	-4.109385	H	7.071462	-4.257672	-0.868593

H	8.160627	-3.474410	0.349081	C	-4.161685	0.169586	-1.089709
H	8.838392	-4.088497	-1.209998	H	-4.506924	1.208865	-1.180747
N	-0.129693	-1.136980	3.370112	C	-5.088487	-0.874348	-1.174677
C	-0.030604	-2.481824	3.737455	H	-6.158133	-0.668095	-1.323355
C	0.098812	-0.346110	4.493735	C	-4.661488	-2.200950	-1.013891
C	0.287147	-2.532552	5.086164	C	-3.291567	-2.511024	-0.843815
H	-0.173655	-3.278780	3.001151	C	-2.354338	-1.451443	-0.751115
C	0.364048	-1.181150	5.567119	C	-0.902052	-1.822800	-0.660626
H	0.021372	0.742442	4.415863	C	-0.324358	-2.289419	-1.884075
H	0.461693	-3.448162	5.664658	C	1.058795	-2.597021	-1.907246
H	0.598633	-0.857756	6.588575	C	1.798462	-2.609733	-0.713641
N	-2.493454	-0.625553	2.242792	H	2.859234	-2.897777	-0.748213
C	-3.179481	-1.794585	2.571032	C	1.216390	-2.213143	0.490124
C	-3.394048	0.440865	2.221705	H	1.834297	-2.210649	1.393458
C	-4.514783	-1.468922	2.749455	C	-0.116513	-1.759042	0.520112
H	-2.656990	-2.754399	2.622100	O	-1.201650	-2.342829	-2.916873
C	-4.651186	-0.054919	2.526785	C	-0.986069	-3.090315	-4.111395
H	-3.043609	1.449323	1.974463	H	-1.987963	-3.200691	-4.569883
H	-5.317047	-2.174418	2.996583	H	-0.566018	-4.094493	-3.898712
H	-5.575748	0.532382	2.578423	H	-0.318396	-2.553616	-4.813709
N	-0.243093	0.612702	-2.099114	O	-2.804184	-3.772151	-0.703456
C	1.154298	0.602230	-2.072657	C	-3.108682	-4.763298	-1.692593
C	-0.683306	-0.052447	-3.247951	H	-2.184422	-5.356396	-1.843227
C	1.597645	-0.063610	-3.203187	H	-3.400597	-4.295248	-2.654685
H	1.682085	1.101815	-1.255520	H	-3.924863	-5.432233	-1.352076
C	0.436911	-0.479431	-3.943328	Cl	1.953824	-2.899214	-3.389220
H	-1.750741	-0.214211	-3.425761	Cl	-5.864194	-3.470850	-0.928568
H	2.647384	-0.242803	-3.464754	C	1.614091	2.180881	3.093194
H	0.423591	-1.054679	-4.876747	C	0.703412	2.741657	2.226541
N	-1.841489	2.718352	-1.481503	C	0.054333	3.186322	1.197765
C	-2.013809	3.025090	-2.830746	C	-0.213887	4.340011	0.353927
C	-2.414480	3.726440	-0.706556	C	0.592812	4.541531	-0.794240
C	-2.688222	4.235908	-2.906909	H	1.423799	3.848888	-0.986231
H	-1.618430	2.364309	-3.608995	C	0.329647	5.616661	-1.654303
C	-2.945937	4.677270	-1.565110	C	-0.732170	6.499229	-1.386112
H	-2.364046	3.680421	0.386583	H	-0.942490	7.336644	-2.069728
H	-2.949710	4.761762	-3.833469	C	-1.528416	6.305205	-0.244257
H	-3.442619	5.605714	-1.259784	H	-2.365114	6.988457	-0.031308
				C	-1.275053	5.232912	0.622683
(S)-L6-TS3B				H	-1.902214	5.071108	1.510617
Ni	-0.476369	1.335982	1.245017	H	0.960051	5.763624	-2.545469
P	-1.587346	1.225728	-0.535842	O	1.986467	0.456417	1.746019
P	-0.676964	-0.704775	1.923161	O	3.032825	2.386089	-0.063840
C	-2.801988	-0.112045	-0.845439	O	3.942828	-1.658191	2.028540

O	8.310334	-1.310400	-1.384207	H	2.100931	-1.509388	3.118672
N	3.131322	0.346474	1.097631	C	-0.077461	-1.997624	5.617891
C	3.607463	1.332067	0.175989	H	-1.960102	-1.448771	4.503412
C	4.057272	-0.710734	1.255377	H	2.168306	-2.330381	5.710356
C	5.156821	-0.427140	0.281264	H	-0.436810	-2.236994	6.626580
C	6.287087	-1.188391	-0.008125	N	-2.328032	-1.230575	2.142200
H	6.461827	-2.136131	0.518529	C	-2.791940	-2.544589	2.195986
C	7.175007	-0.680775	-0.996454	C	-3.399743	-0.357434	2.329526
C	6.903125	0.553007	-1.643725	C	-4.160650	-2.502365	2.406832
H	7.621986	0.901299	-2.400045	H	-2.105855	-3.383951	2.044285
C	5.758311	1.302423	-1.329103	C	-4.546258	-1.118953	2.492110
H	5.551255	2.258887	-1.832278	H	-3.227785	0.724743	2.320526
C	4.883852	0.796349	-0.360239	H	-4.824744	-3.373031	2.463050
C	8.643567	-2.555446	-0.774476	H	-5.559233	-0.727462	2.643977
H	7.861751	-3.323524	-0.962638				
H	8.790637	-2.445792	0.322270				
H	9.592593	-2.881121	-1.238002				
C	1.251904	1.614096	4.428260				
H	0.161072	1.454485	4.521757				
H	1.757205	0.640099	4.589929				
H	1.595428	2.299758	5.235128				
H	2.680244	2.408432	2.911417				
N	-2.570133	2.639566	-0.895042				
C	-2.729754	3.315157	-2.101074				
C	-3.502041	3.120754	0.024537				
C	-3.765154	4.228261	-1.943976				
H	-2.071584	3.103563	-2.949598				
C	-4.260913	4.098478	-0.604403				
H	-3.530831	2.724159	1.045538				
H	-4.110315	4.935383	-2.708059				
H	-5.065846	4.680357	-0.139246				
N	-0.579609	1.092219	-1.951264				
C	-0.949293	0.704369	-3.244023				
C	0.814709	1.151666	-1.871706				
C	0.212979	0.537263	-3.980396				
H	-2.001674	0.544014	-3.498657				
C	1.326985	0.817345	-3.112729				
H	1.293119	1.432095	-0.927981				
H	0.261302	0.236223	-5.034303				
H	2.391562	0.768725	-3.370048				
N	-0.057732	-1.413837	3.434422				
C	1.264906	-1.669343	3.806226				
C	-0.877994	-1.597395	4.558816				
C	1.272839	-2.050988	5.141364				