

# Supporting Information

## Effects of Phosphine Ligands in Nickel-Catalyzed Decarbonylation Reactions of Lactone

Xinghua Wang<sup>2</sup>, Peng Jin<sup>1,3,4</sup>, Shiqiang Li<sup>3</sup>, Yiqiang Wen<sup>2</sup>, Fuke Wang<sup>4</sup>, Huijuan Wei<sup>2,\*</sup>,  
Donghui Wei<sup>2,\*</sup>

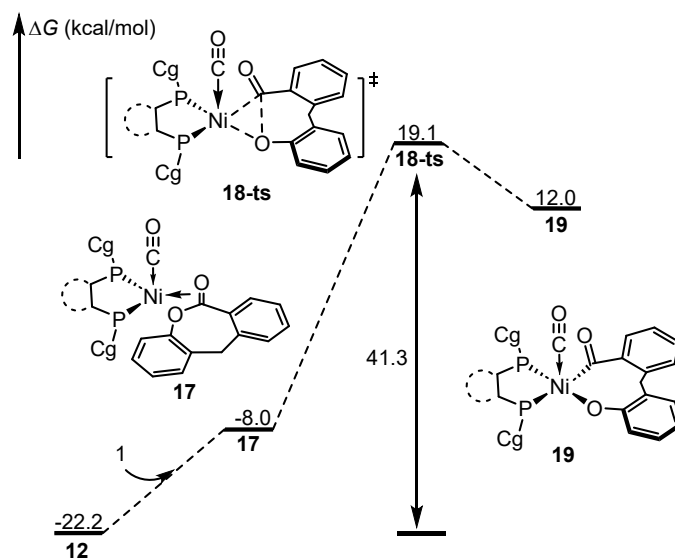
1. State Key Laboratory of Coking Coal Resources Green Exploitation, China Pingmei Shenma Group, Pingdingshan 467000, China
2. College of Chemistry, Zhengzhou University, Zhengzhou 450001, China
3. Henan Shenma Catalytic Technology Co., LTD., Pingdingshan 467000, China
4. Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A\*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Republic of Singapore

\*e-mail: weihuijuan@zzu.edu.cn, donghuiwei@zzu.edu.cn

# Table of Contents

<b>Part 1: Possible Pathways for Oxidative Addition of Intermediate 12(L1) to the Substrate .....</b>	<b>1</b>
<b>Part 2: Test of the Computational Methods .....</b>	<b>2</b>
<b>Part 3: Comparing Triplet and Singlet States of Different Species.....</b>	<b>3</b>
<b>Part 4: IRC Results for Key Transition States .....</b>	<b>4</b>
<b>Part 5: References .....</b>	<b>6</b>
<b>Part 6: The Energetic Information of Optimized Structures .....</b>	<b>7</b>
<b>Part 7: Geometrical Coordinates of the Stationary Points.....</b>	<b>9</b>

## Part 1: Possible Pathways for Oxidative Addition of Intermediate 12(L1) to the Substrate



**Figure S1.** Gibbs free energy profiles of direct oxidative addition of intermediate 12(L1) to the substrate.

## Part 2: Test of the Computational Methods

We have compared the relative Gibbs free energies of **4(L1)**, **5-ts(L1)** and **6(L1)** at different levels including:

M06-L/def2-TZVPP/SMD<sub>toluene</sub> (L1)

M06-L/def2-TZVPP/IEF-PCM<sub>toluene</sub> (L2)<sup>1</sup>

M06/def2-TZVPP/SMD<sub>toluene</sub> (L3)<sup>2</sup>

$\omega$ B97X-D/def2-TZVPP/SMD<sub>toluene</sub> (L4)<sup>3</sup>

B3LYP-D3/def2-TZVPP/SMD<sub>toluene</sub> (L5)<sup>4</sup>

As shown in Table S1, there are the same trend and small energy barrier differences at different levels, indicating the selected method should be proper and reliable in this kind of reaction system.

**Table S1.** Comparison of the relative Gibbs free energies of **4(L1)**, **5-ts(L1)** and **6(L1)** calculated by using different levels (L1-5) (unit: kcal/mol).

Level	<b>4(L1)</b>	<b>5-ts(L1)</b>	<b>6(L1)</b>
L1	0.0	14.0	10.3
L2	0.0	13.5	9.9
L3	0.0	15.2	11.8
L4	0.0	15.8	12.0
L5	0.0	17.1	12.2

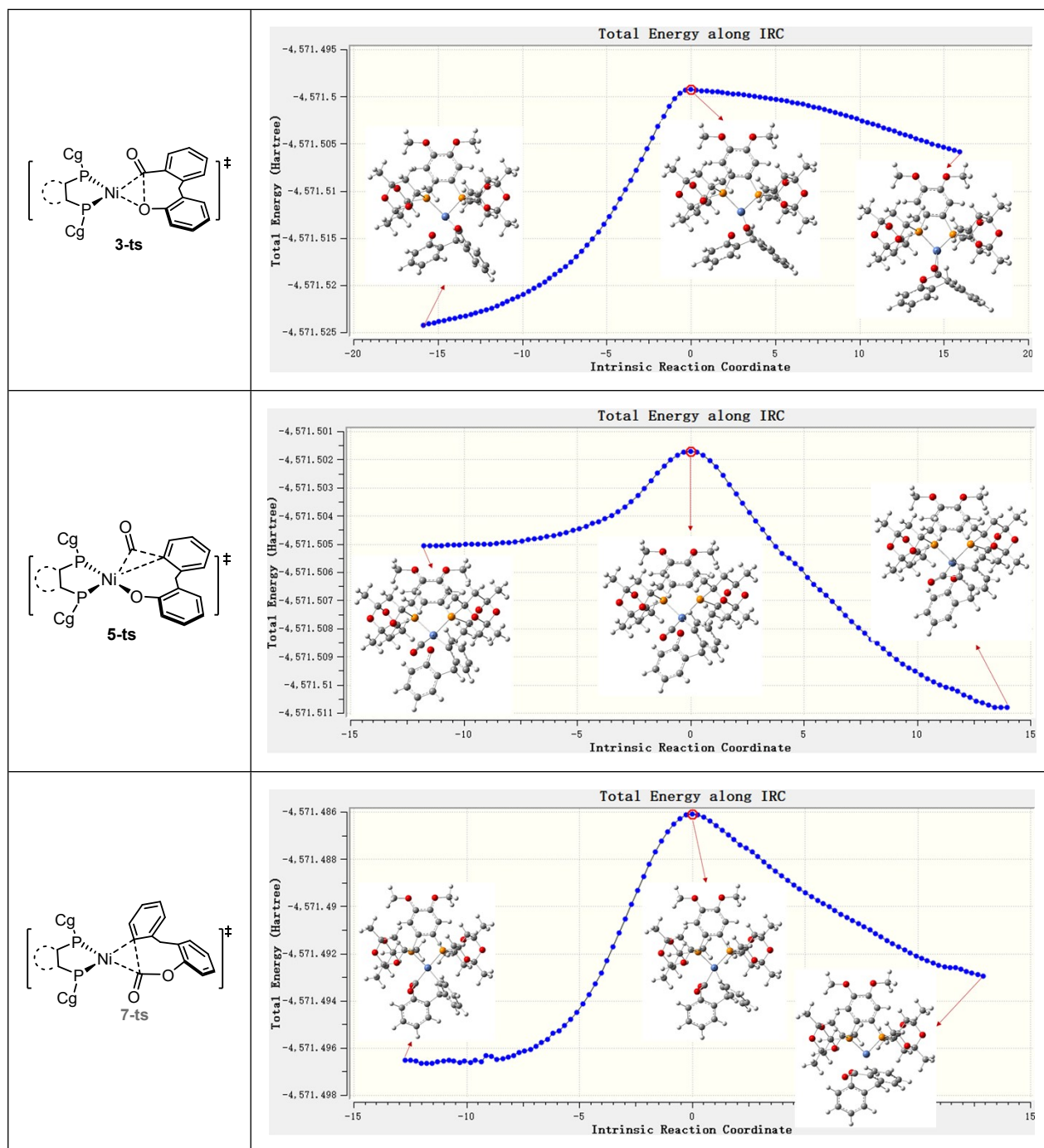
### Part 3: Comparing Triplet and Singlet States of Different Species

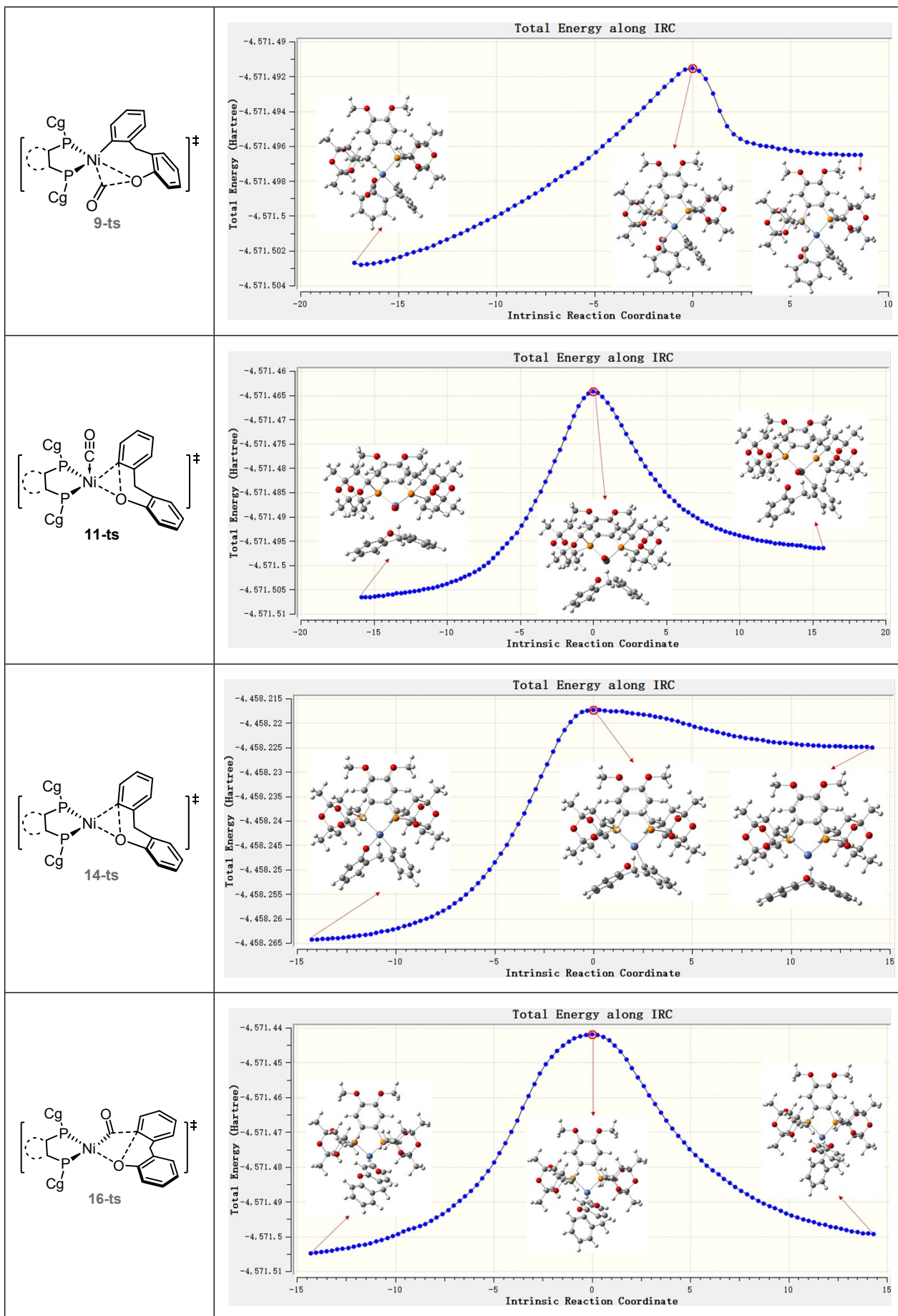
**Table S2.** Free energy difference between triplet and singlet states of different species (unit: kcal/mol)

SP	Ni(COD) <sub>2</sub>	2(L1)	4(L1)	6(L1)	10(L1)	12(L1)
$\Delta G(^3\text{SP}-^1\text{SP})$	30.6	20.7	13.0	13.7	11.5	29.1

## Part 4: IRC Results for Key Transition States

**Table S3.** Intrinsic reaction coordinate (IRC) results for key transition states





## Part 5: References

- (1) (a) Miertuš, S.; Tomasi, J. Approximate evaluations of the electrostatic free energy and internal energy changes in solution processes. *Chem. Phys.* **1982**, *65*, 239-245; (b) Miertuš, S.; Scrocco, E.; Tomasi, J. Electrostatic interaction of a solute with a continuum. A direct utilization of AB initio molecular potentials for the prevision of solvent effects. *Chem. Phys.* **1981**, *55*, 117-129; (c) Pascual-Ahuir, J. L.; Silla, E.; Tuñon, I. GEPOL: An improved description of molecular surfaces. III. A new algorithm for the computation of a solvent-excluding surface. *J. Comput. Chem.* **1994**, *15*, 1127-1138.
- (2) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, *120*, 215-241.
- (3) Chai, J.-D.; Head-Gordon, M. Long-range corrected hybrid density functionals with damped atom-atom dispersion corrections. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620.
- (4) (a) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.* **1994**, *98*, 11623-11627; (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **2010**, *132*, 154104; (c) Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A* **1988**, *38*, 3098-3100; (d) Becke, A. D. Density - functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648-5652; (e) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988**, *37*, 785-789.



## Part 6: The Energetic Information of Optimized Structures

**Table S4.** The quasi-harmonic corrected Gibbs free energies (qh-G(T)), Gibbs free energy corrections (GFEC), single-point energies ( $E$ ), Gibbs free energies ( $G=E + \text{GFEC}$ ) energies, and imaginary frequencies (IF) of the stationary points (SPs) involved in the reaction (unit: a.u.)

SP	qh-G(T)	GFEC	$E$	$G$	IF
Ni(COD) <sub>2</sub>	-2131.418850	0.299676	-2132.582652	-2132.282976	
COD	-311.636876	0.135422	-312.105802	-311.970380	
L1	-2373.383016	0.550112	-2376.003947	-2375.453835	
1	-689.267613	0.144496	-690.150411	-690.005915	
2(L1)	-4570.786546	0.731730	-4574.543803	-4573.812073	
3-ts(L1)	-4570.770140	0.729132	-4574.521627	-4573.792495	173.31 <i>i</i>
4(L1)	-4570.799056	0.727011	-4574.544638	-4573.817627	
5-ts(L1)	-4570.774438	0.727280	-4574.522557	-4573.795277	143.69 <i>i</i>
6(L1)	-4570.779600	0.725188	-4574.526356	-4573.801168	
7-ts(L1)	-4570.756753	0.729329	-4574.507330	-4573.778001	181.14 <i>i</i>
8(L1)	-4570.769698	0.728292	-4574.516836	-4573.788544	
9-ts(L1)	-4570.764540	0.726977	-4574.513850	-4573.786873	226.01 <i>i</i>
CO	-113.225541	-0.021084	-113.339363	-113.360447	
10(L1)	-4570.774867	0.723397	-4574.517859	-4573.794462	
11-ts(L1)	-4570.740895	0.722630	-4574.485319	-4573.762689	402.44 <i>i</i>
12(L1)	-3994.782602	0.549300	-3997.759260	-3997.209960	
P	-576.025220	0.139807	-576.777226	-576.637419	
13(L1)	-4457.543073	0.724280	-4461.162013	-4460.437733	
14-ts(L1)	-4457.497443	0.719867	-4461.115716	-4460.395849	221.35 <i>i</i>
15(L1)	-3881.477033	0.547627	-3884.332391	-3883.784764	
16-ts(L1)	-4570.717408	0.724504	-4574.462999	-4573.738495	306.24 <i>i</i>
17(L1)	-4684.044347	0.734102	-4687.927459	-4687.193357	
18-ts(L1)	-4684.003016	0.731299	-4687.881410	-4687.150111	303.17 <i>i</i>
19(L1)	-4684.016284	0.731482	-4687.892869	-4687.161387	
2(L2)	-3883.949733	0.521986	-3886.713902	-3886.191916	
3-ts(L2)	-3883.931440	0.521290	-3886.693944	-3886.172654	151.43 <i>i</i>
4(L2)	-3883.961433	0.520432	-3886.719073	-3886.198641	
5-ts(L2)	-3883.933497	0.517881	-3886.691466	-3886.173585	144.94 <i>i</i>
6(L2)	-3883.937414	0.516893	-3886.694824	-3886.177931	
10(L2)	-3883.938138	0.516383	-3886.694049	-3886.177666	
11-ts(L2)	-3883.901627	0.514064	-3886.655330	-3886.141266	388.71 <i>i</i>
12(L2)	-3307.938701	0.341925	-3309.926944	-3309.585019	
2(L3)	-3588.846014	0.645931	-3591.444844	-3590.798913	

<b>3-ts(L3)</b>	-3588.827132	0.645597	-3591.422770	-3590.777173	205.43 <i>i</i>
<b>4(L3)</b>	-3588.858676	0.642014	-3591.448886	-3590.806872	
<b>5-ts(L3)</b>	-3588.826898	0.640874	-3591.418145	-3590.777271	112.85 <i>i</i>
<b>6(L3)</b>	-3588.824020	0.640908	-3591.418875	-3590.777967	
<b>10(L3)</b>	-3588.829715	0.638251	-3591.414427	-3590.776176	
<b>11-ts(L3)</b>	-3588.788706	0.636943	-3591.375763	-3590.738820	387.63 <i>i</i>
<b>12(L3)</b>	-3012.841214	0.464934	-3014.660992	-3014.196058	
<b>2(L4)</b>	-4677.216179	0.443328	-4680.843760	-4680.400432	
<b>3-ts(L4)</b>	-4677.199505	0.442285	-4680.824041	-4680.381756	105.03 <i>i</i>
<b>4(L4)</b>	-4677.224602	0.443118	-4680.846108	-4680.402990	
<b>5-ts(L4)</b>	-4677.196794	0.439012	-4680.817921	-4680.378909	153.38 <i>i</i>
<b>6(L4)</b>	-4677.198279	0.439367	-4680.820430	-4680.381063	
<b>10(L4)</b>	-4677.201788	0.438922	-4680.821308	-4680.382386	
<b>11-ts(L4)</b>	-4677.167063	0.436421	-4680.784557	-4680.348136	366.33 <i>i</i>
<b>12(L4)</b>	-4101.203607	0.262904	-4104.055616	-4103.792712	
<b>2(L5)</b>	-4621.301574	0.480610	-4624.847747	-4624.367137	
<b>3-ts(L5)</b>	-4621.281552	0.482445	-4624.827162	-4624.344717	285.95 <i>i</i>
<b>4(L5)</b>	-4621.304212	0.484353	-4624.848129	-4624.363776	
<b>5-ts(L5)</b>	-4621.275909	0.478204	-4624.816826	-4624.338622	160.12 <i>i</i>
<b>6(L5)</b>	-4621.282363	0.476308	-4624.823489	-4624.347181	
<b>10(L5)</b>	-4621.279653	0.479289	-4624.821823	-4624.342534	
<b>11-ts(L5)</b>	-4621.254252	0.479254	-4624.795379	-4624.316125	350.13 <i>i</i>
<b>12(L5)</b>	-4045.285109	0.300518	-4048.056985	-4047.756467	
<b>2(L6)</b>	-4256.664040	0.533704	-4259.892103	-4259.358399	
<b>3-ts(L6)</b>	-4256.648122	0.530093	-4259.871122	-4259.341029	196.52 <i>i</i>
<b>4(L6)</b>	-4256.674987	0.529331	-4259.892686	-4259.363355	
<b>5-ts(L6)</b>	-4256.652561	0.528531	-4259.871447	-4259.342916	132.95 <i>i</i>
<b>6(L6)</b>	-4256.661849	0.527586	-4259.879960	-4259.352374	
<b>10(L6)</b>	-4256.664362	0.525135	-4259.878713	-4259.353578	
<b>11-ts(L6)</b>	-4256.632929	0.525898	-4259.848346	-4259.322448	384.62 <i>i</i>
<b>12(L6)</b>	-3680.661210	0.352027	-3683.111120	-3682.759093	
<b>2(L7)</b>	-3117.808533	0.329391	-3119.592881	-3119.263490	
<b>3-ts(L7)</b>	-3117.792790	0.328697	-3119.574345	-3119.245648	94.67 <i>i</i>
<b>4(L7)</b>	-3117.831802	0.326196	-3119.605348	-3119.279152	
<b>5-ts(L7)</b>	-3117.803651	0.324493	-3119.577159	-3119.252666	171.67 <i>i</i>
<b>6(L7)</b>	-3117.814288	0.324282	-3119.589089	-3119.264807	
<b>10(L7)</b>	-3117.816247	0.323189	-3119.587903	-3119.264714	
<b>11-ts(L7)</b>	-3117.775550	0.322587	-3119.547319	-3119.224732	399.74 <i>i</i>
<b>12(L7)</b>	-2541.798925	0.151824	-2542.809738	-2542.657914	
<b><sup>3</sup>Ni(COD)<sub>2</sub></b>	-2131.366908	0.291400	-2132.525585	-2132.234185	
<b><sup>32</sup>(L1)</b>	-4570.759111	0.724103	-4574.503201	-4573.779098	
<b><sup>34</sup>(L1)</b>	-4570.779137	0.722634	-4574.519504	-4573.796870	

<b><sup>3</sup>6(L1)</b>	-4570.759848	0.719285	-4574.498643	-4573.779358	
<b><sup>3</sup>10(L1)</b>	-4570.757211	0.720583	-4574.496750	-4573.776167	
<b><sup>3</sup>12(L1)</b>	-3994.734090	0.547341	-3997.710864	-3997.163523	

## Part 7: Geometrical Coordinates of the Stationary Points

<b>Ni(COD)<sub>2</sub></b>				H	2.140957	-1.811335	1.586006
Ni	0.000000	0.000000	0.000000				
C	1.171244	0.976480	1.476548	<b>COD</b>			
H	2.025541	1.439040	0.970327	C	1.565723	-0.716254	-0.495018
C	-0.046308	1.634071	1.325277	H	2.346284	-1.072062	-1.179332
H	-0.026035	2.559670	0.737577	C	1.576249	0.597219	-0.222279
C	-1.171244	-0.976480	1.476548	H	2.348710	1.186414	-0.732225
H	-2.025541	-1.439040	0.970327	C	-1.576249	-0.597219	-0.222279
C	0.046308	-1.634071	1.325277	H	-2.348710	-1.186414	-0.732225
H	0.026035	-2.559670	0.737577	C	-1.565723	0.716254	-0.495018
C	-1.634071	-0.046308	-1.325277	H	-2.346284	1.072062	-1.179332
H	-2.559670	-0.026035	-0.737577	C	0.654482	1.389857	0.659554
C	-0.976480	1.171244	-1.476548	H	0.444936	0.863510	1.600624
H	-1.439040	2.025541	-0.970327	H	1.172656	2.311588	0.965335
C	0.976480	-1.171244	-1.476548	C	-0.654482	1.799494	-0.015452
H	1.439040	-2.025541	-0.970327	H	-1.218943	2.464797	0.664260
C	1.634071	0.046308	-1.325277	H	-0.420249	2.446819	-0.879489
H	2.559670	0.026035	-0.737577	C	-0.654482	-1.389857	0.659554
C	0.000000	1.524136	-2.576527	H	-1.172656	-2.311588	0.965335
H	-0.250618	0.976420	-3.497821	H	-0.444936	-0.863510	1.600624
H	-0.124278	2.585264	-2.842486	C	0.654482	-1.799494	-0.015452
C	1.451865	1.275743	-2.169844	H	0.420249	-2.446819	-0.879489
H	2.110044	1.246470	-3.060775	H	1.218943	-2.464797	0.664260
H	1.811335	2.140957	-1.586006	<b>LI</b>			
C	0.000000	-1.524136	-2.576527	P	-1.556418	-0.961248	0.173726
H	0.124278	-2.585264	-2.842486	P	1.643956	-0.857195	0.651963
H	0.250618	-0.976420	-3.497821	O	-5.354175	-1.038678	-0.024585
C	-1.451865	-1.275743	-2.169844	O	-3.857842	0.456952	0.966711
H	-1.811335	-2.140957	-1.586006	O	-3.581235	-2.306676	-0.880648
H	-2.110044	-1.246470	-3.060775	O	-1.291802	4.305039	-0.289487
C	-1.275743	1.451865	2.169844	O	1.311699	4.330343	-0.153866
H	-2.140957	1.811335	1.586006	O	4.091327	0.587965	0.518982
H	-1.246470	2.110044	3.060775	O	5.265625	-1.159743	-0.477069
C	1.524136	0.000000	2.576527	O	3.371086	-2.521583	-0.567161
H	0.976420	0.250618	3.497821	C	-2.955542	-0.579602	1.401393
H	2.585264	0.124278	2.842486	C	-2.394690	-0.118323	2.723288
C	-1.524136	0.000000	2.576527	H	-1.694378	-0.861944	3.129304
H	-2.585264	-0.124278	2.842486	H	-3.204281	0.032771	3.452812
H	-0.976420	-0.250618	3.497821	H	-1.854475	0.833049	2.615303
C	1.275743	-1.451865	2.169844	C	-3.747937	-1.877311	1.512005
H	1.246470	-2.110044	3.060775				

H	-4.494315	-1.783008	2.317638	H	6.277288	-3.154269	0.882790
H	-3.086433	-2.720929	1.756712	H	5.648220	-3.722101	-0.684708
C	-4.488010	-2.143248	0.203840	C	4.094391	-1.569135	1.555693
C	-5.337763	-3.382578	0.236370	H	3.508558	-2.307053	2.123472
H	-5.864685	-3.496888	-0.718893	H	5.010496	-1.349899	2.127842
H	-6.080411	-3.318738	1.040960	C	3.307960	-0.270683	1.367300
H	-4.712172	-4.268552	0.400087	C	3.125271	0.472178	2.668644
C	-4.634422	0.174204	-0.188499	H	2.597863	-0.154216	3.401183
C	-5.643222	1.282529	-0.307713	H	2.545442	1.396313	2.536207
H	-6.308561	1.103084	-1.161005	H	4.104826	0.744331	3.089762
H	-5.140087	2.247762	-0.450283	C	2.493139	-1.452547	-0.951405
H	-6.248773	1.334952	0.605401	C	3.322603	-0.350440	-1.592691
C	-3.761368	0.014782	-1.429320	H	2.705303	0.536149	-1.802036
H	-4.429769	-0.198172	-2.279857	H	3.716021	-0.714387	-2.556343
H	-3.219540	0.939194	-1.670016	C	1.485267	-2.043894	-1.900260
C	-2.808363	-1.151023	-1.260089	H	1.988085	-2.448360	-2.792091
C	-2.116947	-1.512608	-2.549225	H	0.771626	-1.275558	-2.229330
H	-1.501492	-2.413777	-2.428342	H	0.923769	-2.857288	-1.420540
H	-1.473071	-0.688958	-2.890289				
H	-2.859357	-1.712291	-3.336760	<b>I</b>			
C	-0.676981	0.656976	0.036475	O	0.666853	1.702482	0.469319
C	-1.352777	1.886201	-0.113372	C	1.514784	0.672780	0.108927
H	-2.439042	1.891079	-0.121221	C	2.614824	1.013432	-0.675805
C	-0.688891	3.105132	-0.168400	H	2.719678	2.045089	-1.016318
C	-2.694088	4.327633	-0.374364	C	3.552864	0.037358	-1.001408
H	-3.060942	3.788174	-1.264564	H	4.413815	0.300824	-1.619769
H	-2.989012	5.379445	-0.459642	C	3.391162	-1.267684	-0.538599
H	-3.171473	3.900496	0.523904	H	4.125821	-2.035659	-0.789839
C	0.723694	3.120205	-0.083846	C	2.287928	-1.592244	0.249190
C	2.711984	4.387200	-0.043108	H	2.157985	-2.613819	0.617186
H	3.073164	3.968343	0.911373	C	1.337872	-0.628012	0.593276
H	2.989758	5.446072	-0.088096	C	0.117877	-0.931754	1.409511
H	3.214186	3.856643	-0.869405	H	0.073475	-0.250822	2.277933
C	1.401469	1.918976	0.083573	H	0.169069	-1.950527	1.814267
H	2.486589	1.934689	0.169994	C	-1.111621	-0.765425	0.564209
C	0.735246	0.678157	0.167215	C	-1.931794	-1.856517	0.261735
C	4.512270	0.019020	-0.712859	H	-1.675166	-2.838455	0.668926
C	5.435341	1.020672	-1.349308	C	-3.063356	-1.708597	-0.535886
H	6.261925	1.250007	-0.665341	H	-3.685500	-2.578163	-0.760773
H	4.896444	1.949512	-1.576607	C	-3.404924	-0.453023	-1.037825
H	5.851659	0.619411	-2.281341	H	-4.295987	-0.329151	-1.656679
C	4.503312	-2.149301	0.203477	C	-2.607805	0.644332	-0.737891
C	5.364492	-3.376021	0.316782	H	-2.866298	1.640009	-1.104315
H	4.817874	-4.180296	0.824047	C	-1.448738	0.498687	0.038139

C	-0.695225	1.743905	0.333438	H	1.432281	3.734061	0.862807
O	-1.224352	2.818423	0.453597	C	3.433831	3.015665	1.137385
				C	3.163314	5.285701	1.714273
<b>2(L1)</b>				H	2.814645	5.604724	0.717624
Ni	-0.450327	-0.698880	-0.318217	H	3.781783	6.083052	2.140209
P	-0.170571	1.396077	-0.184799	H	2.288062	5.132656	2.366872
P	1.692067	-1.001500	-0.415599	C	4.295008	1.891399	1.050751
O	-2.455000	4.379530	-0.568943	C	6.428579	0.973227	1.445488
O	-0.796380	3.832009	0.984110	H	6.066611	0.135414	2.064172
O	-2.061047	2.416150	-1.776355	H	7.388095	1.316625	1.846982
O	3.976711	4.139641	1.639283	H	6.588460	0.614080	0.414747
O	5.554756	2.075245	1.485925	C	3.796097	0.691889	0.553166
O	3.751906	-2.433715	0.760995	H	4.438499	-0.186585	0.549229
O	3.732665	-4.136422	-0.846844	C	2.461119	0.568109	0.127403
O	2.050336	-3.052039	-2.058699	C	4.324357	-2.909246	-0.453445
O	-2.527106	-1.107556	1.494854	C	5.773051	-3.182233	-0.159619
C	-1.162444	2.440900	1.037193	H	5.854725	-3.919966	0.647768
C	-0.938315	1.976457	2.452783	H	6.283526	-2.262601	0.154203
H	-1.243338	0.925394	2.555031	H	6.277243	-3.578595	-1.049313
H	-1.534966	2.582841	3.149970	C	2.328315	-4.017517	-1.044943
H	0.118459	2.062000	2.744944	C	1.829774	-5.333360	-1.568102
C	-2.613446	2.305769	0.593221	H	0.748303	-5.284884	-1.743498
H	-3.264251	2.773787	1.349681	H	2.036191	-6.133943	-0.847711
H	-2.892595	1.245042	0.511744	H	2.331516	-5.572780	-2.513656
C	-2.829544	3.015806	-0.738739	C	1.707312	-3.620476	0.290509
C	-4.256669	2.984901	-1.203776	H	0.616075	-3.522436	0.198255
H	-4.354198	3.543764	-2.142692	H	1.924267	-4.416551	1.020873
H	-4.917271	3.437550	-0.454017	C	2.320183	-2.316251	0.781713
H	-4.569821	1.947018	-1.378962	C	1.915823	-1.975509	2.193356
C	-1.085834	4.516490	-0.231425	H	0.823696	-1.850959	2.245697
C	-0.830263	5.973522	0.035297	H	2.384667	-1.040435	2.532427
H	-1.064568	6.573216	-0.852600	H	2.210961	-2.777114	2.886179
H	0.221634	6.137701	0.303165	C	2.630819	-1.751624	-1.884262
H	-1.460861	6.314405	0.865386	C	4.112089	-1.915575	-1.593383
C	-0.265965	3.958373	-1.393219	H	4.585783	-0.947143	-1.377704
H	-0.505015	4.551693	-2.291220	H	4.603434	-2.323859	-2.491882
H	0.812741	4.066952	-1.209381	C	2.359745	-0.985908	-3.152156
C	-0.636764	2.508866	-1.653641	H	2.843678	-1.480117	-4.007555
C	-0.058059	1.966609	-2.933542	H	2.749716	0.039399	-3.081399
H	-0.371897	0.924070	-3.085065	H	1.280635	-0.937724	-3.352791
H	1.040649	2.000376	-2.910721	C	-3.362236	-2.040902	2.057053
H	-0.404373	2.558007	-3.794112	C	-2.864894	-3.058292	2.866651
C	1.599369	1.680655	0.228618	H	-1.787172	-3.128777	3.027144
C	2.108209	2.890797	0.735398	C	-3.754279	-3.962185	3.448657

H	-3.373598	-4.764240	4.086084	C	-5.327712	1.199624	-1.155763
C	-5.123823	-3.845988	3.213777	H	-5.598343	1.588094	-2.145352
H	-5.819601	-4.555275	3.668279	H	-6.099795	1.499202	-0.436436
C	-5.609003	-2.822809	2.397099	H	-5.291979	0.104228	-1.203959
H	-6.683967	-2.729298	2.215802	C	-2.870088	3.783736	-0.400631
C	-4.734813	-1.906783	1.809170	C	-3.132147	5.256619	-0.253396
C	-5.168477	-0.763848	0.939252	H	-3.556611	5.663131	-1.179310
H	-4.815762	0.175678	1.405365	H	-2.202877	5.795284	-0.027847
H	-6.265486	-0.699514	0.928758	H	-3.844495	5.426654	0.563320
C	-4.671467	-0.824617	-0.487425	C	-1.897119	3.445114	-1.525773
C	-5.602516	-0.614029	-1.516012	H	-2.304364	3.857174	-2.463911
H	-6.644926	-0.423251	-1.242138	H	-0.918977	3.919676	-1.357143
C	-5.243295	-0.643966	-2.859329	C	-1.755840	1.939021	-1.671157
H	-5.996190	-0.470802	-3.632074	C	-1.036349	1.530016	-2.927399
C	-3.916689	-0.905659	-3.205272	H	-1.000097	0.434224	-3.001482
H	-3.613051	-0.936090	-4.254519	H	-0.009330	1.922342	-2.931016
C	-2.984622	-1.134693	-2.204053	H	-1.557773	1.922768	-3.813279
H	-1.940862	-1.349826	-2.458736	C	0.617937	2.107666	0.228565
C	-3.328310	-1.093702	-0.840670	C	0.623191	3.424418	0.727150
C	-2.215495	-1.343888	0.120422	H	-0.321518	3.954872	0.824653
O	-1.378651	-2.311995	-0.114995	C	1.792518	4.042576	1.157885
<b>3-ts(L1)</b>				C	0.677321	6.060281	1.658033
Ni	-0.338362	-0.867657	-0.543933	H	0.280012	6.205420	0.639317
P	-0.921131	1.152695	-0.144387	H	0.939994	7.039167	2.073764
P	1.759412	-0.290702	-0.499286	H	-0.110946	5.611700	2.285680
O	-4.107184	3.161825	-0.693599	C	3.015228	3.325150	1.117435
O	-2.374917	3.337586	0.857756	C	5.323447	3.280186	1.601777
O	-3.065427	1.357039	-1.750083	H	5.282777	2.357986	2.205115
O	1.856161	5.293467	1.651452	H	6.061524	3.956867	2.046213
O	4.095996	3.966582	1.599985	H	5.653600	3.026058	0.580385
O	4.195706	-0.877786	0.689648	C	3.021379	2.032158	0.606104
O	4.892144	-2.326522	-1.010319	H	3.948553	1.462305	0.618943
O	2.949088	-1.908663	-2.248605	C	1.844275	1.417602	0.140054
O	-0.655054	-2.935261	-0.157211	C	4.937041	-0.997820	-0.522688
C	-2.225276	1.915772	1.026657	C	6.367205	-0.693931	-0.173944
C	-1.861983	1.711007	2.475362	H	6.717467	-1.391095	0.596938
H	-1.715808	0.646199	2.699136	H	6.461488	0.329825	0.210298
H	-2.660223	2.096295	3.127133	H	7.007839	-0.797817	-1.057851
H	-0.932838	2.239084	2.733003	C	3.562794	-2.754476	-1.280581
C	-3.542476	1.260216	0.631284	C	3.641969	-4.119291	-1.903061
H	-4.318672	1.526790	1.367200	H	2.635414	-4.483197	-2.143798
H	-3.450806	0.166831	0.614277	H	4.123039	-4.827016	-1.217028
C	-3.990360	1.745463	-0.744290	H	4.228306	-4.072869	-2.828961
				C	2.796470	-2.732428	0.036602

H	1.754102	-3.037710	-0.129931	P	-1.684294	-0.535127	0.134340
H	3.264812	-3.450440	0.729479	O	3.833708	3.519818	0.238737
C	2.836491	-1.336504	0.646501	O	1.897353	3.473502	-1.074270
C	2.302341	-1.297620	2.055858	O	3.041982	1.716635	1.513521
H	1.248611	-1.615938	2.065840	O	-2.503574	5.240055	-1.168632
H	2.356724	-0.283530	2.477545	O	-4.565683	3.660603	-1.257155
H	2.876276	-1.972858	2.707620	O	-4.290654	-1.123871	-0.571844
C	2.953256	-0.503034	-1.966058	O	-4.590841	-2.739581	1.088812
C	4.371002	-0.089747	-1.611490	O	-2.438042	-2.386273	1.929318
H	4.414680	0.967790	-1.317278	O	0.504959	-2.799027	0.273503
H	5.004168	-0.203721	-2.506582	C	1.864984	2.041033	-1.154847
C	2.431637	0.182828	-3.200489	C	1.326439	1.706847	-2.523075
H	3.091481	-0.023660	-4.056229	H	1.237396	0.619869	-2.657134
H	2.391707	1.271755	-3.054089	H	1.999117	2.098126	-3.300042
H	1.425274	-0.178937	-3.451707	H	0.333923	2.152719	-2.678041
C	-0.761844	-3.615489	1.010797	C	3.266794	1.514543	-0.903261
C	0.050467	-4.750662	1.152501	H	3.921298	1.811216	-1.738524
H	0.672290	-5.052939	0.306842	H	3.268153	0.420237	-0.841952
C	0.055859	-5.470176	2.342824	C	3.827716	2.106558	0.384321
H	0.698499	-6.348984	2.438955	C	5.237680	1.679606	0.672750
C	-0.759948	-5.074577	3.403437	H	5.580077	2.137943	1.608493
H	-0.758893	-5.633947	4.341616	H	5.901462	1.998677	-0.139803
C	-1.587258	-3.963795	3.251646	H	5.295188	0.588796	0.770805
H	-2.238910	-3.652012	4.073732	C	2.530976	4.043837	0.071119
C	-1.602422	-3.219821	2.067797	C	2.666334	5.514181	-0.208561
C	-2.490859	-2.031309	1.872986	H	3.185612	6.012042	0.619027
H	-1.858673	-1.178462	1.543028	H	1.678885	5.976534	-0.332755
H	-2.973016	-1.751549	2.820474	H	3.244351	5.665382	-1.128259
C	-3.522576	-2.277076	0.810357	C	1.749262	3.730877	1.339624
C	-4.869076	-2.467799	1.129318	H	2.275753	4.201215	2.185815
H	-5.173524	-2.442924	2.179847	H	0.738020	4.158799	1.313967
C	-5.823114	-2.674534	0.133625	C	1.704725	2.232449	1.586085
H	-6.871597	-2.818980	0.406015	C	1.163244	1.904809	2.953374
C	-5.438040	-2.687238	-1.207716	H	1.145457	0.823266	3.130316
H	-6.181991	-2.843194	-1.992654	H	0.145589	2.306151	3.062569
C	-4.102308	-2.495614	-1.544263	H	1.796328	2.371077	3.722620
H	-3.776211	-2.489935	-2.586673	C	-0.871305	2.084784	-0.129818
C	-3.136034	-2.304901	-0.545529	C	-1.043574	3.443827	-0.458484
C	-1.750865	-2.063769	-0.971248	H	-0.181090	4.102021	-0.492368
O	-1.328920	-1.981082	-2.134416	C	-2.281107	3.958454	-0.828058
				C	-1.411083	6.126699	-1.149946
<b>4(L1)</b>				H	-0.981536	6.225085	-0.138633
Ni	0.535118	-0.853695	0.340856	H	-1.793942	7.103941	-1.462775
P	0.759763	1.306149	0.214615	H	-0.616663	5.817752	-1.849447



C	-3.406077	3.096345	-0.881395	C	2.454784	-1.909500	-1.675611
C	-5.714006	2.846491	-1.290081	H	1.752831	-1.101721	-1.376956
H	-5.608531	2.006054	-1.995531	H	2.859040	-1.636210	-2.662795
H	-6.541066	3.482833	-1.622276	C	3.587326	-1.987149	-0.681771
H	-5.955282	2.445553	-0.292036	C	4.850222	-2.404822	-1.123849
C	-3.242408	1.752216	-0.566895	H	4.991067	-2.620894	-2.187308
H	-4.092676	1.076170	-0.644249	C	5.916224	-2.559019	-0.243025
C	-1.989993	1.230321	-0.191062	H	6.889579	-2.882757	-0.620258
C	-4.751198	-1.375361	0.757761	C	5.739783	-2.304532	1.119384
C	-6.225377	-1.081458	0.752507	H	6.569990	-2.432832	1.818185
H	-6.725612	-1.714580	0.009654	C	4.498486	-1.884318	1.575391
H	-6.408971	-0.029532	0.499648	H	4.328345	-1.667044	2.632808
H	-6.658694	-1.287500	1.738516	C	3.418424	-1.714729	0.691890
C	-3.227196	-3.149838	1.025413	C	2.147564	-1.209402	1.276918
C	-3.160869	-4.570084	1.507860	O	1.962966	-1.184994	2.478045
H	-2.117482	-4.904844	1.541072				
H	-3.731670	-5.231615	0.845231	<b>5-ts(L1)</b>			
H	-3.580454	-4.634421	2.519205	P	-1.436664	0.675278	-0.052027
C	-2.755218	-2.969558	-0.412615	P	1.592342	0.313961	-0.323972
H	-1.702675	-3.269059	-0.498079	O	-5.182489	1.118253	-0.283350
H	-3.357944	-3.624016	-1.062084	O	-3.552628	1.994662	1.146754
C	-2.943491	-1.525895	-0.862999	O	-3.561996	-0.045093	-1.510289
C	-2.733621	-1.340721	-2.344619	O	-0.436869	5.706170	1.231999
H	-1.718570	-1.654953	-2.627756	O	2.114919	5.427748	0.802128
H	-2.866419	-0.291611	-2.645497	O	4.140331	1.084286	0.385959
H	-3.452908	-1.951453	-2.909062	O	5.208714	-0.398148	-1.072312
C	-2.507536	-0.968234	1.793053	O	3.150903	-1.144306	-1.890677
C	-3.969938	-0.550164	1.779169	C	-2.817743	0.763661	1.236155
H	-4.078569	0.526869	1.585094	C	-2.252714	0.681418	2.629868
H	-4.399457	-0.748833	2.774432	H	-1.632244	-0.220874	2.739331
C	-1.720573	-0.382869	2.935595	H	-3.066536	0.660890	3.369521
H	-2.160011	-0.688268	3.896599	H	-1.617203	1.551505	2.848649
H	-1.725893	0.715540	2.888205	C	-3.757654	-0.384933	0.890459
H	-0.677678	-0.734121	2.904937	H	-4.506638	-0.489622	1.691285
C	0.822040	-3.583109	-0.724297	H	-3.204981	-1.329820	0.812036
C	0.254636	-4.883006	-0.793682	C	-4.483034	-0.110647	-0.421441
H	-0.406648	-5.189524	0.020832	C	-5.490947	-1.164297	-0.779244
C	0.531289	-5.750712	-1.841852	H	-5.976505	-0.906062	-1.728605
H	0.070982	-6.743354	-1.851365	H	-6.258928	-1.235269	0.000472
C	1.386531	-5.365456	-2.878094	H	-4.998921	-2.139013	-0.887104
H	1.599327	-6.039456	-3.710778	C	-4.308307	2.205312	-0.044163
C	1.976748	-4.104140	-2.817170	C	-5.156341	3.421160	0.203948
H	2.670462	-3.792674	-3.606588	H	-5.792782	3.629080	-0.664556
C	1.720602	-3.214699	-1.769527	H	-4.526185	4.298729	0.396801

H	-5.797894	3.252370	1.077139	C	3.700863	1.191221	-1.998926
C	-3.394351	2.332337	-1.257119	H	3.308861	2.216908	-1.932581
H	-4.026378	2.519532	-2.140358	H	4.205468	1.096375	-2.973901
H	-2.712060	3.188515	-1.160433	C	1.681473	0.195066	-3.143299
C	-2.630402	1.037761	-1.491132	H	2.265952	-0.006546	-4.052614
C	-1.910109	1.040128	-2.812655	H	1.196810	1.175181	-3.253382
H	-1.351630	0.107644	-2.961776	H	0.903518	-0.577922	-3.057188
H	-1.206211	1.883165	-2.862741	Ni	-0.060440	-1.136691	-0.108437
H	-2.631555	1.145838	-3.636055	O	0.182170	-1.537509	1.968568
C	-0.393777	2.158121	0.192768	C	0.509827	-2.773823	2.236937
C	-0.883816	3.406761	0.620116	C	1.756992	-3.125733	2.819514
H	-1.943539	3.508250	0.846488	H	2.445522	-2.321369	3.093777
C	-0.037631	4.493053	0.815484	C	2.120464	-4.453381	3.025448
C	-1.814787	5.916366	1.430410	H	3.100868	-4.678804	3.458113
H	-2.382016	5.781903	0.494444	C	1.253886	-5.495117	2.687452
H	-1.929685	6.953263	1.763894	H	1.542159	-6.537378	2.843094
H	-2.231179	5.249693	2.203366	C	-0.002970	-5.173196	2.171199
C	1.355445	4.341794	0.581840	H	-0.714564	-5.973529	1.935743
C	3.504379	5.310100	0.605093	C	-0.389022	-3.850904	1.958777
H	3.952569	4.548646	1.264398	C	-1.770940	-3.498619	1.489234
H	3.939811	6.284855	0.848907	H	-2.004104	-2.508856	1.920585
H	3.748096	5.068566	-0.442884	H	-2.497680	-4.208215	1.913098
C	1.844460	3.106271	0.174658	C	-2.003150	-3.431684	0.002574
H	2.918580	2.969789	0.068200	C	-3.050461	-4.183095	-0.549996
C	0.989388	2.005820	-0.020898	H	-3.641293	-4.819943	0.116474
C	4.726824	0.920349	-0.901792	C	-3.356352	-4.140730	-1.909089
C	5.910279	1.845925	-0.947803	H	-4.174323	-4.749992	-2.302485
H	6.607881	1.594793	-0.139749	C	-2.609451	-3.329542	-2.759241
H	5.589116	2.888138	-0.823166	H	-2.826871	-3.291333	-3.829342
H	6.434510	1.750794	-1.906337	C	-1.561566	-2.580435	-2.232741
C	4.181237	-1.370616	-0.926348	H	-0.938796	-1.989528	-2.911661
C	4.772292	-2.712357	-1.246936	C	-1.257129	-2.597760	-0.863069
H	4.010051	-3.493722	-1.146518	C	0.658776	-2.576332	-0.762979
H	5.601735	-2.933969	-0.564889	O	1.298354	-3.496892	-1.077447
H	5.151154	-2.714023	-2.276282				
C	3.644065	-1.268041	0.497710	<b>6(L1)</b>			
H	2.854944	-2.012969	0.673371	P	-1.347847	0.784465	-0.112073
H	4.467890	-1.485712	1.195896	P	1.645527	0.158457	-0.318095
C	3.126879	0.138148	0.764811	O	-5.021710	1.653529	-0.372600
C	2.794892	0.407348	2.208485	O	-3.320062	2.291822	1.105665
H	1.921251	-0.191099	2.507481	O	-3.519304	0.357920	-1.611806
H	2.560762	1.470126	2.362652	O	0.092008	5.657532	1.364910
H	3.654443	0.158230	2.848335	O	2.615751	5.158988	0.969622
C	2.579338	0.166150	-1.936299	O	4.252372	0.680650	0.395587

O	5.185241	-0.841925	-1.110200	C	4.816680	0.507619	-0.900973
O	3.071284	-1.389987	-1.937206	C	6.073869	1.330599	-0.932131
C	-2.734184	0.981091	1.167912	H	6.755702	0.997177	-0.140480
C	-2.191145	0.804167	2.561650	H	5.844923	2.392087	-0.773328
H	-1.622151	-0.134810	2.639017	H	6.579240	1.220448	-1.899082
H	-3.010777	0.800863	3.295071	C	4.083425	-1.728107	-0.983899
H	-1.507760	1.625827	2.819507	C	4.559805	-3.104536	-1.346280
C	-3.805190	-0.027920	0.785196	H	3.736791	-3.824715	-1.269674
H	-4.581618	-0.027964	1.566475	H	5.367686	-3.416530	-0.673713
H	-3.391202	-1.039473	0.717524	H	4.937353	-3.105949	-2.376041
C	-4.460385	0.358128	-0.536833	C	3.555404	-1.622050	0.443549
C	-5.563028	-0.573621	-0.946063	H	2.700825	-2.296599	0.600823
H	-6.007884	-0.232661	-1.888891	H	4.355102	-1.936170	1.132972
H	-6.344218	-0.600966	-0.177007	C	3.164555	-0.185915	0.757855
H	-5.163704	-1.585897	-1.087961	C	2.874253	0.070957	2.212344
C	-4.035136	2.624897	-0.084207	H	1.975234	-0.484522	2.515609
C	-4.745551	3.918594	0.199648	H	2.700580	1.141444	2.390952
H	-5.339822	4.227048	-0.668880	H	3.732539	-0.238062	2.827081
H	-4.024990	4.712500	0.433698	C	2.609609	-0.036694	-1.942114
H	-5.418018	3.790769	1.056489	C	3.809606	0.894684	-1.981185
C	-3.092616	2.692151	-1.279988	H	3.501088	1.945680	-1.878110
H	-3.684833	2.978696	-2.163918	H	4.299388	0.792476	-2.962850
H	-2.321373	3.462727	-1.144015	C	1.720084	0.106283	-3.147867
C	-2.474298	1.327661	-1.550136	H	2.294230	-0.102237	-4.062148
C	-1.741812	1.297585	-2.865407	H	1.316745	1.125799	-3.219393
H	-1.266886	0.324258	-3.040624	H	0.882417	-0.604956	-3.102740
H	-0.964739	2.074857	-2.885124	Ni	-0.174894	-1.170709	-0.221422
H	-2.441820	1.492463	-3.690965	O	0.141997	-1.573579	1.845258
C	-0.172468	2.153074	0.215037	C	0.271064	-2.830166	2.181306
C	-0.551738	3.430017	0.672489	C	1.480622	-3.359282	2.707422
H	-1.600191	3.626342	0.885411	H	2.319880	-2.676699	2.867312
C	0.387018	4.426935	0.915621	C	1.615618	-4.708395	3.022959
C	-1.263774	5.982030	1.564372	H	2.569854	-5.074362	3.415968
H	-1.834770	5.925190	0.623084	C	0.550761	-5.593581	2.847213
H	-1.289134	7.014858	1.927252	H	0.656195	-6.653660	3.089811
H	-1.739820	5.331387	2.315968	C	-0.664413	-5.088128	2.378242
C	1.764416	4.156819	0.698604	H	-1.524217	-5.759797	2.268542
C	3.992816	4.919384	0.797112	C	-0.824813	-3.739360	2.064758
H	4.349419	4.086300	1.425217	C	-2.151297	-3.177453	1.645506
H	4.511945	5.834926	1.099891	H	-2.201006	-2.144730	2.029262
H	4.239583	4.706563	-0.256235	H	-2.960224	-3.741145	2.134736
C	2.144420	2.894737	0.259157	C	-2.423820	-3.153880	0.162304
H	3.202792	2.662261	0.161600	C	-3.449000	-3.973757	-0.338373
C	1.193821	1.884467	0.019814	H	-3.992965	-4.613336	0.365232

C	-3.785342	-3.995383	-1.689788	H	0.312286	1.347385	3.038973
H	-4.581126	-4.654496	-2.046849	H	-1.397786	1.848594	2.901575
C	-3.094296	-3.173416	-2.575216	H	-0.214337	2.913112	3.703647
H	-3.335231	-3.173788	-3.641648	C	-1.911808	1.264664	-0.264114
C	-2.073838	-2.354629	-2.092638	C	-2.834681	2.230943	-0.710878
H	-1.520476	-1.737725	-2.807410	H	-2.508668	3.262516	-0.824929
C	-1.730409	-2.317419	-0.735054	C	-4.132508	1.891258	-1.076930
C	0.578882	-2.562053	-1.020912	C	-4.692771	4.117234	-1.617325
O	0.997949	-3.561512	-1.409369	H	-4.422771	4.536616	-0.633628
				H	-5.570063	4.653171	-1.995629
				H	-3.854415	4.276490	-2.315821
<b>7-ts(L1)</b>				C	-4.541457	0.535335	-1.004984
P	-0.149347	1.620182	0.123081	C	-6.258651	-1.051989	-1.302532
P	-1.035641	-1.322715	0.236226	H	-5.677744	-1.729901	-1.949625
O	0.956839	5.234687	0.388886	H	-7.300168	-1.050954	-1.641637
O	-0.456352	4.107663	-1.089885	H	-6.225573	-1.430468	-0.267162
O	1.318595	3.277080	1.619244	C	-3.632223	-0.425132	-0.577208
O	-5.055703	2.761586	-1.524113	H	-3.925892	-1.473267	-0.579694
O	-5.805834	0.277866	-1.384165	C	-2.317961	-0.085768	-0.203499
O	-2.740617	-3.347276	-0.599642	C	-3.014679	-3.869858	0.700056
O	-2.073302	-4.863541	1.055073	C	-4.360814	-4.533027	0.608464
O	-0.617320	-3.288268	1.981917	H	-4.333879	-5.318956	-0.156114
C	0.367457	2.930955	-1.144478	H	-5.132877	-3.802174	0.334386
C	0.254249	2.395007	-2.549488	H	-4.631299	-4.986959	1.569562
H	0.844487	1.474139	-2.662749	C	-0.738646	-4.360275	1.052569
H	0.622594	3.135905	-3.274074	C	0.170129	-5.447586	1.546407
H	-0.788798	2.159839	-2.804572	H	1.204034	-5.082142	1.553082
C	1.789275	3.326160	-0.766011	H	0.101982	-6.329057	0.897284
H	2.203930	3.978891	-1.551075	H	-0.113046	-5.737018	2.565787
H	2.432471	2.439424	-0.680287	C	-0.423062	-3.916978	-0.371074
C	1.790022	4.092210	0.552575	H	0.613510	-3.564783	-0.441770
C	3.149292	4.581308	0.962434	H	-0.531287	-4.792581	-1.031361
H	3.072149	5.139681	1.903407	C	-1.409128	-2.849755	-0.822428
H	3.568712	5.242393	0.194392	C	-1.297212	-2.529993	-2.291136
H	3.824345	3.729801	1.113355	H	-0.285936	-2.165503	-2.521983
C	-0.384808	4.877683	0.107018	H	-2.022205	-1.760905	-2.594528
C	-1.143618	6.147167	-0.159758	H	-1.487740	-3.431387	-2.892051
H	-1.104002	6.808429	0.714319	C	-1.539602	-2.206301	1.840241
H	-2.194875	5.928082	-0.386924	C	-2.948351	-2.768691	1.754792
H	-0.701208	6.670820	-1.015836	H	-3.684632	-1.977047	1.553062
C	-0.914193	4.092840	1.305184	H	-3.207633	-3.214832	2.729012
H	-0.861672	4.750620	2.188267	C	-1.338587	-1.304663	3.028374
H	-1.969426	3.816089	1.170094	H	-1.510365	-1.857373	3.963742
C	-0.053790	2.868774	1.560369	H	-2.037052	-0.456617	2.992707
C	-0.357710	2.203012	2.875609				

H	-0.312204	-0.909532	3.042521	H	-1.808917	-0.960723	2.778251
Ni	0.864665	-0.327438	0.311354	H	-3.451398	-0.485645	3.276424
O	2.207993	-1.822074	-1.186047	H	-2.266501	0.760413	2.820651
C	3.435548	-2.111156	-1.718135	C	-3.614287	-1.748429	0.805269
C	3.769656	-3.407314	-2.105341	H	-4.342245	-2.055191	1.573340
H	3.043799	-4.209205	-1.952537	H	-2.800966	-2.487221	0.789007
C	5.020749	-3.652497	-2.671882	C	-4.323624	-1.721894	-0.544302
H	5.289978	-4.668225	-2.972697	C	-4.928316	-3.039946	-0.931219
C	5.928600	-2.608335	-2.844727	H	-5.417889	-2.949460	-1.908500
H	6.908542	-2.800915	-3.288010	H	-5.676154	-3.346119	-0.189730
C	5.584961	-1.313208	-2.451598	H	-4.149536	-3.809564	-0.991477
H	6.296298	-0.492624	-2.587334	C	-4.912856	0.528920	-0.208828
C	4.337412	-1.048544	-1.885211	C	-6.110242	1.416930	-0.015370
C	3.901837	0.313901	-1.418122	H	-6.736928	1.415848	-0.915309
H	2.902023	0.522819	-1.837992	H	-5.795330	2.447930	0.191916
H	4.588408	1.079789	-1.806991	H	-6.708928	1.055484	0.829607
C	3.829970	0.410188	0.085247	C	-4.033903	0.943182	-1.386190
C	4.830836	1.102938	0.779062	H	-4.656939	0.918714	-2.294957
H	5.642065	1.569970	0.210577	H	-3.667548	1.973106	-1.270596
C	4.804934	1.223404	2.166770	C	-2.887684	-0.039296	-1.558021
H	5.590242	1.784622	2.679791	C	-2.124267	0.149486	-2.841403
C	3.786762	0.607863	2.899038	H	-1.310986	-0.587098	-2.924013
H	3.769459	0.680528	3.989311	H	-1.687636	1.157173	-2.884413
C	2.821631	-0.131678	2.230665	H	-2.792545	0.024736	-3.706151
H	2.082882	-0.705013	2.801290	C	-1.271366	1.795964	0.246338
C	2.790170	-0.208027	0.821745	C	-2.187729	2.766582	0.696539
C	2.119174	-1.732497	0.281222	H	-3.223315	2.476964	0.857190
O	2.420592	-2.711905	0.931662	C	-1.795682	4.067887	0.986092
				C	-3.984917	4.725366	1.565692
<b>8(L1)</b>				H	-4.438364	4.439405	0.601961
Ni	0.166318	-1.107242	-0.405199	H	-4.478960	5.633276	1.928062
P	-1.702545	0.039499	-0.065268	H	-4.156003	3.915495	2.294034
P	1.247284	0.817545	-0.372203	C	-0.432334	4.429145	0.835774
O	-5.385068	-0.777276	-0.463646	C	1.223876	6.098113	1.023709
O	-4.188211	0.567015	1.020699	H	1.895945	5.512569	1.672571
O	-3.421254	-1.364378	-1.587219	H	1.268332	7.148514	1.330655
O	-2.619210	5.035273	1.425683	H	1.573783	6.021996	-0.019441
O	-0.118885	5.696785	1.153607	C	0.477589	3.473464	0.399271
O	3.315004	2.423189	0.523809	H	1.531266	3.735696	0.351956
O	4.860378	1.714183	-1.084556	C	0.083102	2.156301	0.093493
O	3.252580	0.325590	-2.063539	C	3.889434	2.688969	-0.757832
O	2.333816	-3.127734	-0.496229	C	4.598743	4.008285	-0.636619
C	-3.099424	-0.359831	1.160599	H	5.354219	3.952155	0.156503
C	-2.626568	-0.252095	2.587924	H	3.889710	4.809347	-0.391528

H	5.099059	4.259235	-1.579716	C	-0.590339	-2.896992	-0.363735
C	4.306675	0.403258	-1.112856	C	1.490751	-2.213222	-1.176283
C	5.365721	-0.546117	-1.593726	O	1.578415	-2.272657	-2.376523
H	4.928941	-1.544678	-1.720307				
H	6.196291	-0.601673	-0.879425				
H	5.752239	-0.211279	-2.563848	<b>9-ts(L1)</b>			
C	3.805799	0.088922	0.290162	Ni	0.730860	-0.698011	0.408604
H	3.387541	-0.922714	0.319184	P	0.534291	1.504048	0.086622
H	4.659179	0.119003	0.986865	P	-1.475944	-0.814782	0.276063
C	2.770566	1.110727	0.726163	O	2.936819	4.411817	0.416966
C	2.416463	1.001820	2.187167	O	1.215489	3.912589	-1.085759
H	2.025891	-0.001433	2.411617	O	2.508879	2.452375	1.620885
H	1.659542	1.743987	2.478937	O	-3.496574	4.522302	-1.523642
H	3.310634	1.165054	2.806256	O	-5.219752	2.599614	-1.212817
C	2.201166	1.285356	-1.955144	O	-3.836174	-1.902142	-0.604059
C	2.820716	2.668400	-1.847712	O	-3.885898	-3.643326	0.962698
H	2.057093	3.440614	-1.678454	O	-1.881720	-2.886831	1.902415
H	3.311003	2.901269	-2.806876	O	0.988971	-2.670995	-1.188271
C	1.337514	1.116954	-3.176776	C	1.544332	2.517121	-1.165192
H	1.927523	1.320373	-4.082527	C	1.251359	2.091937	-2.581179
H	0.492414	1.819493	-3.154293	H	1.480827	1.027661	-2.726989
H	0.958497	0.088174	-3.241737	H	1.863409	2.676499	-3.282941
C	2.705044	-3.153858	0.817879	H	0.194384	2.251377	-2.837170
C	4.078600	-3.398553	0.991562	C	3.001258	2.348161	-0.764595
H	4.679098	-3.525605	0.087951	H	3.635681	2.818080	-1.532869
C	4.657620	-3.466767	2.249683	H	3.272217	1.288181	-0.697894
H	5.729522	-3.655691	2.346886	C	3.272223	3.037339	0.568666
C	3.857386	-3.291898	3.378662	C	4.707697	2.957397	0.997880
H	4.287171	-3.337997	4.381865	H	4.842677	3.492588	1.945662
C	2.493630	-3.085642	3.211424	H	5.361131	3.408203	0.241294
H	1.856712	-2.981641	4.095680	H	4.994742	1.908212	1.140335
C	1.871156	-3.020048	1.951534	C	1.568083	4.594400	0.119966
C	0.376869	-2.810539	1.931821	C	1.356392	6.057863	-0.146860
H	0.160541	-1.726764	1.815808	H	1.634440	6.650204	0.733190
H	-0.003493	-3.075810	2.932047	H	0.305666	6.260292	-0.389101
C	-0.387507	-3.547547	0.866653	H	1.979026	6.372780	-0.992968
C	-0.869873	-4.844070	1.075354	C	0.761975	4.059655	1.298926
H	-0.712145	-5.332240	2.043784	H	1.049558	4.632709	2.195165
C	-1.538054	-5.518928	0.053267	H	-0.316680	4.208405	1.150672
H	-1.912131	-6.533195	0.216749	C	1.091343	2.596254	1.544220
C	-1.704343	-4.896343	-1.185309	C	0.518683	2.085029	2.839610
H	-2.208337	-5.425959	-1.999672	H	0.744399	1.018578	2.974550
C	-1.225947	-3.601174	-1.391950	H	-0.572373	2.219676	2.856735
H	-1.352412	-3.136180	-2.374395	H	0.947176	2.638126	3.688135
				C	-1.221511	1.880827	-0.282566

C	-1.672524	3.132499	-0.746467	C	3.072373	-5.312931	-2.612980
H	-0.950253	3.928402	-0.909862	H	2.999547	-6.373322	-2.871932
C	-3.007900	3.361712	-1.056901	C	4.255592	-4.615111	-2.852370
C	-2.605950	5.600334	-1.685601	H	5.114148	-5.116511	-3.305810
H	-2.175438	5.917328	-0.721256	C	4.333175	-3.263869	-2.504834
H	-3.189836	6.430801	-2.096541	H	5.260655	-2.710488	-2.689638
H	-1.787566	5.363818	-2.385554	C	3.253107	-2.597142	-1.926445
C	-3.947458	2.311305	-0.893577	C	3.334632	-1.155421	-1.500909
C	-6.187053	1.588948	-1.054896	H	2.362575	-0.674797	-1.704609
H	-5.979273	0.713675	-1.692205	H	4.098582	-0.639236	-2.105900
H	-7.146393	2.022077	-1.357488	C	3.648224	-0.987264	-0.031154
H	-6.264455	1.259830	-0.005264	C	4.984168	-1.067644	0.391043
C	-3.506071	1.072424	-0.445475	H	5.768686	-1.217735	-0.358973
H	-4.216034	0.251636	-0.389940	C	5.325534	-0.978215	1.737409
C	-2.151986	0.833254	-0.139293	H	6.372288	-1.047515	2.045217
C	-4.310669	-2.325681	0.675425	C	4.316664	-0.815338	2.687200
C	-5.810614	-2.341129	0.581594	H	4.563449	-0.759890	3.751329
H	-6.125337	-3.013902	-0.225281	C	2.987059	-0.735109	2.276182
H	-6.194808	-1.334873	0.370094	H	2.212449	-0.634941	3.044850
H	-6.248193	-2.693673	1.523287	C	2.627464	-0.783384	0.920645
C	-2.467252	-3.764915	0.939848	C	0.989102	-2.495478	0.632783
C	-2.119512	-5.159582	1.370723	O	1.193142	-3.494078	1.195635
H	-1.030960	-5.291989	1.374344				
H	-2.564883	-5.890254	0.684965	CO			
H	-2.502357	-5.344285	2.381799	C	0.000000	0.000000	-0.647058
C	-1.998854	-3.429255	-0.468070	O	0.000000	0.000000	0.485293
H	-0.914155	-3.549514	-0.579552				
H	-2.485676	-4.128898	-1.166445	<b>10(L1)</b>			
C	-2.423954	-2.020839	-0.843461	P	-1.507286	0.447738	-0.150325
C	-2.180292	-1.702970	-2.295442	P	1.594482	0.418233	-0.416936
H	-1.108736	-1.803635	-2.519411	O	-5.220838	1.038286	-0.879558
H	-2.502868	-0.683179	-2.549810	O	-3.775237	1.729034	0.819128
H	-2.737641	-2.404150	-2.933125	O	-3.480625	-0.135151	-1.910850
C	-2.266780	-1.512147	1.855898	O	-0.943260	5.226169	2.062134
C	-3.780611	-1.422171	1.787378	O	1.650694	5.142217	1.895683
H	-4.113494	-0.381742	1.660698	O	4.049429	1.199747	0.576584
H	-4.195333	-1.783229	2.742369	O	5.290125	0.356615	-1.228663
C	-1.681325	-0.867009	3.083765	O	3.324055	-0.345213	-2.291950
H	-2.095996	-1.330198	3.990939	C	-3.101951	0.463905	0.932948
H	-1.907473	0.207969	3.109129	C	-2.794223	0.298205	2.398606
H	-0.589314	-1.000375	3.099750	H	-2.398161	-0.702146	2.604769
C	2.042161	-3.301681	-1.698361	H	-3.718960	0.426807	2.978960
C	1.979021	-4.665538	-2.041784	H	-2.065035	1.039557	2.754864
H	1.045259	-5.203879	-1.854046	C	-4.054239	-0.597818	0.400960

H	-4.918569	-0.647251	1.082392	H	5.963910	-2.176301	-1.479884
H	-3.591162	-1.589772	0.375435	H	5.504571	-1.490053	-3.060533
C	-4.560349	-0.216428	-0.982455	C	3.839777	-1.111768	-0.042078
C	-5.547349	-1.192023	-1.554641	H	3.127171	-1.944150	-0.123100
H	-5.885699	-0.842706	-2.537674	H	4.682082	-1.426215	0.594941
H	-6.418529	-1.282690	-0.894748	C	3.154652	0.075690	0.614390
H	-5.083279	-2.179042	-1.666260	C	2.805644	-0.151047	2.061772
C	-4.349259	2.059819	-0.444516	H	2.114754	-0.998118	2.156312
C	-5.172713	3.296778	-0.219513	H	2.339284	0.739597	2.506614
H	-5.669639	3.599843	-1.148730	H	3.716213	-0.378732	2.634267
H	-4.539080	4.122943	0.126906	C	2.614537	0.851384	-1.973173
H	-5.939284	3.098863	0.539463	C	3.611557	1.963703	-1.682270
C	-3.264750	2.225867	-1.499026	H	3.101294	2.874651	-1.338766
H	-3.750065	2.512924	-2.445824	H	4.129345	2.215307	-2.621702
H	-2.568403	3.033463	-1.230825	C	1.763337	1.178924	-3.169961
C	-2.529094	0.911476	-1.714890	H	2.408995	1.311553	-4.050171
C	-1.678948	0.946525	-2.953103	H	1.210987	2.114964	-3.009936
H	-1.156870	-0.008134	-3.105118	H	1.049950	0.377056	-3.396831
H	-0.936042	1.751583	-2.886913	Ni	-0.024910	-1.222842	-0.522486
H	-2.311942	1.134722	-3.832384	O	1.287003	-2.539112	0.385297
C	-0.570926	1.947948	0.381282	C	-1.436986	-2.547464	-0.347692
C	-1.173965	3.077511	0.971296	C	-2.176710	-3.017993	-1.438489
H	-2.254871	3.101966	1.081113	H	-2.022169	-2.596436	-2.435846
C	-0.424766	4.138872	1.467003	C	-3.145231	-4.011547	-1.279505
C	-2.344204	5.327112	2.153228	H	-3.706249	-4.364991	-2.149441
H	-2.811582	5.379807	1.156034	C	-3.393194	-4.543081	-0.015239
H	-2.558346	6.258234	2.688497	H	-4.151606	-5.317887	0.122238
H	-2.788805	4.487847	2.713228	C	-2.656332	-4.082859	1.072795
C	0.989024	4.096865	1.373697	H	-2.833082	-4.504998	2.068277
C	3.056406	5.141787	1.810241	C	-1.676019	-3.088673	0.930076
H	3.502785	4.279466	2.332343	C	-0.880169	-2.681478	2.147464
H	3.401031	6.061499	2.294535	H	-0.551725	-1.632473	2.032000
H	3.399304	5.145698	0.762281	H	-1.512752	-2.736277	3.047141
C	1.590544	2.996196	0.776277	C	0.319097	-3.562731	2.312249
H	2.676002	2.935737	0.749985	C	0.434053	-4.508480	3.329487
C	0.834078	1.918484	0.276421	H	-0.367219	-4.580574	4.074252
C	4.657390	1.496646	-0.679796	C	1.541502	-5.356472	3.417759
C	5.725996	2.516546	-0.402128	H	1.619084	-6.087683	4.225610
H	6.447368	2.110619	0.317248	C	2.541968	-5.252026	2.448182
H	5.288881	3.431407	0.017560	H	3.414181	-5.912014	2.491603
H	6.258367	2.772880	-1.325900	C	2.443776	-4.322861	1.417699
C	4.384538	-0.724926	-1.404608	H	3.224248	-4.256584	0.653647
C	5.120791	-1.837195	-2.093478	C	1.335815	-3.440297	1.322251
H	4.444542	-2.683974	-2.265199	C	0.520054	-1.929653	-2.164289



O	0.913073	-2.578881	-3.024003	H	3.290775	5.032537	-1.234102
				H	3.094528	5.914068	-2.774229
<b>11-ts(L1)</b>				H	3.163427	4.128818	-2.776941
P	1.588368	0.296251	0.211123	C	-0.611080	4.091814	-1.377729
P	-1.493310	0.505163	0.502431	C	-2.585475	5.302300	-1.816243
O	5.330136	0.427817	0.953340	H	-3.113077	4.472526	-2.315237
O	4.027012	1.288216	-0.784226	H	-2.856809	6.239837	-2.313270
O	3.438597	-0.426025	2.029643	H	-2.914708	5.353351	-0.764684
O	1.402318	5.039210	-2.112904	C	-1.299789	3.059846	-0.750047
O	-1.187399	5.180066	-1.918836	H	-2.387357	3.091317	-0.713606
O	-3.935708	1.404619	-0.513863	C	-0.631131	1.937574	-0.225189
O	-5.192942	0.640589	1.304594	C	-4.520297	1.751154	0.736346
O	-3.261665	-0.096387	2.402607	C	-5.553040	2.803619	0.444809
C	3.168521	0.135958	-0.860494	H	-6.295035	2.408154	-0.259444
C	2.867406	-0.029795	-2.328448	H	-5.083360	3.689874	-0.000840
H	2.409857	-1.004452	-2.525003	H	-6.066927	3.101789	1.366551
H	3.809539	0.019554	-2.893451	C	-4.321916	-0.461582	1.520574
H	2.201024	0.757652	-2.709481	C	-5.105517	-1.531940	2.224979
C	3.917285	-1.052494	-0.269400	H	-4.465463	-2.401369	2.420015
H	4.752719	-1.319190	-0.936999	H	-5.958774	-1.847399	1.612672
H	3.261993	-1.928800	-0.186717	H	-5.479868	-1.148767	3.182047
C	4.482907	-0.704496	1.101444	C	-3.782079	-0.901085	0.164926
C	5.302975	-1.808770	1.704514	H	-3.094801	-1.748888	0.294386
H	5.699051	-1.487628	2.675692	H	-4.625515	-1.236476	-0.460012
H	6.143022	-2.064272	1.047407	C	-3.072424	0.258942	-0.523413
H	4.682303	-2.700904	1.851855	C	-2.755239	-0.008176	-1.970276
C	4.626592	1.560462	0.475926	H	-2.120416	-0.896555	-2.068407
C	5.636561	2.649033	0.242347	H	-2.239835	0.845585	-2.433175
H	6.166753	2.882899	1.173367	H	-3.684008	-0.192851	-2.530214
H	5.145832	3.560115	-0.122278	C	-2.496488	1.057965	2.036351
H	6.368569	2.319343	-0.505006	C	-3.450929	2.198806	1.721091
C	3.562550	1.918053	1.499774	H	-2.907884	3.079260	1.348761
H	4.068262	2.178219	2.443717	H	-3.952016	2.498356	2.655863
H	2.990103	2.801975	1.181806	C	-1.625265	1.388373	3.217249
C	2.643726	0.733369	1.760483	H	-2.257923	1.597631	4.092278
C	1.806868	0.971477	2.985459	H	-1.019879	2.282366	3.014247
H	1.207238	0.090603	3.239518	H	-0.960741	0.557022	3.477205
H	1.140766	1.831596	2.838050	Ni	-0.002559	-1.245775	0.664712
H	2.460463	1.188131	3.843169	O	-0.926280	-2.982258	-0.007809
C	0.772047	1.850350	-0.342416	C	0.864784	-2.964883	-0.094313
C	1.465133	2.905414	-0.967192	C	1.504580	-3.835276	0.810370
H	2.545200	2.831154	-1.082310	H	1.178252	-3.888521	1.850888
C	0.801051	4.013296	-1.484579	C	2.590008	-4.595246	0.384504
C	2.804951	5.012709	-2.223512	H	3.111044	-5.223711	1.112679

C	3.012002	-4.567656	-0.949194	H	4.619976	-3.996782	0.381479
H	3.861543	-5.170500	-1.276590	C	4.607554	0.485913	0.428583
C	2.299881	-3.789392	-1.863726	C	5.635487	1.582393	0.464247
H	2.574028	-3.795354	-2.924369	H	6.236748	1.515206	1.378964
C	1.215085	-3.007681	-1.463541	H	5.149636	2.566316	0.433748
C	0.308507	-2.316794	-2.439914	H	6.302330	1.493999	-0.402161
H	0.170050	-1.257021	-2.133357	C	3.658645	0.502749	1.624119
H	0.733202	-2.308708	-3.454128	H	4.267279	0.414923	2.539539
C	-1.003961	-3.035522	-2.416730	H	3.112725	1.455136	1.688689
C	-1.704885	-3.423340	-3.561044	C	2.703691	-0.674468	1.557193
H	-1.282934	-3.185277	-4.542484	C	1.914346	-0.863570	2.825134
C	-2.925644	-4.089236	-3.468772	H	1.264610	-1.746042	2.749460
H	-3.467464	-4.373274	-4.373610	H	1.287651	0.016513	3.028296
C	-3.442781	-4.399283	-2.207924	H	2.590209	-1.009286	3.681115
H	-4.392794	-4.933230	-2.120767	C	0.708840	1.052527	0.025827
C	-2.750536	-4.044659	-1.054930	C	1.392433	2.274369	-0.120882
H	-3.136614	-4.290409	-0.062517	H	2.477230	2.263524	-0.207893
C	-1.537080	-3.340785	-1.146546	C	0.717584	3.485185	-0.227972
C	-0.178778	-1.768542	2.401009	C	2.715439	4.721206	-0.429829
O	-0.395829	-2.104971	3.484489	H	3.165259	4.368105	0.513516
				H	2.997684	5.769031	-0.580056
				H	3.120790	4.123802	-1.263407
<b>12(L1)</b>				C	-0.699819	3.491716	-0.197454
P	1.545110	-0.589505	0.048900	C	-2.690970	4.752152	-0.295741
P	-1.546291	-0.582682	0.058190	H	-3.147272	4.176229	-1.117919
O	5.303568	-0.749103	0.453475	H	-2.966719	5.806030	-0.412974
O	3.902140	0.639452	-0.796812	H	-3.096301	4.388932	0.663960
O	3.470250	-1.875819	1.370013	C	-1.381589	2.286533	-0.069504
O	1.310258	4.683599	-0.382933	H	-2.468398	2.288083	-0.121635
O	-1.286217	4.696689	-0.323495	C	-0.704500	1.057587	0.047906
O	-3.891541	0.665841	-0.788155	C	-4.610611	0.490394	0.426305
O	-5.309069	-0.743483	0.420170	C	-5.637175	1.587681	0.472957
O	-3.486093	-1.890437	1.332776	H	-6.284774	1.528012	-0.410289
C	3.000671	-0.423684	-1.152835	H	-5.149613	2.571052	0.485093
C	2.515585	-0.134717	-2.550039	H	-6.258473	1.492671	1.371650
H	1.825675	-0.923349	-2.883094	C	-4.433040	-1.853536	0.268769
H	3.362364	-0.094424	-3.251100	C	-5.261929	-3.100124	0.396011
H	1.984282	0.826786	-2.601256	H	-4.629552	-3.990520	0.294501
C	3.748285	-1.748353	-1.047572	H	-6.036115	-3.124861	-0.380253
H	4.523763	-1.793133	-1.828902	H	-5.748360	-3.123698	1.378842
H	3.053945	-2.588154	-1.200891	C	-3.741119	-1.717811	-1.083724
C	4.426820	-1.860152	0.314424	H	-3.046626	-2.555967	-1.245002
C	5.252463	-3.105373	0.472891	H	-4.508424	-1.746196	-1.873773
H	5.728241	-3.111116	1.461192	C	-2.989758	-0.393294	-1.155708
H	6.034883	-3.145559	-0.294407				

C	-2.490310	-0.079346	-2.542384	P	-1.553050	-0.250741	0.206973
H	-1.797730	-0.862459	-2.883146	P	1.530220	-0.515593	0.386656
H	-1.958502	0.882775	-2.571017	O	-5.326027	-0.358479	0.788973
H	-3.330271	-0.025903	-3.250669	O	-3.905414	-1.269719	-0.825553
C	-2.720350	-0.693906	1.552381	O	-3.498357	0.633702	1.857929
C	-3.674787	0.482361	1.632676	O	-1.546369	-5.165725	-1.776963
H	-3.129019	1.432635	1.723373	O	1.043059	-5.352462	-1.659195
H	-4.293938	0.376462	2.539131	O	3.864552	-1.643904	-0.581477
C	-1.946204	-0.913022	2.825177	O	5.223549	-0.882458	1.167676
H	-2.632812	-1.073010	3.669985	O	3.389025	0.130220	2.211981
H	-1.316055	-0.042309	3.055351	O	1.468628	2.479612	0.198302
H	-1.301737	-1.798321	2.737766	C	-3.082341	-0.095421	-0.939989
Ni	-0.004024	-2.005175	-0.425360	C	-2.668488	0.004381	-2.385328
C	-0.005555	-3.039510	-1.816437	H	-2.104391	0.931261	-2.554825
O	-0.005168	-3.575343	-2.854937	H	-3.559462	0.024269	-3.029189
<b>P</b>				H	-2.042825	-0.844776	-2.695002
O	-0.000002	-1.327319	0.014534	C	-3.929732	1.084921	-0.488798
C	1.183105	-0.643244	0.005650	H	-4.758141	1.195250	-1.206330
C	2.340323	-1.426666	-0.000402	H	-3.362637	2.021471	-0.485924
H	2.233915	-2.513045	0.002014	C	-4.525431	0.813338	0.884652
C	3.588006	-0.815824	-0.008941	C	-5.408962	1.916187	1.389793
H	4.490650	-1.431050	-0.013029	H	-5.810755	1.647974	2.374523
C	3.681926	0.577143	-0.012832	H	-6.245215	2.075859	0.698728
H	4.659197	1.064685	-0.020380	H	-4.837656	2.848167	1.476285
C	2.519822	1.343253	-0.006559	C	-4.564556	-1.487879	0.422791
H	2.587184	2.435400	-0.008293	C	-5.520021	-2.626344	0.199277
C	1.249946	0.754667	0.003861	H	-6.091273	-2.830093	1.112941
C	-0.000005	1.584433	0.020348	H	-4.977162	-3.535952	-0.087040
H	-0.000057	2.243946	0.907124	H	-6.221934	-2.367555	-0.602597
H	0.000017	2.284065	-0.834385	C	-3.554340	-1.745912	1.536778
C	-1.249941	0.754659	0.003719	H	-4.115265	-1.927294	2.467948
C	-2.519820	1.343250	-0.006675	H	-2.955199	-2.645382	1.335476
H	-2.587176	2.435395	-0.008442	C	-2.670791	-0.525167	1.738360
C	-3.681911	0.577142	-0.012836	C	-1.857144	-0.595022	3.001631
H	-4.659184	1.064679	-0.020412	H	-1.209953	0.287495	3.101746
C	-3.587999	-0.815823	-0.008867	H	-1.228705	-1.495240	3.009814
H	-4.490650	-1.431041	-0.012792	H	-2.523888	-0.634760	3.875306
C	-2.340319	-1.426666	-0.000334	C	-0.790787	-1.863980	-0.276296
H	-2.233903	-2.513038	0.002223	C	-1.521433	-2.950721	-0.799726
C	-1.183127	-0.643231	0.005552	H	-2.599175	-2.863840	-0.900448
<b>13(L1)</b>				C	-0.901762	-4.109849	-1.251107
Ni	0.043386	1.227806	0.284512	C	-2.950995	-5.116887	-1.845531
				H	-3.403360	-5.059652	-0.841644
				H	-3.275536	-6.047862	-2.322441

H	-3.311013	-4.267432	-2.449410	C	1.068254	3.730646	-1.835510
C	0.509971	-4.214069	-1.186034	C	-0.234347	3.027130	-2.086813
C	2.440938	-5.505802	-1.588251	H	-0.089811	1.926872	-2.059304
H	2.973242	-4.733403	-2.167149	H	-0.618110	3.285654	-3.085752
H	2.671701	-6.486319	-2.017971	C	-1.199934	3.414989	-0.994866
H	2.798621	-5.485581	-0.545452	C	-2.006322	4.554089	-1.108903
C	1.237898	-3.152665	-0.664150	H	-2.032891	5.101170	-2.058121
H	2.323824	-3.207113	-0.663711	C	-2.743648	5.014097	-0.017953
C	0.614258	-1.976840	-0.202717	H	-3.372422	5.903014	-0.116094
C	4.436275	-1.954204	0.689615	C	-2.646433	4.352033	1.205915
C	5.355158	-3.122071	0.462625	H	-3.193162	4.725899	2.077066
H	6.117008	-2.852528	-0.278814	C	-1.862452	3.199990	1.319493
H	4.795903	-3.990483	0.091754	H	-1.831674	2.676188	2.279478
H	5.858422	-3.400486	1.396360	C	-1.159513	2.705444	0.217840
C	4.469588	0.316581	1.296637				
C	5.365502	1.353604	1.909740				
H	4.812674	2.289564	2.053823	<b>14-ts(L1)</b>			
H	6.227184	1.547151	1.259702	P	1.639504	0.120460	0.174373
H	5.729382	1.004653	2.883860	P	-1.433135	0.549583	0.302703
C	3.951153	0.699745	-0.078924	O	5.377223	-0.254276	0.724870
H	3.358352	1.617365	-0.002266	O	4.108611	0.959484	-0.807780
H	4.811026	0.878233	-0.743699	O	3.451606	-1.066277	1.774464
C	3.109599	-0.424120	-0.663288	O	2.010947	5.185935	-1.336755
C	2.769995	-0.205436	-2.114664	O	-0.570103	5.527000	-1.253158
H	2.221719	0.740068	-2.231935	O	-3.653062	1.973135	-0.640786
H	2.152137	-1.021708	-2.516193	O	-5.139295	1.101232	0.936141
H	3.689483	-0.144701	-2.714187	O	-3.425442	-0.140180	1.940805
C	2.515401	-0.970071	1.960655	C	3.128166	-0.080529	-0.984731
C	3.349946	-2.220937	1.727142	C	2.701918	-0.028772	-2.429475
H	2.718944	-3.074923	1.442672	H	1.987233	-0.836030	-2.644919
H	3.846446	-2.485432	2.675158	H	3.573628	-0.156375	-3.087990
C	1.624020	-1.093489	3.166093	H	2.224231	0.930435	-2.677550
H	2.233910	-1.280588	4.062003	C	3.768546	-1.411128	-0.606784
H	0.923507	-1.931739	3.048609	H	4.542871	-1.659693	-1.350524
H	1.054073	-0.169959	3.330956	H	3.024479	-2.219975	-0.609569
C	1.782662	3.442575	-0.633882	C	4.424716	-1.312190	0.765722
C	2.940269	4.213776	-0.362554	C	5.169714	-2.549333	1.175645
H	3.475613	4.010613	0.569446	H	5.643062	-2.387892	2.152117
C	3.385673	5.197069	-1.236798	H	5.950189	-2.783650	0.441449
H	4.287270	5.766462	-0.990853	H	4.482583	-3.399503	1.247694
C	2.690559	5.462555	-2.418589	C	4.774000	0.993856	0.451745
H	3.035524	6.234663	-3.110258	C	5.876020	2.008091	0.321644
C	1.535233	4.729736	-2.692778	H	6.466257	2.051822	1.244941
H	0.964604	4.939626	-3.604708	H	5.463107	3.005144	0.122299
				H	6.539819	1.730089	-0.505977

C	3.800957	1.297250	1.590927	H	-2.529979	3.084977	1.587042
H	4.382404	1.342919	2.526744	H	-3.756692	2.432312	2.688641
H	3.321499	2.277735	1.457837	C	-1.631502	0.853006	3.100307
C	2.768152	0.190915	1.713084	H	-2.262116	0.967475	3.994696
C	1.944935	0.282977	2.969055	H	-0.879224	1.653986	3.106486
H	1.218350	-0.541608	3.009476	H	-1.115653	-0.115015	3.165145
H	1.397410	1.234912	3.008160	Ni	-0.035709	-1.191057	0.285135
H	2.591008	0.219387	3.857373	O	-0.879489	-2.931085	0.586672
C	1.004160	1.818852	-0.161164	C	0.592582	-3.104321	0.056026
C	1.817405	2.894464	-0.570715	C	1.429427	-3.820061	0.955215
H	2.890594	2.739960	-0.661197	H	1.332664	-3.649686	2.030477
C	1.285822	4.129915	-0.922953	C	2.381101	-4.695770	0.456043
C	3.409589	5.045691	-1.384398	H	3.033821	-5.219343	1.161545
H	3.833081	4.859034	-0.383242	C	2.514023	-4.934886	-0.920767
H	3.809216	5.994008	-1.759931	H	3.268373	-5.628659	-1.296867
H	3.725779	4.235921	-2.062922	C	1.627509	-4.298724	-1.799810
C	-0.117691	4.317326	-0.872809	H	1.677672	-4.503563	-2.874935
C	-1.956040	5.757882	-1.198042	C	0.655732	-3.420756	-1.336912
H	-2.521126	5.065767	-1.844580	C	-0.431162	-2.814723	-2.176371
H	-2.119304	6.781099	-1.553756	H	-0.379240	-1.703599	-2.108696
H	-2.341879	5.679360	-0.167461	H	-0.328439	-3.072530	-3.240754
C	-0.925433	3.262843	-0.465181	C	-1.744489	-3.302743	-1.630356
H	-2.004980	3.390838	-0.482295	C	-2.819980	-3.726666	-2.414697
C	-0.394023	2.009667	-0.102195	H	-2.727294	-3.684681	-3.504184
C	-4.264372	2.172659	0.629450	C	-3.996806	-4.198206	-1.832801
C	-5.101748	3.415153	0.508316	H	-4.830129	-4.513949	-2.464575
H	-5.832262	3.294949	-0.301134	C	-4.098409	-4.279255	-0.442343
H	-4.472140	4.286250	0.286383	H	-5.011239	-4.662845	0.021022
H	-5.642821	3.602640	1.443768	C	-3.035845	-3.875879	0.362527
C	-4.464077	-0.149857	0.964184	H	-3.087418	-3.926443	1.452202
C	-5.459897	-1.181258	1.412440	C	-1.880868	-3.364467	-0.230925
H	-4.975353	-2.159758	1.508718				
H	-6.281351	-1.262818	0.690102	<b>15(L1)</b>			
H	-5.873201	-0.894136	2.387163	P	-1.579405	-0.761493	0.277919
C	-3.900635	-0.401045	-0.429658	P	1.577372	-0.763630	0.264396
H	-3.384633	-1.369534	-0.462105	O	-5.340260	-0.896433	-0.341107
H	-4.738521	-0.441393	-1.144887	O	-3.987719	0.663121	0.745132
C	-2.958640	0.726676	-0.827836	O	-3.492330	-2.193535	-0.941350
C	-2.565988	0.669432	-2.281913	O	-1.301546	4.525812	-0.066075
H	-2.078745	-0.289717	-2.509081	O	1.302751	4.525105	-0.058872
H	-1.871878	1.479055	-2.549010	O	3.984255	0.654162	0.760801
H	-3.457483	0.760867	-2.919726	O	5.341767	-0.897059	-0.331921
C	-2.473178	0.931493	1.855558	O	3.494610	-2.183093	-0.958909
C	-3.223669	2.245867	1.741728	C	-3.122348	-0.333472	1.322910

C	-2.730158	0.186990	2.681519	H	5.113013	2.372179	-0.852582
H	-2.086467	-0.538535	3.198660	H	6.179139	1.190393	-1.656368
H	-3.622850	0.363072	3.300647	C	4.496769	-1.982963	0.026848
H	-2.177319	1.134419	2.605478	C	5.344852	-3.224510	0.031747
C	-3.898253	-1.644832	1.398314	H	4.738845	-4.100443	0.294287
H	-4.717852	-1.549122	2.129439	H	6.161334	-3.128271	0.757549
H	-3.234968	-2.459193	1.725740	H	5.776621	-3.382134	-0.964194
C	-4.500618	-1.979987	0.035435	C	3.887289	-1.660546	1.389681
C	-5.351924	-3.219306	0.048572	H	3.220332	-2.476556	1.705188
H	-5.779596	-3.385288	-0.947793	H	4.703091	-1.573833	2.126197
H	-6.171541	-3.114002	0.769585	C	3.114005	-0.347188	1.322404
H	-4.749429	-4.094244	0.322267	C	2.712438	0.160541	2.683117
C	-4.612167	0.313716	-0.480282	H	2.064165	-0.569362	3.188265
C	-5.609113	1.401416	-0.773046	H	2.160648	1.108980	2.611401
H	-6.162584	1.180286	-1.693943	H	3.600525	0.330259	3.310554
H	-5.101096	2.367211	-0.891442	C	2.677284	-1.037687	-1.276300
H	-6.324100	1.480325	0.055246	C	3.597816	0.130592	-1.581604
C	-3.585244	0.114212	-1.589497	H	3.024121	1.053703	-1.749182
H	-4.132672	-0.106325	-2.521690	H	4.150900	-0.083315	-2.511996
H	-3.007262	1.034010	-1.761122	C	1.837509	-1.436432	-2.458199
C	-2.670446	-1.053492	-1.265935	H	2.473918	-1.714678	-3.312209
C	-1.823145	-1.468935	-2.436561	H	1.187461	-0.605743	-2.767413
H	-1.193244	-2.328330	-2.165907	H	1.201194	-2.295598	-2.203023
H	-1.165854	-0.645508	-2.749554	Ni	0.000258	-1.986337	0.703571
H	-2.453817	-1.753979	-3.292630				
C	-0.709163	0.865925	0.060998	<b>16-ts(L1)</b>			
C	-1.384346	2.100206	0.013573	P	-0.445337	1.475621	-0.336735
H	-2.471652	2.104416	0.063973	P	1.416998	-0.959907	0.049266
C	-0.706769	3.314744	-0.032465	O	-2.914209	4.295891	-0.756494
C	-2.703795	4.563455	-0.135008	O	-1.050426	4.005829	0.628072
H	-3.082180	4.065821	-1.044272	O	-2.525610	2.238106	-1.798470
H	-2.990829	5.620410	-0.170909	O	3.845084	4.493052	0.400451
H	-3.180734	4.100336	0.745603	O	5.424564	2.433936	0.496945
C	0.707290	3.314308	-0.029658	O	3.842405	-2.136257	0.783842
C	2.705503	4.562592	-0.115575	O	3.466936	-4.093822	-0.429431
H	3.174539	4.094431	0.766551	O	1.436362	-3.288930	-1.254706
H	2.993133	5.619629	-0.143371	C	-1.337655	2.624065	0.876645
H	3.091792	4.069865	-1.024241	C	-0.912872	2.334032	2.291631
C	1.383918	2.099176	0.015371	H	-1.054490	1.267835	2.522627
H	2.471089	2.102786	0.068029	H	-1.509840	2.924088	3.002687
C	0.707691	0.865257	0.059781	H	0.147235	2.581507	2.445872
C	4.617404	0.316078	-0.463574	C	-2.817953	2.364137	0.621858
C	5.618493	1.404575	-0.738205	H	-3.417679	2.877811	1.390720
H	6.326601	1.474969	0.096706	H	-3.026161	1.285097	0.684275

C	-3.215575	2.905329	-0.748792	C	1.821764	-3.392991	1.150798
C	-4.678227	2.752015	-1.052890	H	0.739088	-3.322623	1.337137
H	-4.903690	3.204781	-2.026049	H	2.267172	-4.041616	1.921989
H	-5.288152	3.242232	-0.284511	C	2.477621	-2.014785	1.212772
H	-4.940087	1.687331	-1.096403	C	2.534945	-1.431141	2.602075
C	-1.528368	4.540240	-0.605962	H	1.528700	-1.257200	3.006167
C	-1.340829	6.029373	-0.524080	H	3.067403	-0.469513	2.604845
H	-1.717973	6.511363	-1.434202	H	3.068408	-2.113544	3.279806
H	-0.278741	6.280122	-0.407359	C	1.936961	-1.966292	-1.480791
H	-1.891736	6.425842	0.337489	C	3.449105	-2.029636	-1.614332
C	-0.808895	3.899727	-1.787890	H	3.882906	-1.020797	-1.687007
H	-1.192126	4.365369	-2.710523	H	3.698493	-2.561929	-2.546671
H	0.271829	4.095294	-1.754907	C	1.258660	-1.450151	-2.721486
C	-1.107103	2.410359	-1.856863	H	1.514584	-2.079392	-3.586806
C	-0.628055	1.786546	-3.141138	H	1.576197	-0.420178	-2.938198
H	-0.898540	0.725280	-3.187526	H	0.165483	-1.458633	-2.603210
H	0.462493	1.891269	-3.234807	Ni	-0.775028	-0.629443	-0.034392
H	-1.094265	2.293389	-3.998829	O	-1.746967	-2.341232	0.802162
C	1.346738	1.809412	-0.108940	C	-2.257495	-1.674898	1.870032
C	1.895727	3.098090	0.037287	C	-1.410395	-1.545754	2.985370
H	1.231769	3.960129	0.047065	H	-0.438125	-2.041814	2.946622
C	3.258337	3.293888	0.240647	C	-1.816257	-0.827870	4.103775
C	3.029678	5.638666	0.359762	H	-1.142373	-0.734863	4.959644
H	2.531833	5.752138	-0.617865	C	-3.083449	-0.242541	4.133461
H	3.688204	6.499442	0.517706	H	-3.414122	0.319551	5.009692
H	2.264956	5.630120	1.153644	C	-3.935570	-0.406043	3.041596
C	4.121297	2.168910	0.302079	H	-4.940711	0.027517	3.068978
C	6.315959	1.345586	0.541282	C	-3.557596	-1.122426	1.901381
H	6.086996	0.652911	1.368110	C	-4.487744	-1.314140	0.737045
H	7.315680	1.763922	0.700242	H	-4.495892	-0.383359	0.126183
H	6.316902	0.781145	-0.406121	H	-5.522687	-1.430569	1.093189
C	3.580866	0.892831	0.188471	C	-4.081729	-2.468948	-0.121081
H	4.229242	0.024545	0.300977	C	-4.964059	-3.432265	-0.590055
C	2.202679	0.691128	-0.009191	H	-6.019768	-3.345402	-0.310665
C	4.060110	-2.807136	-0.452129	C	-4.538738	-4.506029	-1.377835
C	5.546068	-2.997907	-0.571232	H	-5.249757	-5.254199	-1.732719
H	5.912834	-3.582026	0.281685	C	-3.171590	-4.611928	-1.675013
H	6.058852	-2.027492	-0.578812	H	-2.808770	-5.453800	-2.272734
H	5.792245	-3.534093	-1.495607	C	-2.260772	-3.672968	-1.232766
C	2.062744	-4.034558	-0.214834	H	-1.198824	-3.748510	-1.486120
C	1.524253	-5.433008	-0.315508	C	-2.692107	-2.516519	-0.494014
H	0.440030	-5.435680	-0.147473	C	-2.177154	-1.085555	-1.193710
H	2.000856	-6.080880	0.429887	O	-2.540284	-0.748917	-2.278255
H	1.727210	-5.837524	-1.314680				

## 17(L1)

				H	-1.416977	5.779266	-1.473331
P	0.361614	1.323424	0.323455	C	-3.949805	2.712402	-0.846435
P	-1.890992	-0.761047	0.091186	C	-6.170610	2.218552	-1.465205
O	2.977697	3.899631	1.327420	H	-5.898825	1.446584	-2.204518
O	1.305877	3.894751	-0.304894	H	-7.040122	2.770399	-1.838822
O	2.340977	1.779412	2.085966	H	-6.450720	1.722911	-0.520190
O	-3.274990	4.956178	-0.984665	C	-3.655566	1.382334	-0.568163
O	-5.143379	3.160693	-1.278367	H	-4.417637	0.621689	-0.732207
O	-4.205170	-1.662346	-1.176511	C	-2.372362	0.981911	-0.152446
O	-4.417989	-3.555340	0.181114	C	-4.817486	-2.208102	-0.015283
O	-2.572904	-2.922591	1.467056	C	-6.297586	-2.209917	-0.278230
C	1.490436	2.508381	-0.647214	H	-6.514364	-2.802525	-1.175365
C	1.238669	2.389423	-2.128617	H	-6.659741	-1.185949	-0.438634
H	1.359972	1.346090	-2.452155	H	-6.838590	-2.646616	0.570067
H	1.946708	3.016879	-2.690812	C	-3.009027	-3.675904	0.339821
H	0.219887	2.712120	-2.387306	C	-2.703624	-5.111967	0.658484
C	2.906725	2.116698	-0.251967	H	-1.624185	-5.238897	0.812343
H	3.626845	2.638527	-0.903876	H	-3.028156	-5.767880	-0.158416
H	3.055237	1.038789	-0.378701	H	-3.225497	-5.407721	1.576814
C	3.187729	2.499930	1.195577	C	-2.358058	-3.195482	-0.956186
C	4.598109	2.210949	1.624739	H	-1.262478	-3.261782	-0.881620
H	4.752669	2.560582	2.652968	H	-2.696091	-3.849937	-1.775998
H	5.314098	2.717026	0.965403	C	-2.771828	-1.757570	-1.251076
H	4.789463	1.131422	1.588753	C	-2.389594	-1.286888	-2.629581
C	1.639129	4.263744	1.027397	H	-1.301920	-1.329509	-2.764677
C	1.561850	5.763907	1.085108	H	-2.720427	-0.251507	-2.796191
H	1.850175	6.123904	2.080216	H	-2.869862	-1.920699	-3.389771
H	0.542117	6.107217	0.868566	C	-2.928901	-1.532563	1.480442
H	2.243645	6.198590	0.343897	C	-4.422703	-1.417593	1.226601
C	0.738440	3.566116	2.041582	H	-4.733629	-0.365840	1.142714
H	1.022768	3.924829	3.044315	H	-4.957759	-1.846793	2.089618
H	-0.316903	3.834870	1.889652	C	-2.537935	-0.991023	2.829277
C	0.934953	2.058960	1.992348	H	-3.074389	-1.530183	3.624038
C	0.285262	1.360954	3.156009	H	-2.796909	0.074877	2.904509
H	0.505598	0.285421	3.136611	H	-1.461081	-1.105684	3.008751
H	-0.805323	1.495935	3.133208	Ni	0.294403	-0.891644	0.250868
H	0.663378	1.769850	4.104996	C	0.725675	-1.891653	1.631860
C	-1.349307	1.943767	-0.016614	O	0.935262	-2.553408	2.564622
C	-1.661509	3.291098	-0.283487	O	2.673176	-0.820372	-1.810441
H	-0.872431	4.037120	-0.224558	C	4.044799	-0.740226	-1.743961
C	-2.931260	3.687136	-0.691539	C	4.665442	-0.220563	-2.880901
C	-2.295882	5.953371	-0.830424	H	4.051563	0.003570	-3.755577
H	-1.959966	6.035824	0.216705	C	6.037168	0.013863	-2.875122
H	-2.761314	6.900744	-1.123939	H	6.519003	0.422289	-3.766483



C	6.786789	-0.270381	-1.734566	H	4.840750	-1.946376	2.034000
H	7.863546	-0.088361	-1.721926	C	4.308491	2.258360	0.603549
C	6.154472	-0.788476	-0.605800	C	5.183148	3.455634	0.355281
H	6.735285	-1.007277	0.295080	H	5.680284	3.764870	1.282612
C	4.776252	-1.021138	-0.580944	H	4.589938	4.297887	-0.022912
C	4.075179	-1.567594	0.627640	H	5.951332	3.205064	-0.386513
H	3.261269	-0.874629	0.933766	C	3.209980	2.500294	1.627275
H	4.772373	-1.637996	1.473008	H	3.685568	2.822768	2.567767
C	3.467145	-2.902119	0.323391	H	2.539927	3.312815	1.309722
C	3.885428	-4.071669	0.957860	C	2.432514	1.220229	1.899041
H	4.703231	-4.018545	1.681868	C	1.582883	1.357147	3.131895
C	3.255797	-5.289531	0.705625	H	1.095530	0.408509	3.387331
H	3.591392	-6.192649	1.220898	H	0.815450	2.131160	2.996250
C	2.189333	-5.348475	-0.191707	H	2.213975	1.646520	3.984847
H	1.686392	-6.298437	-0.387754	C	0.461505	2.059776	-0.311856
C	1.762622	-4.193061	-0.835276	C	1.052589	3.209312	-0.873737
H	0.923714	-4.218525	-1.534674	H	2.135639	3.305046	-0.868386
C	2.402728	-2.967261	-0.597585	C	0.297614	4.194912	-1.501061
C	1.837609	-1.765942	-1.253747	C	2.199516	5.505204	-1.981292
O	0.663215	-1.717783	-1.655708	H	2.534157	5.587384	-0.933826
				H	2.412453	6.451265	-2.491005
				H	2.770299	4.702120	-2.476885
<b>18-ts(L1)</b>				C	-1.110272	4.046560	-1.591160
P	1.432997	0.635256	0.360287	C	-3.172837	4.926257	-2.316992
P	-1.666110	0.438892	0.358332	H	-3.495788	4.018689	-2.853305
O	5.140392	1.222896	1.091570	H	-3.518193	5.804000	-2.873744
O	3.742147	1.905133	-0.652863	H	-3.642010	4.936695	-1.319187
O	3.357545	0.159251	2.161195	C	-1.703578	2.922100	-1.029438
O	0.810235	5.302851	-2.067601	H	-2.779685	2.778890	-1.122616
O	-1.771545	5.025102	-2.233935	C	-0.940422	1.932564	-0.381850
O	-4.163384	0.949659	-0.802539	C	-4.836702	1.305263	0.399509
O	-5.376410	0.159054	1.036394	C	-5.989759	2.181559	-0.000867
O	-3.412605	-0.218837	2.250090	H	-6.648660	1.635278	-0.686628
C	3.028033	0.659515	-0.719568	H	-5.628824	3.085732	-0.507512
C	2.714995	0.463907	-2.179948	H	-6.569970	2.478273	0.881212
H	2.170822	-0.471488	-2.346061	C	-4.373930	-0.794206	1.366449
H	3.648226	0.422990	-2.760792	C	-5.028180	-1.907767	2.131881
H	2.106115	1.290700	-2.572301	H	-4.279157	-2.659490	2.410879
C	3.925835	-0.417347	-0.134660	H	-5.805764	-2.386797	1.524941
H	4.793361	-0.565594	-0.798178	H	-5.486110	-1.511875	3.046466
H	3.396145	-1.371889	-0.057724	C	-3.734449	-1.258480	0.059761
C	4.431755	0.000355	1.240877	H	-2.949959	-1.998745	0.270823
C	5.367537	-1.000693	1.855951	H	-4.507727	-1.747713	-0.554595
H	5.740082	-0.621904	2.815525	C	-3.157714	-0.068939	-0.699555
H	6.221924	-1.187210	1.193826				

C	-2.759143	-0.392986	-2.113721	P	-1.657211	0.386152	0.399296
H	-2.054234	-1.231477	-2.133207	O	5.117324	1.545855	0.956258
H	-2.293889	0.470180	-2.611760	O	3.629280	2.036073	-0.774292
H	-3.647201	-0.685015	-2.693061	O	3.450325	0.351287	2.076053
C	-2.787159	0.989325	1.802893	O	0.586745	5.248360	-2.232959
C	-3.869482	1.965638	1.369306	O	-1.991564	4.896506	-2.274503
H	-3.432951	2.877830	0.937461	O	-4.188786	0.839178	-0.662114
H	-4.434981	2.269552	2.265210	O	-5.330429	0.067126	1.231923
C	-2.000265	1.548478	2.957829	O	-3.317770	-0.288514	2.371017
H	-2.674440	1.753450	3.802369	C	3.034309	0.728139	-0.795570
H	-1.520397	2.494185	2.667502	C	2.737918	0.434489	-2.243913
H	-1.227632	0.857062	3.309328	H	2.472549	-0.620376	-2.378332
Ni	0.013207	-1.025625	0.862063	H	3.638473	0.632555	-2.842728
O	-0.534626	-3.003485	0.397540	H	1.922661	1.055210	-2.642345
C	-1.084601	-3.588745	-0.682049	C	4.046418	-0.237090	-0.199189
C	-2.104342	-4.532855	-0.474142	H	4.911534	-0.293681	-0.879462
H	-2.376956	-4.782285	0.554208	H	3.637947	-1.249681	-0.108672
C	-2.749438	-5.120452	-1.557173	C	4.528832	0.266276	1.153488
H	-3.540915	-5.853648	-1.380566	C	5.563566	-0.617219	1.788671
C	-2.386694	-4.782632	-2.863528	H	5.888974	-0.180814	2.740808
H	-2.892964	-5.243455	-3.714706	H	6.435095	-0.720895	1.131175
C	-1.367094	-3.856268	-3.071546	H	5.142272	-1.610633	1.983514
H	-1.073272	-3.583107	-4.090219	C	4.183901	2.483847	0.460932
C	-0.712478	-3.249464	-1.996599	C	4.931058	3.750551	0.150351
C	0.395954	-2.259250	-2.164936	H	5.410094	4.143651	1.055063
H	0.204237	-1.375100	-1.517451	H	4.246770	4.511727	-0.246121
H	0.446843	-1.906939	-3.205372	H	5.707026	3.550707	-0.598654
C	1.692768	-2.894130	-1.761719	C	3.092689	2.658440	1.508984
C	2.622405	-3.250132	-2.746160	H	3.562917	3.038740	2.430081
H	2.401458	-2.997774	-3.787717	H	2.349295	3.403450	1.190722
C	3.808416	-3.906055	-2.430944	C	2.436729	1.322216	1.819281
H	4.519694	-4.158399	-3.221234	C	1.593060	1.379488	3.061691
C	4.072652	-4.247804	-1.104766	H	1.147070	0.398725	3.277854
H	4.989133	-4.781704	-0.842020	H	0.794794	2.125536	2.957741
C	3.159487	-3.908975	-0.115443	H	2.219472	1.663441	3.919504
H	3.347408	-4.166188	0.928363	C	0.409240	2.042322	-0.387828
C	1.970542	-3.219319	-0.418281	C	0.941569	3.193176	-1.004768
C	1.146220	-2.858672	0.774061	H	2.019768	3.322274	-1.044973
O	1.396385	-3.279273	1.879707	C	0.131883	4.141522	-1.620488
C	-0.395238	-1.383062	2.624583	C	1.971883	5.494791	-2.214817
O	-0.744201	-1.696647	3.675302	H	2.349110	5.617350	-1.185730
				H	2.130929	6.432119	-2.758749
				H	2.544575	4.695581	-2.713884
<b>19(L1)</b>				C	-1.274070	3.954361	-1.641507
P	1.446748	0.673699	0.299583				

C	-3.393299	4.760702	-2.284261	C	-0.588442	-3.210206	-2.077549
H	-3.717801	3.831255	-2.780188	C	0.615389	-2.321351	-2.061584
H	-3.787956	5.613857	-2.846012	H	0.411445	-1.408322	-1.468861
H	-3.810906	4.788178	-1.264152	H	0.848752	-1.997060	-3.087165
C	-1.808919	2.829825	-1.025809	C	1.795487	-3.070853	-1.499782
H	-2.883267	2.656217	-1.067573	C	2.539417	-3.832918	-2.416487
C	-0.989976	1.876249	-0.392474	H	2.262763	-3.782868	-3.474127
C	-4.822041	1.205793	0.558902	C	3.590740	-4.650219	-2.024909
C	-5.992241	2.071624	0.186698	H	4.145671	-5.223288	-2.771878
H	-6.673139	1.511272	-0.465329	C	3.922553	-4.738650	-0.672072
H	-5.652858	2.967451	-0.348856	H	4.734949	-5.389145	-0.339136
H	-6.541160	2.381575	1.084071	C	3.212512	-3.986431	0.249003
C	-4.312943	-0.879175	1.529145	H	3.465602	-4.030717	1.309706
C	-4.930603	-1.987832	2.330711	C	2.153149	-3.135845	-0.134712
H	-4.169645	-2.737079	2.582589	C	1.599592	-2.306346	0.998211
H	-5.730398	-2.473689	1.759155	O	2.052031	-2.439483	2.110551
H	-5.352984	-1.586852	3.260131	C	-0.491153	-1.523789	2.546264
C	-3.709590	-1.354123	0.214015	O	-0.831653	-2.018090	3.520514
H	-2.903584	-2.072902	0.415691				
H	-4.493458	-1.863023	-0.368874	<b>2(L2)</b>			
C	-3.175788	-0.174172	-0.586841	P	-2.636572	0.373438	0.058587
C	-2.819541	-0.511437	-2.009104	P	0.044612	0.038759	1.508940
H	-2.045685	-1.287734	-2.044147	C	-2.658681	0.526940	1.907205
H	-2.457101	0.374653	-2.550067	H	-2.520112	1.593488	2.148670
H	-3.704603	-0.896362	-2.536528	H	-3.631763	0.225418	2.327519
C	-2.722779	0.918814	1.895082	C	-1.514212	-0.289741	2.476488
C	-3.826088	1.884817	1.487695	H	-1.724030	-1.367892	2.379295
H	-3.411711	2.796660	1.033920	H	-1.361387	-0.098345	3.550199
H	-4.362106	2.191620	2.400342	C	-4.031998	1.425015	-0.477716
C	-1.900522	1.487207	3.019439	C	-4.766756	1.089645	-1.626217
H	-2.548904	1.696945	3.882470	H	-4.540509	0.165213	-2.166261
H	-1.429844	2.430710	2.708743	C	-5.785563	1.920997	-2.084490
H	-1.117123	0.795982	3.350301	H	-6.350929	1.641325	-2.976922
Ni	0.091936	-1.083235	0.795554	C	-6.086079	3.104269	-1.409282
O	-0.820708	-2.909085	0.279645	H	-6.887441	3.754362	-1.768500
C	-1.225581	-3.459041	-0.827869	C	-5.353730	3.454264	-0.276118
C	-2.348647	-4.329144	-0.837757	H	-5.577643	4.380893	0.258437
H	-2.840831	-4.537596	0.117238	C	-4.333089	2.625121	0.183783
C	-2.813220	-4.900578	-2.015361	H	-3.766913	2.925521	1.069038
H	-3.681374	-5.566429	-1.982789	C	-3.248175	-1.334783	-0.214320
C	-2.185128	-4.635703	-3.237052	C	-2.393588	-2.223034	-0.880001
H	-2.556214	-5.079530	-4.163753	H	-1.421866	-1.851700	-1.228911
C	-1.071638	-3.795782	-3.248880	C	-2.769730	-3.549013	-1.089292
H	-0.561602	-3.580144	-4.195044	H	-2.090886	-4.230439	-1.609253

C	-4.009911	-3.996980	-0.637205	C	3.366558	-2.519665	-0.874698
H	-4.310112	-5.035155	-0.800301	H	4.265328	-2.668808	-0.268299
C	-4.872122	-3.117499	0.021860	C	2.778935	-3.604722	-1.524249
H	-5.846418	-3.468036	0.371883	H	3.218423	-4.601213	-1.432609
C	-4.495554	-1.792659	0.233310	C	1.630960	-3.404764	-2.290642
H	-5.181328	-1.107255	0.742065	H	1.165518	-4.243767	-2.815078
C	0.798848	1.474797	2.359412	C	1.081285	-2.131265	-2.400303
C	0.960616	1.560493	3.749772	H	0.186388	-1.958198	-3.002966
H	0.661349	0.724753	4.390593	C	1.662234	-1.030590	-1.746651
C	1.516901	2.702166	4.322726	C	0.954558	0.270033	-1.803674
H	1.641418	2.760842	5.406914	O	-0.194055	0.367612	-2.380015
C	1.915992	3.768836	3.514661				
H	2.353402	4.662077	3.967713				
C	1.756488	3.693995	2.131889	<b>3-ts(L2)</b>			
H	2.066893	4.525960	1.495341	P	-2.160978	-0.654284	0.385727
C	1.195497	2.553732	1.557865	P	0.839457	-1.393199	0.789612
H	1.060059	2.479457	0.472460	C	-1.650922	-1.277528	2.060012
C	1.068221	-1.402532	1.989255	H	-1.420905	-0.392727	2.674839
C	0.592035	-2.676154	1.637960	H	-2.481762	-1.800213	2.560354
H	-0.370660	-2.775647	1.123946	C	-0.433090	-2.175766	1.903323
C	1.333264	-3.818035	1.924634	H	-0.722016	-3.114272	1.400507
H	0.945640	-4.800038	1.642065	H	-0.000224	-2.465935	2.874407
C	2.574288	-3.706920	2.553218	C	-3.157502	0.832417	0.731134
H	3.160121	-4.602250	2.775105	C	-4.419289	1.059766	0.165620
C	3.065328	-2.447062	2.890522	H	-4.904525	0.275480	-0.421786
H	4.038513	-2.350621	3.379198	C	-5.060021	2.286246	0.340057
C	2.319706	-1.301656	2.610192	H	-6.044853	2.447591	-0.105740
H	2.720557	-0.319644	2.877523	C	-4.448892	3.303119	1.071906
Ni	-0.511154	0.374556	-0.517709	H	-4.952388	4.264056	1.202850
O	1.693031	1.486969	-1.886536	C	-3.185226	3.092785	1.625675
C	3.037772	1.619946	-2.058998	H	-2.687134	3.890960	2.181726
C	3.467230	2.561559	-2.998957	C	-2.541497	1.871793	1.449094
H	2.714331	3.088349	-3.588637	H	-1.534039	1.730673	1.858100
C	4.827116	2.812182	-3.164438	C	-3.330653	-1.943065	-0.178048
H	5.154543	3.548206	-3.903042	C	-3.010555	-2.670424	-1.331111
C	5.764180	2.123040	-2.395923	H	-2.100598	-2.418692	-1.887053
H	6.832259	2.312739	-2.524341	C	-3.838549	-3.705729	-1.765631
C	5.327931	1.188973	-1.456148	H	-3.579329	-4.268371	-2.665656
H	6.055658	0.647590	-0.843960	C	-4.993011	-4.021106	-1.051593
C	3.968944	0.932012	-1.264450	H	-5.642321	-4.831818	-1.391524
C	3.459665	-0.070231	-0.272798	C	-5.320923	-3.301433	0.099253
H	2.702003	0.422713	0.367384	H	-6.225807	-3.547660	0.660591
H	4.270426	-0.405660	0.388590	C	-4.493458	-2.270554	0.535755
C	2.822815	-1.237614	-0.966431	H	-4.756001	-1.710111	1.438943
				C	2.034913	-0.637480	1.954631

C	1.625735	-0.122605	3.194907	H	2.876284	0.006171	-3.553860
H	0.596037	-0.260771	3.537801	C	2.243955	1.087723	-1.808381
C	2.519440	0.569563	4.009618	C	0.893070	0.515667	-1.923568
H	2.183124	0.954017	4.976008	O	0.502792	-0.308746	-2.763177
C	3.837588	0.766596	3.597453				
H	4.538198	1.309411	4.236582	<b>4(L2)</b>			
C	4.255156	0.262414	2.365243	P	1.304051	1.403086	0.431918
H	5.285510	0.411848	2.031286	P	-1.756570	1.221048	0.409657
C	3.363208	-0.430011	1.548906	C	0.376887	2.536037	1.572306
H	3.706056	-0.818086	0.583626	H	0.312660	2.036714	2.552566
C	1.780689	-2.829743	0.151366	H	0.933589	3.470563	1.739579
C	1.755755	-3.074099	-1.226985	C	-1.008522	2.803152	1.006211
H	1.211459	-2.384981	-1.881987	H	-0.951194	3.455222	0.119037
C	2.434085	-4.171623	-1.758444	H	-1.667811	3.322290	1.719946
H	2.416041	-4.350218	-2.836386	C	2.327877	0.384012	1.545934
C	3.134956	-5.033505	-0.917364	C	3.699989	0.190464	1.341484
H	3.665710	-5.893458	-1.333827	H	4.213342	0.717275	0.532252
C	3.164422	-4.795341	0.458319	C	4.414057	-0.685716	2.157627
H	3.717170	-5.468620	1.118482	H	5.482756	-0.832515	1.983536
C	2.493662	-3.697653	0.991714	C	3.769281	-1.380585	3.179615
H	2.530260	-3.510555	2.069854	H	4.332138	-2.069607	3.813986
Ni	-0.263209	-0.207886	-0.602200	C	2.400251	-1.201152	3.383174
O	-0.317488	1.541835	-1.671328	H	1.883690	-1.748030	4.176250
C	-0.310205	2.819634	-1.205624	C	1.682938	-0.328846	2.570125
C	-1.303569	3.670853	-1.705745	H	0.603476	-0.215154	2.724004
H	-2.007932	3.269324	-2.437480	C	2.483826	2.459471	-0.469836
C	-1.384340	4.987756	-1.266593	C	2.614604	2.288639	-1.854356
H	-2.165096	5.641990	-1.663232	H	2.016142	1.520266	-2.355576
C	-0.472260	5.469707	-0.325849	C	3.521493	3.070807	-2.570732
H	-0.528575	6.504439	0.020032	H	3.621592	2.931202	-3.649806
C	0.510082	4.617124	0.174159	C	4.296284	4.024344	-1.913979
H	1.223831	4.981780	0.919472	H	5.004891	4.636495	-2.477472
C	0.605245	3.287176	-0.246279	C	4.172116	4.196275	-0.533710
C	1.628146	2.339336	0.296097	H	4.784218	4.939018	-0.016249
H	1.095935	1.425747	0.636260	C	3.271530	3.416673	0.186631
H	2.136052	2.772329	1.169400	H	3.192411	3.544725	1.270780
C	2.630908	1.925916	-0.740600	C	-2.167531	0.310377	1.942124
C	3.960254	2.351246	-0.671643	C	-2.170110	0.901948	3.212976
H	4.262690	3.001019	0.155164	H	-1.977555	1.971768	3.328704
C	4.901978	1.940336	-1.613274	C	-2.420975	0.133338	4.349629
H	5.938322	2.277607	-1.530824	H	-2.413823	0.606837	5.334400
C	4.519609	1.093476	-2.654741	C	-2.679893	-1.231203	4.231254
H	5.252163	0.765541	-3.396209	H	-2.872519	-1.831039	5.123867
C	3.199253	0.669493	-2.748296	C	-2.698227	-1.826443	2.969303

H	-2.908730	-2.893797	2.865783	P	-1.532791	0.585128	1.047837
C	-2.438859	-1.062247	1.835142	C	0.706984	1.679502	2.186601
H	-2.444807	-1.537231	0.848770	H	0.790433	0.803005	2.850546
C	-3.356802	1.733991	-0.292522	H	1.250569	2.508908	2.666684
C	-3.351490	2.361730	-1.547466	C	-0.755544	2.018354	1.935647
H	-2.408125	2.501639	-2.082827	H	-0.832433	2.916978	1.301406
C	-4.544894	2.790535	-2.121490	H	-1.293294	2.240934	2.870076
H	-4.530297	3.278820	-3.098700	C	3.165334	0.670093	0.913468
C	-5.755779	2.581845	-1.460426	C	4.063519	0.603007	-0.162002
H	-6.691963	2.912883	-1.916554	H	3.750274	0.930311	-1.158370
C	-5.769771	1.943347	-0.221661	C	5.351118	0.110501	0.026893
H	-6.715767	1.772854	0.298060	H	6.040242	0.059475	-0.819170
C	-4.576772	1.518866	0.361115	C	5.754606	-0.327025	1.288881
H	-4.600644	1.018815	1.333297	H	6.763998	-0.718744	1.435649
Ni	-0.251045	0.236073	-0.766894	C	4.864642	-0.269857	2.360336
O	1.033831	-0.550285	-1.980047	H	5.173758	-0.616889	3.349157
C	1.961413	-1.364123	-1.540324	C	3.573175	0.222306	2.175612
C	3.254549	-1.344999	-2.118211	H	2.882744	0.243569	3.022221
H	3.436494	-0.639299	-2.933719	C	1.686014	2.835572	-0.258925
C	4.259343	-2.196997	-1.674780	C	0.909003	3.151967	-1.379037
H	5.245878	-2.155475	-2.146935	H	0.203616	2.406345	-1.763135
C	4.019830	-3.098782	-0.635266	C	1.038324	4.393872	-2.001088
H	4.809196	-3.765039	-0.279122	H	0.431483	4.628642	-2.878767
C	2.749914	-3.135839	-0.057933	C	1.949120	5.327198	-1.509406
H	2.546323	-3.839331	0.757735	H	2.056976	6.297448	-2.000280
C	1.720695	-2.294963	-0.485156	C	2.730560	5.018984	-0.394088
C	0.355710	-2.365686	0.142402	H	3.448695	5.747453	-0.010037
H	0.019940	-1.354102	0.462366	C	2.601554	3.780699	0.228338
H	0.424298	-2.950383	1.073483	H	3.224684	3.541749	1.096116
C	-0.695535	-2.995049	-0.739964	C	-2.141608	-0.452090	2.430327
C	-0.841913	-4.388531	-0.682849	C	-3.248452	-0.072109	3.206783
H	-0.201462	-4.954011	0.001240	H	-3.800825	0.842529	2.967601
C	-1.769701	-5.062522	-1.469194	C	-3.652730	-0.860101	4.281021
H	-1.859614	-6.149206	-1.394156	H	-4.517690	-0.561681	4.878768
C	-2.582750	-4.347047	-2.350121	C	-2.954486	-2.028762	4.594384
H	-3.313808	-4.865998	-2.975107	H	-3.274114	-2.645355	5.438400
C	-2.450749	-2.968061	-2.425635	C	-1.853053	-2.405884	3.830073
H	-3.069219	-2.379288	-3.107622	H	-1.303411	-3.319072	4.072015
C	-1.518784	-2.274863	-1.633769	C	-1.444684	-1.625680	2.746454
C	-1.490664	-0.780433	-1.790343	H	-0.576414	-1.916215	2.140716
O	-2.133312	-0.237278	-2.665001	C	-3.048629	1.208306	0.253530
				C	-3.145778	2.508292	-0.262484
<b>5-ts(L2)</b>				H	-2.337962	3.229080	-0.108195
P	1.470150	1.219689	0.571616	C	-4.270567	2.898212	-0.989109

H	-4.333601	3.916905	-1.379524	C	2.855906	-1.643631	0.224576
C	-5.309220	1.996272	-1.214833	C	4.091088	-0.982767	0.157624
H	-6.188763	2.303306	-1.785675	H	4.208384	0.005182	0.612726
C	-5.217048	0.697841	-0.713510	C	5.166088	-1.563216	-0.511017
H	-6.021538	-0.019467	-0.892719	H	6.120599	-1.033668	-0.557854
C	-4.095377	0.304874	0.010887	C	5.020639	-2.802432	-1.134020
H	-4.028103	-0.722382	0.383590	H	5.863595	-3.253803	-1.662633
Ni	0.074795	-0.211896	-0.338309	C	3.790353	-3.457402	-1.091367
O	0.930160	-1.771008	0.788604	H	3.663384	-4.421523	-1.589577
C	1.528829	-2.595689	-0.031037	C	2.713621	-2.880397	-0.422181
C	2.937292	-2.759222	-0.036416	H	1.747337	-3.394162	-0.430991
H	3.519591	-2.200774	0.702225	C	2.018477	0.174852	2.343963
C	3.571843	-3.574481	-0.967188	C	1.336871	1.355067	2.665893
H	4.664310	-3.652304	-0.953588	H	0.509927	1.690829	2.026676
C	2.834592	-4.287135	-1.916268	C	1.711769	2.092241	3.790497
H	3.333525	-4.925887	-2.649029	H	1.174256	3.012348	4.033662
C	1.442309	-4.179114	-1.899405	C	2.765307	1.663283	4.593505
H	0.845700	-4.750622	-2.620413	H	3.060324	2.245925	5.469847
C	0.781999	-3.365399	-0.979050	C	3.444596	0.484342	4.278886
C	-0.719725	-3.299469	-0.922457	H	4.269637	0.142159	4.908671
H	-1.001360	-3.057546	0.118788	C	3.071609	-0.261996	3.163735
H	-1.144883	-4.291942	-1.136257	H	3.604006	-1.189913	2.932276
C	-1.412255	-2.298472	-1.809457	C	-2.074281	-2.631758	-0.403654
C	-2.537523	-2.696202	-2.545876	C	-2.015603	-3.908588	0.171798
H	-2.846322	-3.745293	-2.499782	H	-1.738215	-4.035263	1.221115
C	-3.267747	-1.797702	-3.321082	C	-2.316470	-5.041696	-0.584070
H	-4.132333	-2.148862	-3.890336	H	-2.260974	-6.029142	-0.119776
C	-2.891706	-0.455989	-3.373606	C	-2.689525	-4.916633	-1.920533
H	-3.457221	0.260212	-3.974875	H	-2.924316	-5.805479	-2.510577
C	-1.780236	-0.037300	-2.650757	C	-2.763622	-3.650519	-2.500943
H	-1.463385	1.009454	-2.708180	H	-3.061224	-3.539934	-3.546135
C	-1.037735	-0.936474	-1.867597	C	-2.450625	-2.520292	-1.751554
C	0.718199	-0.415078	-1.932944	H	-2.521001	-1.535284	-2.220107
O	1.378456	-0.460513	-2.897911	C	-3.267589	-0.394208	1.016554
				C	-3.271493	0.635616	1.972059
<b>6(L2)</b>				H	-2.329599	1.008753	2.377466
P	1.397433	-0.826062	0.942795	C	-4.473062	1.209103	2.377244
P	-1.666282	-1.105161	0.518741	H	-4.462853	2.009802	3.120487
C	0.488894	-2.170442	1.844316	C	-5.680521	0.778867	1.826985
H	0.494054	-3.078426	1.221630	H	-6.620903	1.237301	2.142366
H	1.015086	-2.422383	2.777990	C	-5.682666	-0.235698	0.871844
C	-0.928122	-1.695996	2.098816	H	-6.623944	-0.580950	0.437755
H	-0.933555	-0.832169	2.783811	C	-4.483935	-0.822070	0.468217
H	-1.560390	-2.461522	2.574509	H	-4.507091	-1.624270	-0.273463

Ni	-0.057598	0.181369	-0.466683	C	-4.495923	2.686344	-1.872243
O	-0.885131	1.798839	0.562194	H	-4.503208	3.602328	-2.467444
C	-1.224724	2.742106	-0.283233	C	-3.386366	2.384177	-1.086191
C	-2.569147	2.956803	-0.676676	H	-2.531998	3.067040	-1.084265
H	-3.341302	2.307771	-0.253249	C	-2.447077	-0.288342	1.965850
C	-2.906059	3.953984	-1.587382	C	-1.976506	-1.595703	2.121540
H	-3.954665	4.090586	-1.870890	H	-1.273451	-2.002874	1.393656
C	-1.922225	4.774686	-2.142310	C	-2.409834	-2.380455	3.190579
H	-2.186375	5.558572	-2.856322	H	-2.035491	-3.401141	3.297851
C	-0.591001	4.578140	-1.765779	C	-3.318711	-1.864559	4.111295
H	0.193091	5.214393	-2.193055	H	-3.656763	-2.478046	4.949944
C	-0.228801	3.591558	-0.849906	C	-3.803809	-0.564193	3.957270
C	1.200920	3.358798	-0.451187	H	-4.524732	-0.159853	4.671798
H	1.225919	3.049672	0.605402	C	-3.373778	0.219819	2.890728
H	1.763301	4.302046	-0.515864	H	-3.772230	1.231998	2.770967
C	1.916934	2.324943	-1.290290	C	2.198227	2.674027	0.214416
C	3.050153	2.730825	-2.016557	C	2.714170	3.671011	1.054378
H	3.386083	3.768093	-1.910756	H	2.492512	3.662859	2.125678
C	3.739249	1.868532	-2.865619	C	3.529775	4.673502	0.534403
H	4.611461	2.226230	-3.419153	H	3.925194	5.448143	1.195967
C	3.290773	0.559744	-3.017094	C	3.847491	4.682756	-0.824245
H	3.800165	-0.133579	-3.692481	H	4.491191	5.467821	-1.228586
C	2.178226	0.133985	-2.292097	C	3.351197	3.684927	-1.661603
H	1.835424	-0.899152	-2.416899	H	3.607767	3.681234	-2.723527
C	1.497830	0.985372	-1.411797	C	2.526835	2.684420	-1.148478
C	-0.745814	0.283479	-2.105345	H	2.159650	1.879524	-1.792860
O	-1.147153	0.495092	-3.163935	C	2.314095	0.214270	1.711620
				C	1.878988	-0.643230	2.733866
<b>10(L2)</b>				H	0.851247	-0.586990	3.107003
P	-1.848945	0.757290	0.590848	C	2.745382	-1.591797	3.272002
P	1.152241	1.319901	0.851808	H	2.395912	-2.249402	4.071806
C	-1.316449	2.306502	1.454925	C	4.047128	-1.711655	2.784601
H	-1.232418	3.091945	0.686045	H	4.720414	-2.465313	3.199550
H	-2.080882	2.645087	2.171942	C	4.480680	-0.875956	1.756944
C	0.031876	2.067138	2.116795	H	5.490693	-0.977451	1.352960
H	-0.068656	1.359527	2.955033	C	3.621548	0.080449	1.222583
H	0.444140	2.993473	2.543569	H	3.966662	0.720451	0.405851
C	-3.361579	1.214615	-0.311434	Ni	-0.133973	0.174286	-0.655909
C	-4.461527	0.346511	-0.353399	O	1.530686	-0.346780	-1.525792
H	-4.450327	-0.580839	0.226134	C	2.278871	-1.420916	-1.517097
C	-5.568213	0.651407	-1.143239	C	3.516214	-1.390820	-2.208392
H	-6.417486	-0.035286	-1.169249	H	3.778414	-0.470445	-2.738795
C	-5.588177	1.819902	-1.903759	C	4.374894	-2.483661	-2.212903
H	-6.455415	2.055196	-2.525075	H	5.323303	-2.417570	-2.755501



C	4.037773	-3.656541	-1.533667	C	3.624588	3.788530	-1.236315
H	4.709265	-4.518290	-1.534008	H	3.783825	4.053938	-2.284140
C	2.815940	-3.707717	-0.860264	C	4.319653	4.456327	-0.230169
H	2.531075	-4.618994	-0.321910	H	5.025042	5.250672	-0.486202
C	1.936879	-2.624207	-0.834609	C	4.116706	4.108052	1.106724
C	0.626058	-2.697720	-0.106893	H	4.665146	4.626731	1.896927
H	0.582861	-1.859636	0.614049	C	3.220438	3.094898	1.435771
H	0.586205	-3.628259	0.482100	H	3.086883	2.813438	2.485306
C	-0.572365	-2.601773	-1.020602	C	-2.420151	-0.454013	2.026872
C	-1.129932	-3.762403	-1.573490	C	-3.499904	-0.042866	2.826207
H	-0.700949	-4.735275	-1.307793	H	-3.978173	0.924804	2.643077
C	-2.207759	-3.695900	-2.454841	C	-3.974174	-0.859487	3.848920
H	-2.633129	-4.612747	-2.871649	H	-4.813292	-0.525901	4.464510
C	-2.729946	-2.453092	-2.806670	C	-3.384100	-2.102952	4.086394
H	-3.567851	-2.382631	-3.506644	H	-3.760596	-2.743903	4.887347
C	-2.175869	-1.288649	-2.267503	C	-2.320221	-2.524991	3.293901
H	-2.594600	-0.322809	-2.573452	H	-1.857593	-3.500142	3.465283
C	-1.106639	-1.344606	-1.368310	C	-1.845226	-1.705104	2.269665
C	-0.446789	1.473318	-2.122695	H	-1.016121	-2.044153	1.647286
O	-0.447654	1.623297	-3.262101	C	-3.302224	1.245965	-0.058011
				C	-3.598593	2.602287	-0.247995
<b>11-ts(L2)</b>				H	-2.934114	3.376248	0.144676
P	1.342416	1.057787	0.797067	C	-4.746867	2.981821	-0.942925
P	-1.758366	0.649309	0.704063	H	-4.967724	4.043397	-1.079146
C	0.297721	1.678835	2.204429	C	-5.608221	2.015954	-1.460823
H	0.224357	0.879763	2.959822	H	-6.503743	2.316923	-2.009688
H	0.789400	2.526954	2.704799	C	-5.318002	0.662991	-1.280465
C	-1.087406	2.058747	1.698053	H	-5.983227	-0.102001	-1.688926
H	-1.017260	2.933381	1.030770	C	-4.174160	0.280056	-0.586376
H	-1.763774	2.333521	2.523787	H	-3.950131	-0.784101	-0.456980
C	2.440178	-0.196567	1.548150	Ni	-0.149482	0.445674	-0.837893
C	3.772532	-0.318738	1.122181	O	0.839940	-0.584024	-2.269593
H	4.185133	0.400669	0.408944	C	1.824380	-1.464056	-2.034799
C	4.576108	-1.353821	1.592316	C	3.026007	-1.294059	-2.746778
H	5.609694	-1.432454	1.246315	H	3.098404	-0.461819	-3.450821
C	4.064992	-2.289591	2.491893	C	4.090404	-2.167255	-2.549792
H	4.697250	-3.101580	2.859306	H	5.019944	-2.013272	-3.104899
C	2.739961	-2.186393	2.913167	C	3.973832	-3.233726	-1.656140
H	2.328357	-2.915623	3.615872	H	4.807706	-3.922304	-1.500772
C	1.931887	-1.153402	2.441789	C	2.776172	-3.414937	-0.967888
H	0.891083	-1.098848	2.775470	H	2.669352	-4.249207	-0.266917
C	2.507108	2.424726	0.430615	C	1.696756	-2.544565	-1.135026
C	2.719642	2.779360	-0.906818	C	0.408863	-2.703030	-0.386724
H	2.172637	2.251012	-1.695137	H	0.412460	-1.979528	0.453288

H	0.339962	-3.705506	0.061199	H	-3.270147	1.547368	-1.978222
C	-0.763973	-2.421335	-1.276286	C	2.034708	-1.804118	-0.353291
C	-1.748854	-3.362612	-1.571629	C	2.908466	-2.209262	-1.371666
H	-1.704780	-4.338281	-1.075965	H	3.359096	-1.464267	-2.035552
C	-2.761718	-3.089983	-2.496666	C	3.212531	-3.558771	-1.538095
H	-3.522469	-3.841927	-2.716905	H	3.897932	-3.867980	-2.331316
C	-2.762724	-1.862492	-3.164497	C	2.641648	-4.515904	-0.696310
H	-3.533510	-1.641383	-3.908798	H	2.881295	-5.573652	-0.831370
C	-1.793333	-0.899951	-2.890961	C	1.769839	-4.121680	0.317315
H	-1.797158	0.058392	-3.416786	H	1.323937	-4.867061	0.980281
C	-0.852836	-1.150068	-1.880206	C	1.472276	-2.770848	0.490459
C	-0.537281	1.971956	-1.752764	H	0.792874	-2.437823	1.286666
O	-0.845692	3.008987	-2.161634	C	3.042690	0.911289	-0.264686
				C	3.012840	2.216379	-0.780263
<b>12(L2)</b>				H	2.079407	2.637863	-1.164345
P	-1.556152	-0.045237	-0.076822	C	4.165763	2.999060	-0.804769
P	1.506507	-0.064570	-0.108946	H	4.122034	4.011069	-1.214979
C	-0.720898	-0.434293	-1.698726	C	5.367816	2.496320	-0.308394
H	-0.588794	-1.528097	-1.753863	H	6.271214	3.110405	-0.328053
H	-1.351483	-0.143654	-2.554883	C	5.406622	1.205765	0.219303
C	0.630339	0.257122	-1.727688	H	6.342325	0.803594	0.615776
H	0.493552	1.346450	-1.828736	C	4.255901	0.421236	0.244832
H	1.243285	-0.067295	-2.584127	H	4.300863	-0.587381	0.666514
C	-3.193941	-0.838667	-0.239865	Ni	-0.003178	-0.080965	1.468815
C	-4.281777	-0.308435	0.472624	C	0.105069	-0.187656	3.200766
H	-4.146679	0.598746	1.069750	O	0.205396	-0.272345	4.358830
C	-5.530079	-0.921051	0.424171				
H	-6.366737	-0.487745	0.977991	<b>2(L3)</b>			
C	-5.713451	-2.083963	-0.325774	P	-1.001962	1.595893	-0.845390
H	-6.693450	-2.565678	-0.362484	P	-2.563787	-0.922907	0.234430
C	-4.637712	-2.628281	-1.024398	C	-2.810072	1.431433	-1.290271
H	-4.770951	-3.539982	-1.612182	H	-3.295033	2.419671	-1.373368
C	-3.387391	-2.011441	-0.984107	H	-2.827653	1.010158	-2.308323
H	-2.558803	-2.455345	-1.542432	C	-0.936607	3.192348	0.196166
C	-1.919674	1.740001	-0.294936	C	-2.957160	-2.352110	-0.954652
C	-1.276736	2.637361	0.568610	C	-3.227151	-1.322478	1.963006
H	-0.630706	2.232859	1.361450	C	-0.183214	1.916537	-2.535501
C	-1.459427	4.012036	0.424858	C	-3.589176	0.516337	-0.342257
H	-0.954233	4.703258	1.103840	H	-4.539637	0.191871	-0.799684
C	-2.294827	4.499437	-0.579698	H	-3.872227	1.066899	0.568869
H	-2.445511	5.576168	-0.690379	C	1.238283	2.409093	-2.290483
C	-2.943997	3.612552	-1.440604	H	1.799429	2.428385	-3.238852
H	-3.603012	3.994921	-2.224189	H	1.773049	1.731638	-1.607242
C	-2.756067	2.238500	-1.302353	H	1.272921	3.426772	-1.876857

C	-0.100269	0.559105	-3.234275	Ni	-0.470256	-0.251991	0.125870
H	0.513980	0.648886	-4.145032	O	2.055114	-0.851675	-0.887122
H	-1.087605	0.201831	-3.560859	C	3.255558	-1.508694	-0.865301
H	0.362490	-0.209106	-2.595212	C	3.347322	-2.857237	-1.204842
C	0.413474	3.259203	0.906620	H	2.433539	-3.404973	-1.445934
H	0.438348	4.126495	1.586829	C	4.599726	-3.471824	-1.227810
H	1.262584	3.363933	0.219182	H	4.679756	-4.529304	-1.492662
H	0.591840	2.359725	1.512679	C	5.744877	-2.741802	-0.910968
C	-2.710705	-0.215528	2.883382	H	6.724881	-3.224866	-0.929290
H	-2.908804	-0.479268	3.934763	C	5.640531	-1.391965	-0.567838
H	-3.211297	0.746782	2.701433	H	6.538274	-0.818410	-0.318186
H	-1.624902	-0.064070	2.773828	C	4.397085	-0.760235	-0.542666
C	-2.014298	3.032659	1.265392	C	4.181165	0.677756	-0.173661
H	-1.920590	3.832286	2.017855	H	3.637078	1.170894	-0.998477
H	-1.907133	2.074022	1.792550	H	5.145345	1.197780	-0.085801
H	-3.034633	3.095930	0.857972	C	3.415203	0.831501	1.119261
C	-1.192438	4.480649	-0.574349	C	3.966139	1.630301	2.129537
H	-1.294132	5.318115	0.136105	H	4.904096	2.155498	1.922335
H	-2.122831	4.451018	-1.161743	C	3.374020	1.756278	3.383256
H	-0.367768	4.744406	-1.250561	H	3.832003	2.390881	4.145907
C	-4.747299	-1.369570	2.080807	C	2.211229	1.036095	3.657928
H	-5.032570	-1.463438	3.141983	H	1.746050	1.090141	4.645757
H	-5.201475	-2.218513	1.556853	C	1.644686	0.244605	2.668328
H	-5.225077	-0.450110	1.709837	H	0.736035	-0.327503	2.874199
C	-0.936320	2.881040	-3.447325	C	2.200270	0.148625	1.377812
H	-0.451343	2.899065	-4.437528	C	1.419902	-0.631500	0.380857
H	-0.944017	3.915257	-3.084428	O	0.651821	-1.599441	0.792769
H	-1.979539	2.576829	-3.618653				
C	-2.599944	-2.640855	2.411703	<b>3-ts(L3)</b>			
H	-2.807242	-2.811304	3.480403	P	-0.426483	-1.911925	0.581417
H	-1.506313	-2.629887	2.283428	P	-2.439987	0.463709	-0.114773
H	-2.999499	-3.508823	1.868879	C	-2.210212	-2.056063	1.136889
C	-4.304591	-3.030182	-0.746761	H	-2.542528	-3.107381	1.091947
H	-4.484565	-3.751035	-1.561871	H	-2.205790	-1.798412	2.207020
H	-5.143227	-2.317512	-0.762756	C	-0.243752	-3.334996	-0.687519
H	-4.358216	-3.600445	0.190630	C	-2.818991	1.686831	1.287715
C	-2.918610	-1.756305	-2.359259	C	-3.410495	0.935812	-1.675288
H	-2.963034	-2.561884	-3.109590	C	0.463714	-2.440929	2.201766
H	-1.981439	-1.208382	-2.527310	C	-3.193819	-1.150080	0.396322
H	-3.762306	-1.079860	-2.563482	H	-4.115193	-1.007329	0.987381
C	-1.818715	-3.368191	-0.851151	H	-3.515939	-1.632623	-0.540016
H	-1.961631	-4.166431	-1.597682	C	1.932454	-2.711917	1.889153
H	-1.754930	-3.852142	0.132605	H	2.506905	-2.813625	2.824741
H	-0.840501	-2.898558	-1.036745	H	2.400365	-1.905711	1.304798

H	2.071318	-3.648669	1.331203	H	-0.789094	2.474021	1.186430
C	0.361116	-1.269734	3.181294	Ni	-0.281039	0.027852	-0.382374
H	1.014811	-1.456794	4.048691	O	0.817946	1.740699	-0.901166
H	-0.656907	-1.154101	3.581375	C	1.508236	2.634851	-0.153576
H	0.661038	-0.305532	2.748829	C	1.280718	3.993899	-0.416464
C	1.091866	-3.187607	-1.413407	H	0.590278	4.256987	-1.221257
H	1.213170	-4.012980	-2.134566	C	1.919980	4.974523	0.334816
H	1.964030	-3.212853	-0.746126	H	1.731377	6.029251	0.118156
H	1.124555	-2.250138	-1.982849	C	2.800936	4.613082	1.355396
C	-2.920636	0.003064	-2.784262	H	3.305959	5.378790	1.948652
H	-3.350287	0.322166	-3.747655	C	3.033994	3.263078	1.609454
H	-3.239709	-1.038541	-2.629463	H	3.723357	2.967274	2.406577
H	-1.824569	0.019257	-2.883719	C	2.395978	2.260663	0.873069
C	-1.348873	-3.103940	-1.717069	C	2.642842	0.804855	1.113220
H	-1.198566	-3.768525	-2.583362	H	1.656809	0.296252	1.175418
H	-1.325552	-2.069141	-2.089029	H	3.173299	0.649873	2.063720
H	-2.354235	-3.317702	-1.321781	C	3.388675	0.179012	-0.025784
C	-0.378129	-4.744602	-0.128167	C	4.721927	-0.219750	0.091388
H	-0.456707	-5.461126	-0.963090	H	5.237742	-0.072692	1.045374
H	-1.278383	-4.881111	0.490299	C	5.392676	-0.811414	-0.978564
H	0.495967	-5.052673	0.461804	H	6.433396	-1.124586	-0.862780
C	-4.924660	0.791675	-1.553129	C	4.732791	-1.002485	-2.193375
H	-5.391187	0.944572	-2.540579	H	5.254516	-1.460973	-3.037081
H	-5.381211	1.520344	-0.872991	C	3.406751	-0.607117	-2.327563
H	-5.224413	-0.213499	-1.219510	H	2.866099	-0.753365	-3.265865
C	-0.137873	-3.654734	2.911970	C	2.723324	-0.016614	-1.253619
H	0.347695	-3.772707	3.895436	C	1.288902	0.265284	-1.424971
H	0.010360	-4.599962	2.379858	O	0.618178	0.037966	-2.447105
H	-1.213621	-3.545007	3.112351				
C	-3.023118	2.362669	-2.057924	<b>4(L3)</b>			
H	-3.424538	2.606702	-3.054638	P	0.378659	2.149141	0.147675
H	-1.928789	2.479009	-2.107238	P	2.264730	-0.460938	0.253890
H	-3.418884	3.115536	-1.361579	C	2.030826	2.221653	1.007975
C	-4.247697	2.207525	1.351125	H	2.448356	3.240778	0.948727
H	-4.379939	2.808605	2.266457	H	1.803493	2.062776	2.072720
H	-4.992906	1.398399	1.392468	C	0.565158	3.416268	-1.271650
H	-4.501669	2.863120	0.506967	C	2.499905	-1.424043	1.867573
C	-2.497911	0.950422	2.585368	C	3.322555	-1.234518	-1.118798
H	-2.505014	1.656750	3.430872	C	-0.754537	2.914762	1.487452
H	-1.495495	0.501069	2.539219	C	3.049233	1.186211	0.547422
H	-3.226288	0.158751	2.818728	H	3.890301	1.123556	1.258823
C	-1.826404	2.841788	1.153267	H	3.495732	1.490063	-0.411305
H	-1.952228	3.554413	1.984936	C	-2.057012	3.411489	0.866748
H	-1.942125	3.408395	0.219238	H	-2.778998	3.639192	1.667510

H	-2.530277	2.659183	0.219240	H	1.906948	-3.392422	1.052811
H	-1.927014	4.336620	0.288403	H	0.563884	-2.413435	1.648689
C	-1.090125	1.799559	2.473000	Ni	0.104433	0.022855	-0.417045
H	-1.762203	2.186135	3.255779	O	-0.047305	-1.813290	-1.024376
H	-0.199567	1.408977	2.986626	C	-0.821368	-2.804080	-0.674297
H	-1.603942	0.963158	1.983775	C	-0.703806	-4.041560	-1.361187
C	-0.660367	3.413160	-2.186069	H	0.004955	-4.090603	-2.192651
H	-0.529616	4.194097	-2.952691	C	-1.466315	-5.148308	-1.014716
H	-1.601016	3.635225	-1.667217	H	-1.346204	-6.079293	-1.577461
H	-0.781095	2.458185	-2.709644	C	-2.381512	-5.080588	0.040006
C	2.831355	-0.607723	-2.424320	H	-2.982292	-5.948970	0.319445
H	3.347838	-1.076164	-3.277595	C	-2.515706	-3.874830	0.724828
H	3.056621	0.467170	-2.473073	H	-3.232241	-3.799992	1.551232
H	1.749400	-0.749353	-2.570810	C	-1.763168	-2.742974	0.397470
C	1.752975	2.941143	-2.105305	C	-1.962975	-1.457938	1.153986
H	1.820440	3.541346	-3.026554	H	-1.007793	-0.887465	1.157249
H	1.628195	1.892344	-2.410262	H	-2.199400	-1.675391	2.207696
H	2.715962	3.050490	-1.584507	C	-3.053726	-0.596617	0.572338
C	0.830733	4.841453	-0.798091	C	-4.312962	-0.549375	1.182469
H	1.109725	5.458183	-1.668061	H	-4.467739	-1.095004	2.118633
H	1.659641	4.921545	-0.079733	C	-5.367582	0.167340	0.620452
H	-0.056931	5.314153	-0.356309	H	-6.335809	0.195417	1.126957
C	4.816835	-0.951774	-0.974354	C	-5.189850	0.836120	-0.591321
H	5.350393	-1.394434	-1.831583	H	-6.017768	1.385245	-1.046764
H	5.260873	-1.386092	-0.069635	C	-3.948552	0.795452	-1.214489
H	5.054585	0.121949	-0.984015	H	-3.778040	1.312619	-2.163171
C	-0.101786	4.050534	2.275870	C	-2.870326	0.108288	-0.635430
H	-0.827695	4.427193	3.014789	C	-1.547997	0.233341	-1.321602
H	0.194802	4.908894	1.663412	O	-1.486230	0.395704	-2.525691
H	0.776981	3.725601	2.849387				
C	3.086377	-2.741027	-1.192605	<b>5-ts(L3)</b>			
H	3.555689	-3.133119	-2.109491	P	-0.480703	1.841912	-0.798708
H	2.015715	-2.981067	-1.240053	P	-2.174356	-0.794496	0.169784
H	3.538398	-3.287078	-0.353016	C	-2.249607	1.608666	-1.311115
C	3.944799	-1.800750	2.170953	H	-2.745344	2.583010	-1.449147
H	4.006967	-2.236390	3.181944	H	-2.182289	1.169965	-2.317275
H	4.623361	-0.933905	2.159201	C	-0.497076	3.375535	0.340921
H	4.342617	-2.555777	1.480227	C	-2.533706	-2.161388	-1.092325
C	1.979446	-0.527151	2.988835	C	-3.077798	-1.174477	1.805254
H	1.955807	-1.091911	3.934487	C	0.278014	2.332456	-2.481792
H	0.950360	-0.191103	2.789571	C	-3.080986	0.704431	-0.419626
H	2.614137	0.354816	3.161400	H	-4.016991	0.411114	-0.924677
C	1.617026	-2.671005	1.826252	H	-3.390091	1.245334	0.486583
H	1.671472	-3.193292	2.794818	C	1.619815	3.032344	-2.276766

H	2.160588	3.073744	-3.235386	H	-1.693582	-4.084550	-1.599299
H	2.277402	2.521961	-1.559222	H	-1.878204	-3.869924	0.143807
H	1.496064	4.070784	-1.940211	H	-0.573181	-3.017641	-0.732546
C	0.481881	1.046906	-3.282808	Ni	0.037218	-0.204134	0.286623
H	0.986386	1.287024	-4.232344	O	0.893744	-1.378261	-1.311705
H	-0.475577	0.574398	-3.549807	C	1.992065	-2.059151	-1.141924
H	1.071096	0.288310	-2.750664	C	2.066306	-3.450894	-1.420176
C	0.918820	3.721475	0.811197	H	1.175019	-3.943597	-1.820190
H	0.859179	4.348687	1.714861	C	3.228127	-4.181572	-1.193991
H	1.479817	4.297519	0.066433	H	3.236468	-5.255206	-1.409092
H	1.517673	2.841830	1.070235	C	4.377307	-3.563892	-0.695239
C	-2.532301	-0.218328	2.863245	H	5.288528	-4.138244	-0.511433
H	-3.014435	-0.426076	3.831678	C	4.342871	-2.188164	-0.455735
H	-2.737581	0.835545	2.626634	H	5.244572	-1.679100	-0.093727
H	-1.447306	-0.333151	3.004507	C	3.192714	-1.433239	-0.681007
C	-1.330519	2.951820	1.550374	C	3.177110	0.059173	-0.498864
H	-1.253648	3.708659	2.347105	H	2.408440	0.460343	-1.179570
H	-0.984758	1.994340	1.966330	H	4.144949	0.483233	-0.809250
H	-2.399434	2.858974	1.305094	C	2.860730	0.545883	0.887141
C	-1.121764	4.625857	-0.269457	C	3.848543	1.213122	1.626035
H	-1.246171	5.384006	0.521200	H	4.835313	1.352086	1.171830
H	-2.119461	4.460093	-0.702139	C	3.605291	1.699243	2.909067
H	-0.484155	5.084164	-1.037032	H	4.399056	2.210172	3.460026
C	-4.589338	-0.960592	1.705954	C	2.351247	1.514776	3.486336
H	-5.047970	-1.200430	2.678658	H	2.146202	1.871060	4.499321
H	-5.076289	-1.600955	0.961194	C	1.356311	0.856207	2.763647
H	-4.861517	0.080766	1.485336	H	0.381587	0.699988	3.237257
C	-0.631351	3.248548	-3.304676	C	1.577861	0.399232	1.457318
H	-0.110999	3.504767	-4.241923	C	0.497970	-1.406487	1.438457
H	-0.879314	4.196403	-2.812971	O	0.809584	-2.312904	2.089380
H	-1.571872	2.763376	-3.599505				
C	-2.796178	-2.604587	2.258036	<b>6(L3)</b>			
H	-3.181294	-2.743365	3.280663	P	0.418959	-1.850482	-0.770973
H	-1.723251	-2.839040	2.287657	P	2.221448	0.733739	0.131101
H	-3.293543	-3.355312	1.629994	C	2.180816	-1.676165	-1.329569
C	-3.989010	-2.606287	-1.156942	H	2.639542	-2.666795	-1.477376
H	-4.114509	-3.299370	-2.004983	H	2.103266	-1.237244	-2.334860
H	-4.687395	-1.772665	-1.327923	C	0.414212	-3.397793	0.353745
H	-4.313363	-3.150683	-0.259661	C	2.601842	2.081461	-1.143215
C	-2.122950	-1.585145	-2.447468	C	3.167356	1.088343	1.751840
H	-2.160318	-2.382946	-3.206330	C	-0.396329	-2.297059	-2.441957
H	-1.087314	-1.215764	-2.420626	C	3.062375	-0.799767	-0.460740
H	-2.804291	-0.792132	-2.792820	H	3.999468	-0.544341	-0.983678
C	-1.619691	-3.346079	-0.784679	H	3.365460	-1.345261	0.444612

C	-1.758644	-2.949144	-2.209260	C	1.735625	3.297420	-0.819853
H	-2.338321	-2.931829	-3.145409	H	1.836566	4.041960	-1.626000
H	-2.366797	-2.449100	-1.443892	H	2.016511	3.799084	0.114369
H	-1.659071	-4.004471	-1.919661	H	0.678363	3.003220	-0.771977
C	-0.551957	-0.999718	-3.236825	Ni	-0.009677	0.206415	0.339540
H	-1.119308	-1.204338	-4.158590	O	-0.863394	1.466171	-1.224853
H	0.423063	-0.601188	-3.555830	C	-1.965885	2.141878	-1.062484
H	-1.057392	-0.196727	-2.683796	C	-2.024701	3.548270	-1.262196
C	-1.001249	-3.731054	0.834974	H	-1.111180	4.061919	-1.577103
H	-0.937906	-4.370231	1.729903	C	-3.198765	4.268583	-1.067605
H	-1.574872	-4.292890	0.088949	H	-3.194962	5.352503	-1.223297
H	-1.588774	-2.849625	1.111549	C	-4.375888	3.626379	-0.676899
C	2.606129	0.155707	2.823522	H	-5.298400	4.191121	-0.521370
H	3.126909	0.336578	3.777299	C	-4.351553	2.240762	-0.501325
H	2.755526	-0.905529	2.577197	H	-5.271401	1.715349	-0.216727
H	1.532150	0.317478	3.000572	C	-3.188699	1.496919	-0.694211
C	1.271480	-3.006550	1.557435	C	-3.172435	0.000607	-0.553604
H	1.202199	-3.780511	2.338059	H	-2.390586	-0.379738	-1.227598
H	0.941244	-2.056601	2.002002	H	-4.133446	-0.418718	-0.890901
H	2.336861	-2.916860	1.296228	C	-2.877986	-0.505304	0.831581
C	1.006691	-4.652396	-0.281073	C	-3.903348	-1.106180	1.577701
H	1.124234	-5.422249	0.499157	H	-4.894761	-1.200878	1.121523
H	2.002189	-4.504425	-0.724889	C	-3.692599	-1.576958	2.871978
H	0.348419	-5.087516	-1.044383	H	-4.513300	-2.037914	3.427694
C	4.666791	0.811321	1.621088	C	-2.435356	-1.436309	3.454131
H	5.157801	1.048108	2.578519	H	-2.254619	-1.775283	4.477920
H	5.161137	1.419111	0.854085	C	-1.403626	-0.846623	2.721591
H	4.892073	-0.243469	1.412836	H	-0.424640	-0.733065	3.199963
C	0.454318	-3.247490	-3.288692	C	-1.591304	-0.417097	1.400539
H	-0.095241	-3.467126	-4.218445	C	-0.327291	1.483187	1.480137
H	0.661272	-4.211653	-2.810792	O	-0.614294	2.401526	2.117051
H	1.413027	-2.808214	-3.596428				
C	2.963192	2.530687	2.205982	<b>10(L3)</b>			
H	3.384577	2.653535	3.216274	P	2.184747	0.173546	0.274589
H	1.905244	2.817714	2.268312	P	-0.075762	-2.151477	0.206462
H	3.476056	3.256183	1.560993	C	2.490308	-1.453172	1.124159
C	4.071022	2.473369	-1.236514	H	3.567096	-1.689383	1.090061
H	4.203813	3.164496	-2.084953	H	2.266149	-1.274387	2.185027
H	4.736446	1.616728	-1.424249	C	3.513889	0.146742	-1.107556
H	4.432469	3.002334	-0.344245	C	-1.017708	-2.471844	1.836125
C	2.144571	1.515654	-2.487696	C	-0.594759	-3.491582	-1.051766
H	2.193695	2.308987	-3.250350	C	2.730079	1.400115	1.642313
H	1.098281	1.180002	-2.440627	C	1.664975	-2.621947	0.605648
H	2.790640	0.697696	-2.842392	H	1.706458	-3.469969	1.310373

H	2.091643	-3.000153	-0.335619	H	0.680774	-2.162568	3.198582
C	2.940447	2.795605	1.062101	C	-2.442811	-1.925675	1.769647
H	3.181160	3.492945	1.880439	H	-2.960857	-2.176650	2.709405
H	2.045601	3.184746	0.558574	H	-3.043096	-2.335666	0.950196
H	3.781721	2.837805	0.355945	H	-2.464823	-0.835134	1.670797
C	1.587181	1.449635	2.655142	Ni	-0.019137	0.137901	-0.442341
H	1.759303	2.276000	3.362486	O	-1.929672	-0.105460	-0.723330
H	1.526128	0.531262	3.256788	C	-3.017291	0.547605	-0.406190
H	0.614095	1.622712	2.179414	C	-4.201856	0.296530	-1.142423
C	3.288980	1.273076	-2.111605	H	-4.133246	-0.387563	-1.992964
H	4.125806	1.288749	-2.827810	C	-5.410275	0.892078	-0.801967
H	3.232547	2.268780	-1.652293	H	-6.303843	0.669075	-1.393174
H	2.375804	1.114652	-2.700165	C	-5.489121	1.771918	0.279827
C	-0.083467	-3.080780	-2.430460	H	-6.436562	2.244680	0.549256
H	-0.255762	-3.905403	-3.140369	C	-4.329545	2.042239	1.008166
H	0.996400	-2.868645	-2.448778	H	-4.370679	2.737322	1.854638
H	-0.616339	-2.205774	-2.821063	C	-3.105572	1.447756	0.697000
C	3.371134	-1.182575	-1.846960	C	-1.845640	1.802724	1.431269
H	3.965158	-1.150572	-2.773947	H	-1.286767	0.881528	1.674986
H	2.329723	-1.381822	-2.139198	H	-2.083104	2.312068	2.377970
H	3.747868	-2.033981	-1.261798	C	-0.997333	2.672729	0.540429
C	4.938249	0.239985	-0.569445	C	-1.150510	4.065203	0.601685
H	5.640035	0.014699	-1.388835	H	-1.792740	4.491360	1.380720
H	5.149402	-0.481001	0.233424	C	-0.533906	4.902108	-0.323942
H	5.191013	1.245932	-0.209312	H	-0.662066	5.985874	-0.260916
C	-0.001690	-4.864775	-0.730326	C	0.216812	4.333376	-1.350241
H	-0.373725	-5.593373	-1.468756	H	0.677618	4.965289	-2.115231
H	-0.273933	-5.250213	0.258148	C	0.384783	2.947598	-1.403954
H	1.095110	-4.879277	-0.807579	H	0.977290	2.544233	-2.227105
C	3.991430	0.981654	2.403444	C	-0.176026	2.091646	-0.446309
H	4.091014	1.636614	3.283979	C	0.150839	0.060504	-2.448303
H	4.916640	1.095192	1.829093	O	-0.384952	0.408845	-3.405781
H	3.952476	-0.046111	2.790527				
C	-2.117539	-3.573305	-1.131240	<b>11-ts(L3)</b>			
H	-2.401819	-4.192883	-1.996891	P	-2.056924	-0.353091	0.454176
H	-2.569245	-2.580390	-1.271660	P	-0.079760	2.219399	0.236298
H	-2.571011	-4.041252	-0.247241	C	-2.465520	1.192735	1.409120
C	-1.056124	-3.940223	2.248269	H	-3.558864	1.336126	1.446771
H	-1.463603	-4.011311	3.270039	H	-2.168362	0.977883	2.446770
H	-0.061053	-4.408731	2.275618	C	-3.462505	-0.417361	-0.858054
H	-1.708017	-4.550802	1.609689	C	1.074090	2.441993	1.739242
C	-0.275043	-1.694235	2.920350	C	0.098174	3.731660	-0.911344
H	-0.887235	-1.657011	3.835421	C	-2.444280	-1.692377	1.772361
H	-0.083785	-0.655117	2.614447	C	-1.779948	2.469131	0.930359



H	-1.762284	3.221328	1.737850	H	0.198997	0.563633	2.435647
H	-2.364167	2.929408	0.119167	H	-0.395457	1.997290	3.312291
C	-2.508827	-3.049756	1.077958	C	2.439710	1.888950	1.345362
H	-2.464380	-3.859125	1.824850	H	3.098380	1.816791	2.226378
H	-1.669602	-3.204841	0.383277	H	2.960863	2.504351	0.599666
H	-3.443962	-3.188126	0.517378	H	2.341913	0.883779	0.921125
C	-1.273750	-1.693637	2.753224	Ni	-0.068521	-0.007944	-0.650905
H	-1.393329	-2.523972	3.467985	O	1.892132	-0.660759	-1.169168
H	-1.225751	-0.772133	3.352349	C	3.087610	-0.838469	-0.601004
H	-0.310097	-1.831971	2.253356	C	4.233880	-0.423007	-1.300837
C	-3.147737	-1.492961	-1.895387	H	4.109485	0.007332	-2.297364
H	-3.926347	-1.491413	-2.675406	C	5.491048	-0.549332	-0.718352
H	-3.119613	-2.504571	-1.470024	H	6.373611	-0.213006	-1.269690
H	-2.186462	-1.325494	-2.396928	C	5.632837	-1.108755	0.554578
C	-0.781118	3.500265	-2.139159	H	6.621909	-1.208359	1.007772
H	-0.669566	4.352143	-2.828959	C	4.498525	-1.541162	1.241059
H	-1.852041	3.439272	-1.894364	H	4.595455	-1.983339	2.237965
H	-0.505036	2.600766	-2.700896	C	3.225873	-1.408028	0.684517
C	-3.482473	0.946813	-1.547601	C	1.954969	-1.812172	1.361288
H	-4.124620	0.903993	-2.442057	H	1.400552	-0.899656	1.657840
H	-2.485322	1.265549	-1.881598	H	2.151156	-2.384139	2.279895
H	-3.895436	1.734034	-0.898585	C	1.141843	-2.604038	0.378888
C	-4.856792	-0.670667	-0.296440	C	0.986312	-3.986248	0.495690
H	-5.599558	-0.515816	-1.096587	H	1.334113	-4.471628	1.414163
H	-5.126256	0.016674	0.519589	C	0.442036	-4.748461	-0.538591
H	-4.992097	-1.701068	0.058073	H	0.324111	-5.828804	-0.431012
C	-0.342244	5.058050	-0.293200	C	0.110330	-4.109594	-1.737741
H	-0.286381	5.848541	-1.059711	H	-0.267029	-4.690817	-2.584304
H	0.278398	5.391913	0.544266	C	0.260739	-2.733966	-1.881952
H	-1.387865	5.034819	0.048523	H	0.022731	-2.266743	-2.839435
C	-3.708959	-1.460512	2.599344	C	0.666505	-1.949305	-0.782571
H	-3.732813	-2.196373	3.420469	C	-0.283800	0.209737	-2.446870
H	-4.642863	-1.590340	2.043914	O	-0.369436	0.272588	-3.599191
H	-3.733468	-0.469258	3.075135				
C	1.553976	3.801390	-1.365328	<b>12(L3)</b>			
H	1.661705	4.527061	-2.187203	Ni	0.000672	-0.055253	1.255963
H	1.912015	2.827507	-1.738600	P	1.602880	-0.005880	-0.263499
H	2.229451	4.127179	-0.561919	P	-1.598114	0.041521	-0.266541
C	1.219763	3.851910	2.291867	C	0.741287	-0.116478	-1.924373
H	1.793403	3.814434	3.233175	H	1.294861	0.434576	-2.704444
H	0.253562	4.322038	2.530240	H	0.819799	-1.176786	-2.211759
H	1.773616	4.517193	1.615780	C	2.365654	1.735863	-0.236328
C	0.487606	1.549160	2.831729	C	-2.364350	-1.696113	-0.403850
H	1.233645	1.381221	3.625151	C	-2.981206	1.346424	-0.334576

C	2.986760	-1.299044	-0.453194	C	-1.195647	-2.603016	-0.783808
C	-0.731118	0.306269	-1.907063	H	-1.476072	-3.662730	-0.668144
H	-1.279953	-0.168497	-2.739135	H	-0.334862	-2.409078	-0.123724
H	-0.807276	1.389107	-2.093723	H	-0.874250	-2.467534	-1.827553
C	4.013776	-1.080931	0.654893	C	-2.837880	-2.123165	0.986064
H	4.715359	-1.930010	0.688677	H	-3.140525	-3.183090	0.971371
H	3.536982	-1.008465	1.644841	H	-3.697939	-1.546915	1.349567
H	4.619055	-0.176463	0.499990	H	-2.029314	-2.007304	1.724422
C	2.337357	-2.666030	-0.236613	C	-0.012380	-0.185271	2.984295
H	3.111825	-3.450247	-0.231134	O	-0.025775	-0.286223	4.149532
H	1.629580	-2.927185	-1.037462				
H	1.801814	-2.721374	0.723966	<b>2(L4)</b>			
C	2.812086	2.035625	1.195002	P	2.433046	-0.367490	0.188138
H	3.115457	3.091776	1.282271	P	-0.423365	-0.286306	1.285749
H	3.663738	1.425582	1.522682	C	2.216809	-0.736226	1.992484
H	1.988010	1.852874	1.902304	H	2.089165	-1.826555	2.090427
C	-2.335083	2.684348	0.025820	H	3.111015	-0.464059	2.575896
H	-3.110319	3.462916	0.112698	C	0.974690	-0.018051	2.485134
H	-1.626354	3.029834	-0.741170	H	1.145320	1.070917	2.519495
H	-1.800107	2.638069	0.987239	H	0.701262	-0.318921	3.508203
C	1.199367	2.668752	-0.555768	C	3.931831	-1.308801	-0.267903
H	1.464948	3.713923	-0.327520	C	4.760453	-0.830083	-1.293035
H	0.324175	2.401873	0.057580	H	4.573777	0.126256	-1.786657
H	0.906117	2.634115	-1.615858	C	5.848720	-1.593844	-1.693396
C	3.500311	1.993339	-1.215962	C	6.150921	-2.825065	-1.123478
H	3.755297	3.066719	-1.212735	H	7.010529	-3.409246	-1.450946
H	3.234817	1.736447	-2.253121	C	5.305538	-3.278219	-0.119731
H	4.420953	1.453112	-0.955041	C	4.205470	-2.551869	0.318939
C	-3.658414	1.487501	-1.695197	H	3.587662	-2.977038	1.111031
H	-4.414058	2.289839	-1.650892	C	3.019861	1.374443	0.212867
H	-4.182857	0.579809	-2.018397	C	2.211852	2.312711	-0.436223
H	-2.954507	1.769202	-2.491693	H	1.308214	1.995279	-0.965710
C	3.673880	-1.301245	-1.816030	C	2.571956	3.654764	-0.403473
H	4.421366	-2.111483	-1.850180	C	3.713008	4.096770	0.251698
H	4.209425	-0.369324	-2.035253	H	3.985500	5.151927	0.270188
H	2.974017	-1.488695	-2.643461	C	4.500799	3.137339	0.881677
C	-4.018732	1.017636	0.735480	C	4.180904	1.785149	0.879203
H	-4.713497	1.864702	0.855933	H	4.842794	1.077977	1.384697
H	-3.553359	0.834720	1.716531	C	-1.242545	-1.816804	1.877185
H	-4.630122	0.141305	0.477578	C	-1.503953	-2.082277	3.227452
C	-3.482768	-1.858964	-1.422179	H	-1.273150	-1.366223	4.019435
H	-3.734588	-2.927794	-1.527678	C	-2.096569	-3.292683	3.565814
H	-3.200229	-1.501459	-2.424260	C	-2.438438	-4.248241	2.615758
H	-4.408909	-1.346851	-1.125587	H	-2.901021	-5.191945	2.905066

C	-2.167731	-3.954842	1.285213	F	-1.513324	4.686627	1.534121
C	-1.570190	-2.760758	0.896597	F	-2.487547	-4.856181	0.356301
H	-1.365152	-2.564928	-0.160636	F	-2.351317	-3.553340	4.850633
C	-1.560203	1.072623	1.752301				
C	-1.103773	2.377359	1.512920	<b>3-ts(L4)</b>			
H	-0.112590	2.575688	1.094398	P	1.902800	0.690491	0.551192
C	-1.946038	3.446560	1.776304	P	-1.172880	0.945698	0.766587
C	-3.239505	3.277067	2.257738	C	1.198397	0.952797	2.247071
H	-3.893325	4.128688	2.445475	H	1.061834	-0.045357	2.693695
C	-3.671330	1.973143	2.456099	H	1.902224	1.494733	2.898410
C	-2.861770	0.867643	2.219212	C	-0.131298	1.684578	2.120341
H	-3.266789	-0.131819	2.390569	H	0.042057	2.731897	1.821460
Ni	0.406028	-0.330669	-0.663539	H	-0.673607	1.724945	3.078440
O	-1.560231	-1.217752	-2.463313	C	3.132253	-0.641762	0.742723
C	-2.859409	-1.343519	-2.871554	C	4.400549	-0.569497	0.153121
C	-3.098402	-2.108983	-4.014921	H	4.769313	0.345237	-0.315286
H	-2.243894	-2.506731	-4.565774	C	5.206171	-1.702867	0.152265
C	-4.406900	-2.356726	-4.423363	C	4.802667	-2.910955	0.706454
H	-4.588365	-2.955848	-5.319006	H	5.448121	-3.788701	0.689952
C	-5.477450	-1.840102	-3.695079	C	3.536574	-2.953628	1.278444
H	-6.505150	-2.031318	-4.012003	C	2.694185	-1.850890	1.306185
C	-5.229407	-1.078128	-2.553617	H	1.701327	-1.961170	1.750522
H	-6.063096	-0.671406	-1.973383	C	2.867932	2.220130	0.254652
C	-3.926021	-0.826521	-2.121522	C	2.484785	3.010459	-0.833885
C	-3.609393	0.001110	-0.913475	H	1.666871	2.708767	-1.494559
H	-2.936327	-0.581785	-0.256213	C	3.168449	4.198219	-1.074121
H	-4.520610	0.208479	-0.335130	C	4.217044	4.624815	-0.270624
C	-2.926321	1.279724	-1.299315	H	4.744023	5.557296	-0.474232
C	-3.537904	2.514356	-1.075938	C	4.570882	3.818425	0.806292
H	-4.526704	2.532983	-0.606396	C	3.918502	2.625447	1.088800
C	-2.910433	3.710281	-1.421809	H	4.241314	2.028941	1.945521
H	-3.402411	4.665466	-1.220752	C	-2.368582	-0.123828	1.651263
C	-1.649236	3.675104	-2.015147	C	-2.036030	-0.747464	2.862255
H	-1.140417	4.602581	-2.289632	H	-1.114105	-0.521524	3.402383
C	-1.035351	2.452031	-2.267210	C	-2.910241	-1.683227	3.401773
H	-0.056771	2.413269	-2.752232	C	-4.103461	-2.037320	2.783522
C	-1.656657	1.239295	-1.920275	H	-4.775673	-2.775168	3.220623
C	-0.894336	-0.017294	-2.109585	C	-4.406236	-1.399102	1.585952
O	0.323832	0.005003	-2.522098	C	-3.570086	-0.454050	1.007773
F	5.567621	-4.458365	0.450441	H	-3.859347	-0.000723	0.055946
F	6.640422	-1.129593	-2.663653	C	-2.243124	2.342555	0.247193
F	5.605938	3.541284	1.513903	C	-2.198638	2.733048	-1.094661
F	1.791333	4.547583	-1.017785	H	-1.577250	2.201375	-1.822185
F	-4.922409	1.771472	2.885638	C	-2.988771	3.804976	-1.500000

C	-3.807808	4.501418	-0.621590	C	-0.424329	1.447008	-2.436411
H	-4.419749	5.338151	-0.958275	H	-0.345518	0.548867	-3.069139
C	-3.825265	4.085059	0.705504	H	-1.000566	2.182734	-3.016910
C	-3.063268	3.017925	1.160613	C	0.955205	1.979845	-2.075357
H	-3.127108	2.725031	2.211315	H	0.882735	2.984696	-1.628556
Ni	0.184236	0.123891	-0.653177	H	1.610324	2.086962	-2.954186
O	0.591700	-1.346095	-1.983488	C	-2.238061	-0.554536	-1.330330
C	0.866019	-2.647634	-1.675456	C	-3.579934	-0.736472	-0.983932
C	2.021660	-3.187831	-2.249557	H	-4.176513	0.056433	-0.528225
H	2.608039	-2.560583	-2.924447	C	-4.159525	-1.982250	-1.197462
C	2.410087	-4.487898	-1.942496	C	-3.460056	-3.052857	-1.740781
H	3.317254	-4.900816	-2.391361	H	-3.933125	-4.023496	-1.886944
C	1.644790	-5.257884	-1.065590	C	-2.125412	-2.839903	-2.062924
H	1.947918	-6.276952	-0.815144	C	-1.500645	-1.615727	-1.876263
C	0.492688	-4.714842	-0.501179	H	-0.439140	-1.520073	-2.121698
H	-0.107598	-5.308771	0.194712	C	-2.624369	2.212089	-0.613844
C	0.085568	-3.408853	-0.789509	C	-2.855059	2.593883	0.712077
C	-1.122060	-2.782114	-0.166756	H	-2.251968	2.180178	1.526917
H	-0.799831	-1.829466	0.308144	C	-3.887028	3.488363	0.974123
H	-1.524705	-3.428413	0.625888	C	-4.677079	4.030027	-0.031096
C	-2.189963	-2.461287	-1.170944	H	-5.479397	4.732755	0.193465
C	-3.402667	-3.154804	-1.174784	C	-4.409159	3.638028	-1.338475
H	-3.562921	-3.939932	-0.429569	C	-3.403467	2.734349	-1.654690
C	-4.412728	-2.842147	-2.081474	H	-3.261386	2.443215	-2.697707
H	-5.358694	-3.388138	-2.050647	C	2.154620	-0.630922	-1.649642
C	-4.219733	-1.820619	-3.012480	C	2.119895	-0.749040	-3.044860
H	-5.007600	-1.569536	-3.726527	H	1.929566	0.098479	-3.705326
C	-3.018454	-1.120791	-3.028054	C	2.325352	-2.001016	-3.617068
H	-2.845634	-0.314302	-3.744513	C	2.560743	-3.140879	-2.859747
C	-1.993305	-1.438072	-2.123228	H	2.698150	-4.114349	-3.329682
C	-0.794439	-0.583021	-2.142172	C	2.609738	-2.987546	-1.478861
O	-0.603112	0.415200	-2.847453	C	2.417497	-1.759117	-0.861762
F	-2.594074	-2.264526	4.564379	H	2.452730	-1.701610	0.228781
F	-5.545750	-1.722598	0.968543	C	3.303171	1.733565	-0.404424
F	-4.609763	4.739752	1.567258	C	3.248193	2.945100	0.296888
F	-2.964555	4.180915	-2.780627	H	2.303808	3.369684	0.641971
F	3.119433	-4.100220	1.820636	C	4.436384	3.601728	0.585867
F	6.416756	-1.633557	-0.408918	C	5.677871	3.091245	0.224155
F	5.572800	4.216028	1.594889	H	6.599403	3.620303	0.466651
F	2.806173	4.957960	-2.108637	C	5.696271	1.877425	-0.449258
				C	4.535377	1.185194	-0.774970
<b>4(L4)</b>				H	4.615833	0.238534	-1.312114
P	-1.326780	0.963888	-0.892154	Ni	0.220467	0.598399	0.733655
P	1.717312	0.915531	-0.770882	O	-1.061791	0.426596	2.174181

C	-1.942035	-0.548455	2.163633	C	-4.144801	0.289158	0.089552
C	-3.264661	-0.317790	2.613824	H	-3.899453	1.013814	0.869244
H	-3.516402	0.681591	2.981066	C	-5.388252	-0.327416	0.104221
C	-4.219367	-1.328850	2.599987	C	-5.760072	-1.278668	-0.839248
H	-5.233112	-1.114738	2.951676	H	-6.740971	-1.752124	-0.809399
C	-3.896425	-2.606651	2.138683	C	-4.830408	-1.602868	-1.818293
H	-4.649437	-3.397847	2.112619	C	-3.571895	-1.014977	-1.878927
C	-2.594088	-2.855122	1.705057	H	-2.882821	-1.331915	-2.662237
H	-2.324453	-3.855192	1.345921	C	-1.844803	2.462976	-0.692839
C	-1.614657	-1.860013	1.707527	C	-0.952412	3.191926	0.098798
C	-0.217604	-2.148915	1.234602	H	-0.155547	2.682766	0.649076
H	0.088095	-1.400928	0.471282	C	-1.099965	4.571890	0.184367
H	-0.209333	-3.116119	0.705435	C	-2.111197	5.249847	-0.483167
C	0.821952	-2.195208	2.328636	H	-2.221297	6.330830	-0.398341
C	1.035803	-3.418681	2.977863	C	-2.985297	4.494781	-1.258839
H	0.444937	-4.286094	2.668285	C	-2.873466	3.115199	-1.383539
C	1.974537	-3.554056	3.995214	H	-3.590650	2.574730	-2.005433
H	2.119493	-4.525148	4.475185	C	2.125225	-1.430149	-1.880464
C	2.731881	-2.451368	4.394839	C	3.229714	-1.317154	-2.737717
H	3.473066	-2.548033	5.191805	H	3.755628	-0.371875	-2.889803
C	2.531162	-1.229042	3.770446	C	3.663952	-2.448768	-3.413076
H	3.103190	-0.345900	4.064919	C	3.044151	-3.685525	-3.269178
C	1.583763	-1.079845	2.742189	H	3.400638	-4.562500	-3.809878
C	1.468454	0.286649	2.138731	C	1.954231	-3.757639	-2.412234
O	2.037390	1.242067	2.621053	C	1.476079	-2.657318	-1.705813
F	-1.411420	-3.856384	-2.559282	H	0.611929	-2.751984	-1.033338
F	-5.439441	-2.162535	-0.866115	C	2.940724	0.988309	-0.563782
F	2.821132	-4.062834	-0.720245	C	3.019620	2.380098	-0.694632
F	2.280845	-2.114471	-4.945913	H	2.253833	2.971619	-1.198959
F	6.875339	1.359228	-0.802946	C	4.117088	3.042678	-0.154619
F	4.392681	4.764671	1.238230	C	5.131575	2.381392	0.524823
F	-5.155507	4.147012	-2.322367	H	5.976769	2.921328	0.951104
F	-4.130996	3.839526	2.237830	C	5.016258	1.001231	0.647023
				C	3.951716	0.291042	0.111874
				H	3.913182	-0.791764	0.253331
<b>5-ts(L4)</b>				Ni	-0.109290	-0.179588	0.586394
P	-1.569626	0.657296	-0.833242	O	-0.837411	-2.114725	0.186234
P	1.453543	0.049235	-1.030874	C	-1.374388	-2.544128	1.302773
C	-0.809812	0.479906	-2.504744	C	-2.771245	-2.740212	1.434906
H	-0.842505	-0.591692	-2.762896	H	-3.395618	-2.572370	0.552774
H	-1.386320	1.021777	-3.270989	C	-3.343683	-3.099805	2.650299
C	0.631991	0.960360	-2.420122	H	-4.430709	-3.213701	2.718098
H	0.661518	2.040584	-2.203630	C	-2.548711	-3.310781	3.779476
H	1.171620	0.809838	-3.367793	H	-2.997767	-3.590516	4.735322
C	-3.234065	-0.057308	-0.917608				

C	-1.164511	-3.169991	3.659999	H	1.766277	3.333684	-0.600195
H	-0.524495	-3.352545	4.531138	C	2.113843	-0.997582	-1.876528
C	-0.566869	-2.804363	2.453640	C	1.451225	-2.228401	-1.823213
C	0.926750	-2.686602	2.319051	H	0.594605	-2.384939	-1.153747
H	1.181847	-2.874237	1.260120	C	1.915077	-3.263212	-2.629698
H	1.419954	-3.478379	2.902886	C	3.002141	-3.122114	-3.480873
C	1.548454	-1.368725	2.703110	H	3.352088	-3.948572	-4.099555
C	2.697510	-1.354055	3.507974	C	3.629237	-1.881408	-3.513110
H	3.085295	-2.307699	3.879879	C	3.209081	-0.812527	-2.733283
C	3.355646	-0.169862	3.833748	H	3.742348	0.137629	-2.807208
H	4.246751	-0.199614	4.465840	C	-2.200590	2.377003	-0.418723
C	2.870820	1.048974	3.360982	C	-2.096638	3.370632	-1.399708
H	3.368760	1.986635	3.620513	H	-1.718446	3.176059	-2.404152
C	1.734938	1.060410	2.557279	C	-2.502539	4.665696	-1.093522
H	1.338718	2.017737	2.201511	C	-3.014779	5.015537	0.147338
C	1.081443	-0.131532	2.209244	H	-3.327964	6.036152	0.365936
C	-0.771431	0.286287	2.118860	C	-3.116601	4.006465	1.098020
O	-1.408237	0.620714	3.035094	C	-2.710899	2.702465	0.845406
F	-5.160661	-2.511342	-2.738662	H	-2.818685	1.957721	1.635873
F	-6.263700	0.000374	1.055344	C	-3.200859	-0.284530	-0.984409
F	-3.965578	5.125560	-1.906959	C	-3.106864	-1.560203	-1.558498
F	-0.245468	5.266907	0.936663	H	-2.151222	-2.006962	-1.829926
F	1.344387	-4.935386	-2.262922	C	-4.270711	-2.293347	-1.745641
F	4.712679	-2.351334	-4.235752	C	-5.522788	-1.823338	-1.366600
F	5.959801	0.339380	1.318865	H	-6.422597	-2.419308	-1.518514
F	4.199057	4.368301	-0.293800	C	-5.578375	-0.560424	-0.793890
				C	-4.446707	0.221386	-0.596060
				H	-4.568036	1.212318	-0.156833
<b>6(L4)</b>				Ni	-0.062023	-0.111086	0.719770
P	1.418794	0.394337	-0.908398	O	-0.757798	-1.999505	0.265083
P	-1.660581	0.652943	-0.718851	C	-1.074116	-2.668349	1.352523
C	0.521514	1.315875	-2.243194	C	-2.415794	-2.833302	1.771573
H	0.457205	2.377245	-1.957644	H	-3.206959	-2.376303	1.169173
H	1.083731	1.270834	-3.188321	C	-2.728436	-3.552705	2.921962
C	-0.860458	0.703391	-2.374999	H	-3.775995	-3.664847	3.218257
H	-0.787801	-0.343866	-2.712345	C	-1.719878	-4.125918	3.698161
H	-1.492842	1.217282	-3.115369	H	-1.964353	-4.691587	4.600424
C	2.851161	1.431089	-0.477908	C	-0.389544	-3.963774	3.304100
C	4.053990	0.825250	-0.094558	H	0.412893	-4.403381	3.907575
H	4.197414	-0.256608	-0.132618	C	-0.052276	-3.254755	2.151774
C	5.081912	1.621087	0.392360	C	1.373537	-3.047072	1.731027
C	4.967192	3.000889	0.511624	H	1.426610	-3.069518	0.631469
H	5.785611	3.609148	0.895934	H	1.994353	-3.880042	2.092177
C	3.759103	3.570832	0.131498	C	1.979918	-1.755575	2.231419
C	2.697364	2.818365	-0.354901				

C	3.100163	-1.836966	3.077722	C	2.202839	-2.703516	-3.314774
H	3.497788	-2.830098	3.312409	C	1.959995	-1.393936	-2.914831
C	3.704855	-0.709359	3.626356	H	1.628816	-0.679668	-3.669541
H	4.570226	-0.818445	4.284891	C	-2.741751	2.020550	-0.915905
C	3.184984	0.549600	3.340970	C	-3.454418	2.417424	-2.054202
H	3.628156	1.451181	3.773553	H	-3.234430	2.028949	-3.050727
C	2.083729	0.653763	2.492048	C	-4.490115	3.332067	-1.903122
H	1.685807	1.650043	2.270103	C	-4.847664	3.854795	-0.666512
C	1.485137	-0.475196	1.917820	H	-5.660664	4.574333	-0.570020
C	-0.809841	0.399398	2.255405	C	-4.127717	3.427116	0.442626
O	-1.258851	0.600933	3.295764	C	-3.078817	2.520003	0.347468
F	1.296350	-4.444913	-2.580711	H	-2.556785	2.179277	1.246459
F	4.675648	-1.715951	-4.327154	C	-2.206308	-0.807372	-1.098004
F	6.220784	1.041255	0.773272	C	-1.471905	-1.909737	-1.556155
F	3.612877	4.893544	0.243759	H	-0.468017	-1.809666	-1.974790
F	-2.402101	5.607365	-2.033471	C	-2.017824	-3.178612	-1.433615
F	-3.618608	4.306228	2.294705	C	-3.269543	-3.400093	-0.871336
F	-4.189175	-3.500289	-2.307988	H	-3.678510	-4.404839	-0.768357
F	-6.767150	-0.069134	-0.434821	C	-3.972706	-2.286395	-0.429944
				C	-3.469316	-0.993897	-0.530138
				H	-4.053960	-0.163451	-0.130907
<b>10(L4)</b>				Ni	0.123678	0.780724	0.664319
P	1.637868	0.579679	-0.912885	O	-1.467273	0.176277	1.744125
P	-1.378718	0.811278	-1.009815	C	-1.911594	-0.969767	2.191558
C	0.928082	1.483444	-2.360472	C	-3.206279	-1.029109	2.767655
H	0.949000	2.545454	-2.069242	H	-3.777993	-0.097772	2.828499
H	1.572726	1.406500	-3.249734	C	-3.743073	-2.223236	3.234836
C	-0.506173	1.048014	-2.628609	H	-4.748261	-2.225518	3.667581
H	-0.546594	0.096537	-3.181390	C	-3.016438	-3.412244	3.145603
H	-1.029791	1.785713	-3.254327	H	-3.434824	-4.354142	3.507608
C	3.196357	1.467083	-0.564772	C	-1.735287	-3.369592	2.592148
C	4.415705	0.802012	-0.407991	H	-1.146822	-4.291465	2.517241
H	4.518969	-0.273874	-0.556494	C	-1.169328	-2.183917	2.121382
C	5.538419	1.537747	-0.042762	C	0.208628	-2.163044	1.526910
C	5.500055	2.909217	0.170014	H	0.146397	-1.772810	0.495173
H	6.392229	3.466909	0.453577	H	0.586524	-3.195595	1.448987
C	4.274842	3.541955	-0.002295	C	1.205732	-1.314541	2.274998
C	3.123781	2.851947	-0.358199	C	1.977370	-1.879058	3.300377
H	2.192129	3.413373	-0.456490	H	1.813855	-2.929817	3.563776
C	2.138408	-1.051072	-1.566379	C	2.945417	-1.135378	3.972111
C	2.580808	-2.023283	-0.658943	H	3.540270	-1.598848	4.763213
H	2.728250	-1.797745	0.398844	C	3.154851	0.197186	3.622492
C	2.800160	-3.318227	-1.106777	H	3.915573	0.791612	4.136250
C	2.613795	-3.693331	-2.432087	C	2.382575	0.778745	2.613824
H	2.777885	-4.718610	-2.762821				

H	2.562682	1.827606	2.350457	C	3.552001	-3.401598	-2.852389
C	1.405561	0.038535	1.942836	H	3.989047	-4.270155	-3.344934
C	0.165475	2.554599	1.237114	C	2.366103	-3.491469	-2.138593
O	0.210649	3.626933	1.644779	C	1.798624	-2.397850	-1.491464
F	-5.166712	3.727097	-2.983937	H	0.878474	-2.541629	-0.923877
F	-4.457145	3.912969	1.639240	C	3.174874	1.270467	-0.324604
F	-1.307334	-4.226310	-1.864489	C	3.451216	2.558282	-0.796460
F	-5.175745	-2.465609	0.114669	H	2.836509	3.055740	-1.548070
F	3.181169	-4.243635	-0.225621	C	4.551504	3.236386	-0.283078
F	2.024379	-3.022979	-4.598638	C	5.383359	2.691183	0.686067
F	6.700894	0.901023	0.104999	H	6.235063	3.244466	1.080648
F	4.202548	4.860640	0.183636	C	5.078463	1.410935	1.135418
				C	3.998837	0.688309	0.649709
				H	3.805634	-0.312187	1.044576
<b>11-ts(L4)</b>				Ni	0.118167	0.736676	0.784272
P	-1.426055	0.613955	-0.902657	O	-0.842283	0.272982	2.488873
P	1.676614	0.336186	-0.773510	C	-1.747379	-0.711306	2.581677
C	-0.454852	0.616358	-2.486492	C	-2.991414	-0.387768	3.154014
H	-0.384302	-0.418953	-2.856018	H	-3.153496	0.638299	3.493227
H	-0.984575	1.180953	-3.268266	C	-3.984880	-1.353932	3.271433
C	0.934088	1.191221	-2.236754	H	-4.951341	-1.081218	3.704128
H	0.856028	2.261435	-1.984001	C	-3.751915	-2.661514	2.840692
H	1.576376	1.111870	-3.127989	H	-4.532932	-3.420797	2.926241
C	-2.508683	-0.856189	-0.995524	C	-2.512937	-2.986464	2.291894
C	-3.779595	-0.808796	-0.403627	H	-2.317444	-4.009841	1.954513
H	-4.185603	0.110962	0.022756	C	-1.501361	-2.033331	2.149180
C	-4.535395	-1.970969	-0.335114	C	-0.171646	-2.355477	1.535498
C	-4.091245	-3.186639	-0.843113	H	-0.182988	-1.986097	0.489508
H	-4.701995	-4.086896	-0.781548	H	-0.015827	-3.443250	1.489938
C	-2.828641	-3.204208	-1.417961	C	0.943667	-1.674898	2.270472
C	-2.026578	-2.072023	-1.501846	C	1.979363	-2.354842	2.912552
H	-1.043277	-2.168899	-1.966284	H	2.023560	-3.445250	2.824438
C	-2.635585	1.983746	-1.088430	C	2.930240	-1.672392	3.677834
C	-2.823197	2.847094	-0.004627	H	3.730919	-2.222437	4.176578
H	-2.261252	2.728009	0.925774	C	2.821131	-0.288413	3.833337
C	-3.754625	3.875022	-0.118196	H	3.546126	0.256308	4.444969
C	-4.494937	4.082405	-1.273766	C	1.798218	0.419078	3.203230
H	-5.216117	4.896291	-1.346944	H	1.709522	1.500878	3.332686
C	-4.287434	3.203867	-2.331940	C	0.924698	-0.270375	2.352826
C	-3.377520	2.157744	-2.263864	C	0.495826	2.494436	1.054774
H	-3.277300	1.487217	-3.120108	O	0.807627	3.605405	1.101330
C	2.434288	-1.155338	-1.565508	F	4.823100	4.461177	-0.743269
C	3.632968	-1.033151	-2.283296	F	5.849828	0.863057	2.078088
H	4.166189	-0.083185	-2.364237	F	-3.941884	4.694881	0.917252
C	4.164547	-2.154230	-2.905980				



F	-4.997385	3.375690	-3.450008	H	2.101949	2.574326	-1.182126
F	-5.740465	-1.925615	0.237683	C	4.160357	2.914136	-0.728527
F	-2.365237	-4.356490	-1.913735	C	5.353277	2.464609	-0.178182
F	1.748049	-4.672872	-2.067678	H	6.251720	3.080699	-0.184195
F	5.306217	-2.034044	-3.587702	C	5.346797	1.194767	0.386854
				C	4.216180	0.388669	0.406326
				H	4.276336	-0.597591	0.872059
<b>12(L4)</b>				Ni	-0.015195	-0.119738	1.547043
P	-1.557269	-0.068534	0.005179	C	0.093707	-0.261140	3.282417
P	1.491900	-0.112917	-0.021540	O	0.190836	-0.369968	4.435888
C	-0.735798	-0.471587	-1.614882	F	-0.817607	4.818125	1.313536
H	-0.625540	-1.568461	-1.663753	F	-3.676903	4.071427	-2.318712
H	-1.356485	-0.170559	-2.474281	F	-6.335676	-0.738270	1.690088
C	0.627067	0.198906	-1.647091	F	-5.104432	-3.234312	-2.075512
H	0.504389	1.288503	-1.760151	F	4.131403	4.130142	-1.281830
H	1.235536	-0.142675	-2.499506	F	6.477614	0.735776	0.929655
C	-3.215517	-0.825573	-0.144822	F	4.122170	-3.938906	-2.356322
C	-4.169704	-0.482312	0.824069	F	1.261667	-5.077534	1.172642
H	-3.945348	0.232469	1.619516				
C	-5.423388	-1.073241	0.774476				
C	-5.770357	-2.010874	-0.193256	<b>2(L5)</b>			
H	-6.758575	-2.469381	-0.211199	P	2.331261	-0.775064	0.316003
C	-4.802115	-2.337925	-1.131371	P	-0.565876	-0.409125	1.186390
C	-3.534190	-1.764997	-1.133061	C	1.939468	-1.236090	2.065293
H	-2.829159	-2.068410	-1.907940	H	1.712971	-2.314628	2.052743
C	-1.904951	1.723414	-0.216084	H	2.797707	-1.108201	2.743225
C	-1.250599	2.603717	0.653968	C	0.725408	-0.451007	2.531963
H	-0.610097	2.222256	1.459180	H	0.998576	0.596479	2.739602
C	-1.437340	3.971806	0.488836	H	0.319749	-0.851182	3.473531
C	-2.251766	4.492147	-0.508942	C	3.868031	-1.706307	-0.040397
H	-2.389511	5.567343	-0.622791	C	4.830286	-1.169754	-0.904396
C	-2.889649	3.589841	-1.353082	H	4.708725	-0.166121	-1.319094
C	-2.733933	2.214211	-1.230752	C	5.970035	-1.909137	-1.253599
H	-3.263258	1.551301	-1.919344	C	6.161806	-3.200792	-0.746507
C	2.044289	-1.848558	-0.261682	H	7.049369	-3.774454	-1.013555
C	2.943401	-2.224981	-1.266554	C	5.196008	-3.742373	0.109685
H	3.409418	-1.495170	-1.932840	C	4.055671	-3.000899	0.456574
C	3.256537	-3.570909	-1.407992	H	3.322980	-3.458558	1.124083
C	2.701282	-4.556586	-0.598696	C	2.907698	0.968260	0.429744
H	2.959974	-5.607403	-0.728957	C	2.582885	1.808620	-0.643283
C	1.809424	-4.149787	0.384956	H	2.071254	1.395519	-1.520018
C	1.473160	-2.813886	0.574699	C	2.886774	3.178705	-0.592930
H	0.775772	-2.519426	1.366945	C	3.490446	3.725035	0.547910
C	3.028677	0.865310	-0.168274	H	3.693546	4.794939	0.604669
C	3.001494	2.147214	-0.735253	C	3.821254	2.882955	1.616770

C	3.544311	1.504743	1.550667	C	-1.382417	1.270717	-2.154290
H	3.823406	0.871796	2.396765	C	-0.781775	-0.083075	-2.224329
C	-1.791285	-1.693111	1.651156	O	0.451578	-0.236205	-2.552777
C	-2.250434	-1.904823	2.953631	C	-3.752901	-4.264334	-0.219079
H	-1.888984	-1.293185	3.784528	N	-4.170059	-4.885326	-1.111212
C	-3.202620	-2.905519	3.212271	C	-3.662564	-3.115637	4.548778
C	-3.704196	-3.692765	2.167112	N	-4.028482	-3.278149	5.642132
H	-4.449725	-4.462412	2.369361	C	-4.612391	2.815476	2.486735
C	-3.241142	-3.482129	0.862322	N	-5.722616	2.930100	2.819486
C	-2.274530	-2.495077	0.612051	C	-0.361669	4.719000	0.909438
H	-1.905526	-2.337858	-0.407164	N	0.352474	5.580795	0.586313
C	-1.398551	1.192487	1.519469	C	5.369007	-5.056571	0.643804
C	-0.648332	2.321734	1.170997	N	5.499607	-6.125253	1.087343
H	0.364799	2.197742	0.776237	C	6.945091	-1.337841	-2.128729
C	-1.178282	3.610774	1.291935	N	7.738410	-0.867491	-2.839355
C	-2.493843	3.787518	1.739753	C	4.439984	3.420900	2.787233
H	-2.923289	4.786596	1.818152	N	4.944479	3.839674	3.749553
C	-3.255566	2.659328	2.066644	C	2.545252	4.017399	-1.698115
C	-2.710367	1.365905	1.958371	N	2.257309	4.681411	-2.610160
H	-3.337369	0.506500	2.209610				
Ni	0.399284	-0.532594	-0.687631	<b>3-ts(L5)</b>			
O	-1.558537	-1.211514	-2.539046	P	1.888305	0.896812	0.718893
C	-2.876201	-1.262956	-2.919799	P	-1.189726	1.054956	0.880586
C	-3.183060	-2.168073	-3.937725	C	1.176160	1.234850	2.404871
H	-2.367101	-2.713248	-4.415246	H	1.187580	0.284824	2.961689
C	-4.508425	-2.365322	-4.313451	H	1.822394	1.920198	2.973976
H	-4.743458	-3.076886	-5.107935	C	-0.237017	1.797366	2.292243
C	-5.527433	-1.658232	-3.676824	H	-0.194391	2.872843	2.055432
H	-6.568983	-1.808629	-3.967850	H	-0.780921	1.715078	3.246781
C	-5.210948	-0.759637	-2.659762	C	2.584124	-0.787831	0.863357
H	-6.005987	-0.207212	-2.150837	C	3.858287	-1.158415	0.432363
C	-3.888377	-0.555003	-2.256184	H	4.585493	-0.406177	0.117328
C	-3.522231	0.386106	-1.147994	C	4.217438	-2.516977	0.377054
H	-2.965919	-0.180867	-0.377174	C	3.306225	-3.514706	0.745448
H	-4.430003	0.766988	-0.658775	H	3.582320	-4.567517	0.682804
C	-2.663654	1.523189	-1.614537	C	2.030207	-3.139508	1.182373
C	-3.116956	2.841256	-1.521535	C	1.674782	-1.786041	1.231941
H	-4.115596	3.025552	-1.113515	H	0.658851	-1.518224	1.539188
C	-2.324424	3.912246	-1.930957	C	3.360352	1.968538	0.520230
H	-2.696621	4.936147	-1.843956	C	3.544173	2.561024	-0.731779
C	-1.053372	3.668120	-2.450980	H	2.812493	2.393131	-1.527439
H	-0.419014	4.495898	-2.776632	C	4.668253	3.366235	-0.978727
C	-0.591502	2.360352	-2.561936	C	5.611166	3.583908	0.032714
H	0.391801	2.159975	-2.994908	H	6.484814	4.209055	-0.155167

C	5.424293	2.992046	1.289363	H	-2.645019	0.854846	-3.895657
C	4.302004	2.183824	1.530721	C	-1.898262	-0.645898	-2.540738
H	4.184405	1.719830	2.513408	C	-0.739264	0.193246	-2.234841
C	-2.187860	-0.297314	1.615325	O	-0.442925	1.295177	-2.689793
C	-1.753821	-1.035063	2.722655	C	4.850646	3.969208	-2.261772
H	-0.869434	-0.731856	3.288696	N	4.998574	4.461603	-3.306125
C	-2.449196	-2.184069	3.137085	C	6.379471	3.208440	2.330602
C	-3.594224	-2.606206	2.451193	N	7.145596	3.384010	3.189600
H	-4.133545	-3.498192	2.770292	C	5.513914	-2.885079	-0.097070
C	-4.039487	-1.859328	1.351427	N	6.570211	-3.178606	-0.490415
C	-3.339646	-0.718343	0.934563	C	1.046717	-4.113174	1.538607
H	-3.705709	-0.167419	0.062584	N	0.200318	-4.864024	1.816979
C	-2.504848	2.302838	0.568116	C	-5.202649	-2.278263	0.633715
C	-2.614666	2.856202	-0.708798	N	-6.140069	-2.624363	0.035705
H	-1.920763	2.557703	-1.500648	C	-1.980553	-2.911400	4.274954
C	-3.625526	3.792785	-0.988172	N	-1.584676	-3.484059	5.208399
C	-4.512626	4.195458	0.016008	C	-5.286362	4.053968	2.338187
H	-5.294798	4.924707	-0.197828	N	-6.009726	4.378992	3.190903
C	-4.391297	3.647552	1.300569	C	-3.749688	4.326700	-2.308412
C	-3.395722	2.695775	1.570839	N	-3.850372	4.753473	-3.387041
H	-3.333443	2.264428	2.573714				
Ni	0.208838	0.585499	-0.643912	<b>4(L5)</b>			
O	0.764404	-0.673430	-2.137575	P	-1.413188	0.700916	-0.996271
C	1.003668	-2.002658	-2.141653	P	1.628505	0.868384	-0.914629
C	2.216456	-2.431949	-2.704442	C	-0.548809	0.941152	-2.618816
H	2.895600	-1.676794	-3.107379	H	-0.421807	-0.048378	-3.086092
C	2.533227	-3.785618	-2.746101	H	-1.167361	1.526146	-3.315420
H	3.483398	-4.103873	-3.183723	C	0.797496	1.614973	-2.384825
C	1.640435	-4.731438	-2.236714	H	0.661180	2.678568	-2.129134
H	1.881161	-5.796266	-2.272665	H	1.433727	1.602553	-3.283375
C	0.438065	-4.305374	-1.676315	C	-2.187275	-0.947987	-1.093619
H	-0.257426	-5.036635	-1.253704	C	-3.493416	-1.197318	-0.665760
C	0.108620	-2.948250	-1.604274	H	-4.153893	-0.377833	-0.371961
C	-1.144127	-2.464986	-0.940783	C	-3.971710	-2.515964	-0.593009
H	-0.861931	-1.668642	-0.222023	C	-3.144357	-3.596608	-0.927891
H	-1.609516	-3.281037	-0.368882	H	-3.514286	-4.619405	-0.852045
C	-2.137589	-1.884692	-1.905578	C	-1.832613	-3.342701	-1.343586
C	-3.327273	-2.558131	-2.194096	C	-1.362285	-2.024902	-1.428830
H	-3.523678	-3.517346	-1.705940	H	-0.323734	-1.858755	-1.728555
C	-4.272338	-2.020248	-3.066030	C	-2.810394	1.874304	-0.949428
H	-5.204213	-2.559480	-3.252168	C	-3.067078	2.514926	0.266515
C	-4.033185	-0.792385	-3.684324	H	-2.440330	2.292629	1.137943
H	-4.767142	-0.368894	-4.373244	C	-4.130785	3.427550	0.365599
C	-2.852050	-0.108611	-3.422429	C	-4.922499	3.714517	-0.752444

H	-5.739503	4.433215	-0.678979	C	2.600365	-0.207530	3.962782
C	-4.660860	3.068381	-1.968359	H	3.088488	0.764865	4.060280
C	-3.609025	2.144209	-2.064531	C	1.649467	-0.364915	2.937571
H	-3.432134	1.640481	-3.018551	C	1.431639	0.818996	2.058630
C	2.185191	-0.782731	-1.489647	O	1.934775	1.897457	2.286904
C	2.196538	-1.153997	-2.836424	C	2.445566	-2.847235	-4.587390
H	1.981682	-0.427550	-3.623166	N	2.418592	-3.123635	-5.718038
C	2.469702	-2.483534	-3.205454	C	2.989169	-4.044092	0.141261
C	2.735777	-3.450835	-2.229163	N	3.156481	-4.816049	0.996578
H	2.906212	-4.490012	-2.512054	C	6.866618	1.526776	-0.785593
C	2.755541	-3.071322	-0.880276	N	7.921782	1.061588	-0.946700
C	2.483204	-1.744439	-0.516292	C	3.992380	5.292323	0.469229
H	2.483584	-1.473205	0.543755	N	3.863108	6.395521	0.818192
C	3.152291	1.843981	-0.689736	C	-5.460708	3.354525	-3.117834
C	3.013017	3.159405	-0.231039	N	-6.105776	3.578109	-4.061020
H	2.022911	3.586647	-0.056075	C	-4.400218	4.074943	1.611698
C	4.146987	3.942372	0.025251	N	-4.622526	4.596153	2.628686
C	5.429741	3.407502	-0.151549	C	-5.311085	-2.755682	-0.154666
H	6.312428	4.012407	0.057670	N	-6.406212	-2.948546	0.191842
C	5.566294	2.087385	-0.594787	C	-0.919534	-4.397536	-1.651212
C	4.428916	1.308637	-0.865299	N	-0.113464	-5.201915	-1.897968
H	4.565478	0.282008	-1.212839				
Ni	0.157195	0.747984	0.641654	<b>5-ts(L5)</b>			
O	-1.120148	0.760265	2.087851	P	-1.600049	0.624438	-0.693079
C	-1.914683	-0.264758	2.298477	P	1.386373	-0.051129	-0.962567
C	-3.258253	-0.051730	2.693464	C	-0.953972	0.334627	-2.387833
H	-3.594109	0.978765	2.841402	H	-1.085788	-0.744081	-2.574895
C	-4.120931	-1.117114	2.925543	H	-1.524972	0.882874	-3.153807
H	-5.152779	-0.918304	3.229262	C	0.518825	0.719450	-2.413348
C	-3.680126	-2.434155	2.776299	H	0.619272	1.813535	-2.341666
H	-4.359654	-3.270262	2.956021	H	0.999859	0.425251	-3.357665
C	-2.357829	-2.663112	2.395564	C	-3.361580	0.184043	-0.718867
H	-1.997070	-3.691884	2.280703	C	-4.109248	0.411937	0.441292
C	-1.471373	-1.612776	2.146771	H	-3.655536	0.889110	1.313866
C	-0.055677	-1.881644	1.722292	C	-5.451874	0.014893	0.506706
H	0.177895	-1.293366	0.806734	C	-6.051436	-0.625778	-0.585695
H	0.028944	-2.938357	1.420308	H	-7.093306	-0.942724	-0.533336
C	0.990357	-1.605107	2.777589	C	-5.300294	-0.855206	-1.743553
C	1.316900	-2.643640	3.659257	C	-3.955762	-0.451771	-1.809966
H	0.817028	-3.609493	3.542287	H	-3.392901	-0.656923	-2.722567
C	2.262277	-2.477919	4.666070	C	-1.570301	2.453446	-0.524807
H	2.499386	-3.313404	5.328834	C	-0.569326	2.996609	0.282679
C	2.908665	-1.250498	4.822396	H	0.110764	2.322752	0.816778
H	3.650144	-1.111950	5.612411	C	-0.434226	4.387044	0.422426

C	-1.319298	5.244735	-0.239046	H	3.387870	0.886058	4.057786
H	-1.225041	6.325806	-0.132571	C	1.723509	0.319804	2.804015
C	-2.332701	4.699613	-1.040933	H	1.418697	1.357932	2.625353
C	-2.456882	3.307827	-1.186056	C	0.990666	-0.730185	2.228702
H	-3.253814	2.908715	-1.819471	C	-0.824175	-0.156658	2.228452
C	2.236482	-1.501308	-1.702225	O	-1.435933	0.052156	3.195872
C	3.521991	-1.414863	-2.243541	C	-5.899984	-1.500758	-2.868955
H	4.082714	-0.477486	-2.218438	N	-6.379624	-2.019541	-3.794419
C	4.115526	-2.541212	-2.835309	C	-6.208446	0.247301	1.696931
C	3.420149	-3.755215	-2.895179	N	-6.831216	0.438823	2.661706
H	3.881091	-4.630301	-3.354861	C	1.413213	-5.069816	-2.416409
C	2.128915	-3.832916	-2.359501	N	0.834124	-6.078475	-2.468791
C	1.533660	-2.710240	-1.759179	C	5.431763	-2.440174	-3.383220
H	0.527649	-2.778894	-1.319298	N	6.503055	-2.345825	-3.829631
C	2.754514	1.062033	-0.496815	C	5.638610	0.853532	1.863548
C	2.815916	2.409889	-0.859317	N	6.375166	0.399691	2.642793
H	2.102204	2.843770	-1.562302	C	3.842644	4.621655	-0.725294
C	3.813987	3.247824	-0.333013	N	3.840091	5.736742	-1.060094
C	4.761967	2.744917	0.564572	C	-3.241339	5.567666	-1.723096
H	5.530271	3.397131	0.979885	N	-3.982750	6.267103	-2.285645
C	4.705390	1.392114	0.924709	C	0.621145	4.896236	1.240881
C	3.707084	0.559200	0.401150	N	1.509409	5.262814	1.898797
H	3.678236	-0.489040	0.712043				
Ni	-0.179957	-0.402192	0.637087	<b>6(L5)</b>			
O	-1.039166	-2.164620	-0.191117	P	-1.392674	0.105386	0.820763
C	-1.640537	-2.733861	0.834566	P	1.621184	0.660402	0.606910
C	-3.049307	-2.855694	0.898596	C	-0.525702	0.918418	2.250053
H	-3.632769	-2.527030	0.033925	H	-0.542766	2.010021	2.103006
C	-3.686792	-3.371906	2.023104	H	-1.054881	0.717650	3.193511
H	-4.779794	-3.433645	2.040988	C	0.910805	0.423661	2.286862
C	-2.946535	-3.808699	3.122581	H	0.950961	-0.656172	2.504382
H	-3.444081	-4.211225	4.007464	H	1.506377	0.939007	3.056832
C	-1.553919	-3.745863	3.059970	C	-2.833668	1.149761	0.430321
H	-0.957371	-4.116121	3.901199	C	-3.855086	0.596399	-0.356373
C	-0.891362	-3.233696	1.943957	H	-3.828690	-0.457998	-0.642611
C	0.610991	-3.237632	1.868140	C	-4.928326	1.388140	-0.789475
H	0.894474	-3.279475	0.801784	C	-4.996925	2.743477	-0.441390
H	1.001111	-4.161147	2.321058	H	-5.830257	3.359203	-0.779967
C	1.338403	-2.072544	2.489200	C	-3.982485	3.295042	0.348864
C	2.462888	-2.305553	3.294840	C	-2.904973	2.501431	0.777499
H	2.762798	-3.340678	3.484753	H	-2.136473	2.972471	1.393272
C	3.199527	-1.261186	3.850933	C	-2.118440	-1.366417	1.647133
H	4.069083	-1.479889	4.475407	C	-1.299953	-2.491240	1.804978
C	2.825904	0.060982	3.613167	H	-0.302587	-2.509743	1.343581

C	-1.769754	-3.603464	2.523725	C	-3.031086	-0.180306	-3.574639
C	-3.056204	-3.603087	3.075649	H	-3.561314	0.618265	-4.100432
H	-3.421287	-4.470303	3.626919	C	-1.981037	0.130177	-2.708262
C	-3.870471	-2.475711	2.911920	H	-1.714368	1.184348	-2.565271
C	-3.400457	-1.357959	2.203472	C	-1.282682	-0.869679	-2.019095
H	-4.053524	-0.487588	2.107836	C	0.940624	0.260449	-2.299814
C	1.741594	2.486851	0.474481	O	1.480559	0.518381	-3.280673
C	2.730011	3.233092	1.122967	C	5.471040	-2.365553	2.491458
H	3.514928	2.740537	1.703074	N	5.803522	-3.158269	3.276469
C	2.728625	4.634490	1.031325	C	6.469525	0.547650	-1.319287
C	1.729026	5.298958	0.306135	N	7.214604	0.957048	-2.114508
H	1.726200	6.387489	0.244275	C	-0.930439	-4.749734	2.684291
C	0.737416	4.550198	-0.337747	N	-0.249254	-5.683649	2.822735
C	0.756280	3.148015	-0.262620	C	-5.183579	-2.452236	3.475107
H	-0.009883	2.565121	-0.786578	N	-6.253448	-2.420651	3.933569
C	3.338429	0.084528	0.658826	C	-5.942994	0.806454	-1.611213
C	3.743905	-0.892144	1.571834	N	-6.758203	0.325596	-2.289223
H	3.050823	-1.296454	2.310303	C	-4.037977	4.667191	0.743040
C	5.059778	-1.380202	1.541904	N	-4.067164	5.780396	1.083022
C	5.968085	-0.908780	0.586374	C	-0.309559	5.188534	-1.072002
H	6.988673	-1.291170	0.561189	N	-1.189284	5.666048	-1.666724
C	5.552822	0.057803	-0.338466	C	3.748931	5.386371	1.692097
C	4.239246	0.549724	-0.304086	N	4.581669	5.990517	2.236699
H	3.932915	1.292401	-1.045596				
Ni	0.149644	-0.266941	-0.799305	<b>10(L5)</b>			
O	1.073839	-1.999396	-0.049477	P	-1.586342	0.590429	0.953839
C	1.511754	-2.702991	-1.081793	P	1.437450	0.609710	0.939297
C	2.885434	-2.774099	-1.408623	C	-0.764751	1.225728	2.483850
H	3.599253	-2.246004	-0.772790	H	-0.720837	2.318196	2.354746
C	3.335839	-3.499021	-2.508229	H	-1.374187	1.056579	3.385156
H	4.406523	-3.530103	-2.730550	C	0.646211	0.667055	2.617380
C	2.433280	-4.181958	-3.323451	H	0.638949	-0.353849	3.030306
H	2.782093	-4.751164	-4.187761	H	1.241344	1.271352	3.317834
C	1.074146	-4.133792	-3.009484	C	-3.108526	1.596468	0.806408
H	0.353753	-4.671878	-3.635340	C	-4.356539	1.027180	0.545372
C	0.600441	-3.419122	-1.908884	H	-4.487382	-0.056138	0.520388
C	-0.865332	-3.367345	-1.586431	C	-5.474044	1.842191	0.301288
H	-0.981484	-3.302660	-0.493976	C	-5.355156	3.235980	0.329394
H	-1.346007	-4.307125	-1.893732	H	-6.222876	3.868390	0.140083
C	-1.609396	-2.221058	-2.231148	C	-4.107369	3.807664	0.605766
C	-2.680652	-2.511084	-3.093616	C	-2.989914	2.990363	0.833335
H	-2.954057	-3.560289	-3.246383	H	-2.028706	3.474710	1.022844
C	-3.390971	-1.512294	-3.756724	C	-2.161552	-1.095697	1.381757
H	-4.218225	-1.776731	-4.419586	C	-2.674604	-1.914310	0.366789

H	-2.831421	-1.513404	-0.637171	H	-3.865239	-0.852466	-4.779492
C	-2.968458	-3.263071	0.613775	C	-3.347932	0.771522	-3.450777
C	-2.751773	-3.816812	1.881503	H	-4.125973	1.442764	-3.824616
H	-2.942745	-4.874182	2.065540	C	-2.489847	1.200634	-2.434474
C	-2.266395	-2.994429	2.904781	H	-2.618369	2.211049	-2.029786
C	-1.978174	-1.641641	2.657096	C	-1.494312	0.357113	-1.938229
H	-1.597867	-1.037952	3.482894	C	-0.159841	2.757164	-0.993386
C	2.885140	1.722706	0.949732	O	-0.256333	3.852315	-1.317004
C	3.699720	1.857495	2.076128	C	5.630195	2.859921	3.205113
H	3.496730	1.292696	2.989464	N	6.290105	2.971307	4.157904
C	4.807959	2.719202	2.044365	C	4.608363	4.003549	-1.449356
C	5.109966	3.435641	0.879434	N	4.860067	4.590566	-2.422563
H	5.971946	4.103075	0.854464	C	0.969781	-4.535083	1.356642
C	4.300204	3.283540	-0.252975	N	0.197751	-5.362498	1.633804
C	3.187188	2.427502	-0.219340	C	5.289157	-2.808654	-0.247925
H	2.574585	2.281433	-1.114777	N	6.377238	-2.972525	-0.628630
C	2.181610	-1.055783	0.836704	C	-3.453244	-4.075453	-0.458443
C	1.375498	-2.149305	1.159846	N	-3.838865	-4.718414	-1.349071
H	0.351492	-1.994818	1.511832	C	-2.028191	-3.534001	4.206806
C	1.851946	-3.460519	1.027153	N	-1.822663	-3.955234	5.272666
C	3.153536	-3.690157	0.564863	C	-6.741281	1.240875	0.025722
H	3.532347	-4.706851	0.458431	N	-7.772831	0.748922	-0.196085
C	3.959051	-2.595128	0.229892	C	-3.962564	5.228777	0.655999
C	3.471044	-1.282506	0.350863	N	-3.834790	6.384884	0.705836
H	4.119043	-0.450445	0.065951				
Ni	-0.130806	0.908853	-0.647190	<b>11-ts(L5)</b>			
O	1.360904	0.474543	-1.886829	P	1.541002	0.670012	0.842850
C	1.779579	-0.613726	-2.489287	P	-1.524942	0.508602	0.946375
C	3.053283	-0.593402	-3.110644	C	0.755092	0.700343	2.529419
H	3.624690	0.339166	-3.069806	H	0.820307	-0.307804	2.967865
C	3.562358	-1.710164	-3.762670	H	1.338463	1.352568	3.196061
H	4.550760	-1.655501	-4.228137	C	-0.693415	1.182997	2.445703
C	2.824633	-2.894638	-3.820714	H	-0.715769	2.276986	2.314610
H	3.219979	-3.775424	-4.331279	H	-1.242217	0.974045	3.377178
C	1.567342	-2.929556	-3.217297	C	2.228001	-1.015033	0.687208
H	0.972966	-3.849311	-3.255854	C	3.453358	-1.268841	0.060277
C	1.029460	-1.821613	-2.556399	H	4.098967	-0.447408	-0.259643
C	-0.321576	-1.893692	-1.905050	C	3.874129	-2.587938	-0.168650
H	-0.214167	-1.670082	-0.825070	C	3.066955	-3.672158	0.204531
H	-0.696077	-2.927547	-1.975014	H	3.391715	-4.694933	0.011430
C	-1.348288	-0.940420	-2.461841	C	1.833645	-3.418416	0.811622
C	-2.206013	-1.350503	-3.493112	C	1.422471	-2.098397	1.052526
H	-2.093835	-2.359943	-3.903147	H	0.449075	-1.937527	1.520130
C	-3.200858	-0.507239	-3.983812	C	3.042765	1.714849	0.946528

C	3.245669	2.659957	-0.061169	C	-3.322459	-0.218258	-3.808569
H	2.521683	2.754907	-0.876759	H	-4.221473	-0.509303	-4.355348
C	4.382364	3.486553	-0.039303	C	-2.917255	1.119610	-3.786324
C	5.316318	3.368682	0.996065	H	-3.498051	1.877749	-4.318051
H	6.197816	4.010555	1.017204	C	-1.779273	1.503694	-3.080084
C	5.112826	2.416888	2.004698	H	-1.456810	2.547484	-3.073090
C	3.979901	1.589375	1.976647	C	-1.089538	0.536518	-2.337624
H	3.846916	0.843921	2.765518	C	-0.398254	2.919105	-0.597756
C	-2.095078	-1.168300	1.449589	O	-0.691103	4.014331	-0.382730
C	-1.781564	-1.739072	2.689106	C	0.943774	-4.477801	1.168533
H	-1.278957	-1.162637	3.468672	N	0.168301	-5.296249	1.463342
C	-2.096335	-3.082232	2.960916	C	5.127995	-2.824020	-0.812308
C	-2.746753	-3.869413	2.005260	N	6.151135	-3.008847	-1.337516
H	-2.963878	-4.918066	2.207078	C	-3.742987	-4.063619	-0.234049
C	-3.092139	-3.290493	0.777104	N	-4.259477	-4.671847	-1.082116
C	-2.766780	-1.954619	0.504074	C	-1.716835	-3.649501	4.216983
H	-3.025471	-1.544682	-0.475780	N	-1.394469	-4.096266	5.242905
C	-3.112824	1.408867	0.810646	C	-5.792475	1.751546	-1.767905
C	-3.583661	2.280429	1.794970	N	-6.374985	1.602332	-2.765154
H	-3.033413	2.433799	2.725885	C	-5.259520	3.860150	2.626155
C	-4.790235	2.976285	1.605891	N	-5.632188	4.576899	3.464887
C	-5.534187	2.802539	0.433184	C	4.584252	4.448454	-1.076933
H	-6.469630	3.343632	0.288115	N	4.747402	5.228632	-1.925410
C	-5.058204	1.931374	-0.554362	C	6.062126	2.283319	3.064921
C	-3.849252	1.244454	-0.369185	N	6.826392	2.168304	3.935707
H	-3.488657	0.588179	-1.166615				
Ni	-0.101396	1.130000	-0.671415	<b>12(L5)</b>			
O	0.780350	0.728716	-2.409561	P	-1.566160	-0.103396	0.033229
C	1.454358	-0.400418	-2.669710	P	1.476432	-0.128442	0.010155
C	2.742762	-0.262451	-3.220762	C	-0.744617	-0.520223	-1.582927
H	3.127160	0.746185	-3.392113	H	-0.630992	-1.617195	-1.619032
C	3.493465	-1.386360	-3.546789	H	-1.364217	-0.233599	-2.447765
H	4.497157	-1.263599	-3.962730	C	0.617698	0.151341	-1.624369
C	2.967401	-2.665546	-3.353498	H	0.496760	1.238163	-1.763470
H	3.552505	-3.548539	-3.620087	H	1.225856	-0.207170	-2.469790
C	1.691244	-2.802754	-2.811208	C	-3.233714	-0.844871	-0.120037
H	1.266164	-3.800952	-2.661884	C	-4.215536	-0.440230	0.793549
C	0.923457	-1.692106	-2.448619	H	-3.990198	0.327142	1.539270
C	-0.449754	-1.834158	-1.858761	C	-5.493562	-1.013953	0.770374
H	-0.389979	-1.676845	-0.759225	C	-5.799930	-2.021027	-0.156156
H	-0.821971	-2.859146	-2.005996	H	-6.790657	-2.475500	-0.171561
C	-1.393001	-0.830690	-2.453152	C	-4.816422	-2.436188	-1.059104
C	-2.546054	-1.183556	-3.163284	C	-3.540715	-1.844500	-1.046762
H	-2.821189	-2.241915	-3.224705	H	-2.804354	-2.185890	-1.776478



C	-1.902996	1.692124	-0.183122	C	4.232785	-3.986041	-2.368934
C	-1.236835	2.565564	0.681143	N	4.984583	-4.287891	-3.205314
H	-0.592719	2.155101	1.471507				
C	-1.391062	3.955023	0.546900	<b>2(L6)</b>			
C	-2.230007	4.472683	-0.448136	Ni	-0.498404	-0.666556	0.432355
H	-2.357368	5.550740	-0.552114	P	0.323409	1.246844	0.046654
C	-2.906641	3.595489	-1.305907	P	1.476247	-1.498914	0.182501
C	-2.739318	2.206029	-1.176162	O	-1.086477	4.484750	-1.308465
H	-3.272719	1.537860	-1.857875	O	0.450204	4.006332	0.382270
C	2.057611	-1.859927	-0.206330	O	-1.309584	2.222489	-1.843254
C	2.952931	-2.248571	-1.206093	O	5.176289	3.091867	1.146803
H	3.390784	-1.510220	-1.883504	O	6.174506	0.698802	1.244269
C	3.308775	-3.599781	-1.348690	O	3.486098	-3.407356	0.467756
C	2.757530	-4.569600	-0.500016	O	2.654789	-4.800782	-1.209526
H	3.030359	-5.619286	-0.614389	O	0.923021	-3.320192	-1.714279
C	1.855442	-4.179021	0.496431	O	-3.018944	-0.058705	1.567531
C	1.515284	-2.824637	0.645417	C	-0.274281	2.850950	0.821190
H	0.818018	-2.512270	1.431903	C	-1.736794	2.996259	0.433922
C	3.006448	0.865220	-0.142077	H	-2.186211	3.843632	0.973243
C	2.968459	2.151515	-0.691305	H	-2.299144	2.087034	0.689659
H	2.047563	2.558438	-1.114747	C	-1.800701	3.286087	-1.057783
C	4.117413	2.957938	-0.709967	C	0.274957	4.318121	-0.985609
C	5.322633	2.488812	-0.175100	C	0.864836	3.252229	-1.896362
H	6.215968	3.113293	-0.191736	H	0.755517	3.587606	-2.939161
C	5.359879	1.206854	0.388081	H	1.937663	3.111087	-1.702760
C	4.209152	0.404723	0.408088	C	0.085719	1.968008	-1.686534
H	4.268587	-0.586784	0.863928	C	2.128590	1.152929	0.367430
Ni	-0.027479	-0.138622	1.572136	C	2.966381	2.255771	0.608422
C	0.097485	-0.297495	3.316381	H	2.541515	3.258820	0.587645
O	0.205895	-0.414285	4.463576	C	4.316572	2.087265	0.901708
C	4.051067	4.261584	-1.292592	C	4.691461	4.410271	1.063880
N	3.983703	5.319626	-1.774020	H	4.289857	4.639167	0.062529
C	6.578703	0.705930	0.942313	H	5.542356	5.071492	1.259604
N	7.568258	0.292616	1.395604	H	3.909061	4.612158	1.813556
C	-0.690242	4.836608	1.426448	C	4.863074	0.776908	0.959417
N	-0.109252	5.545063	2.144963	C	6.753617	-0.581174	1.333370
C	-3.766010	4.117411	-2.321884	H	6.292401	-1.186893	2.129899
N	-4.465213	4.533943	-3.154609	H	7.812433	-0.432298	1.570442
C	-6.488547	-0.574038	1.698069	H	6.681078	-1.133131	0.381592
N	-7.297298	-0.212467	2.453511	C	4.036010	-0.317926	0.724603
C	-5.109768	-3.461531	-2.010938	H	4.442010	-1.328639	0.781773
N	-5.341210	-4.295236	-2.790220	C	2.673054	-0.145954	0.428904
C	1.279987	-5.157834	1.364190	C	3.535902	-3.743600	-0.904399
N	0.801767	-5.951633	2.068947	C	1.319201	-4.426929	-0.929587

C	1.192235	-4.162932	0.564031	P	-0.181181	1.379542	-0.297442
H	0.161625	-3.873373	0.814801	P	1.432869	-1.126175	-0.621319
H	1.435353	-5.089389	1.104824	O	-1.700158	4.658700	-1.463641
C	2.178448	-3.062464	0.937538	O	-0.445593	4.080337	0.415429
C	1.757833	-2.173260	-1.560354	O	-1.565159	2.489939	-2.319697
C	3.205042	-2.559624	-1.799089	O	4.004795	3.462655	2.206390
H	3.884329	-1.716710	-1.607509	O	5.354325	1.252617	2.017172
H	3.340452	-2.867037	-2.847220	O	3.495884	-2.881516	0.006534
C	-4.300996	-0.435440	1.886282	O	3.396762	-4.021765	-2.026372
C	-4.552466	-1.225890	3.005163	O	1.715193	-2.615647	-2.831092
H	-3.710718	-1.572328	3.608144	O	-1.930595	-2.239853	0.067872
C	-5.869552	-1.554366	3.327325	C	-1.082153	2.803166	0.555830
H	-6.075344	-2.173362	4.204215	C	-2.461687	2.869905	-0.083945
C	-6.918744	-1.100376	2.529236	H	-3.106992	3.569057	0.469190
H	-7.949936	-1.360935	2.779007	H	-2.946972	1.886313	-0.089740
C	-6.652861	-0.308343	1.410643	C	-2.301133	3.376948	-1.509184
H	-7.476257	0.054857	0.788336	C	-0.408368	4.568503	-0.910738
C	-5.342375	0.038997	1.076875	C	0.453597	3.703626	-1.815695
C	-4.976736	0.915310	-0.085191	H	0.501944	4.179166	-2.807484
H	-4.427040	1.790577	0.307579	H	1.480311	3.630578	-1.429230
H	-5.888245	1.319977	-0.547664	C	-0.198151	2.338428	-1.928960
C	-4.150348	0.231685	-1.149106	C	1.545802	1.434326	0.335243
C	-4.533639	0.383689	-2.488750	C	2.120159	2.532527	0.999475
H	-5.405495	1.006027	-2.713776	H	1.544759	3.452372	1.099213
C	-3.854568	-0.243518	-3.528764	C	3.397120	2.458074	1.550557
H	-4.181429	-0.100722	-4.561707	C	3.320514	4.687124	2.318722
C	-2.771987	-1.073095	-3.234285	H	3.111838	5.133810	1.332090
H	-2.240218	-1.595960	-4.033428	H	3.975452	5.363436	2.878478
C	-2.376564	-1.240429	-1.915118	H	2.370526	4.582369	2.867629
H	-1.534298	-1.895611	-1.669070	C	4.137774	1.251573	1.443285
C	-3.030401	-0.579835	-0.856380	C	6.116601	0.072200	1.947740
C	-2.429949	-0.774988	0.490764	H	5.615179	-0.773532	2.446097
O	-1.868163	-1.904459	0.782026	H	7.060277	0.274625	2.465950
H	4.552805	-4.123608	-1.076559	H	6.341074	-0.212864	0.906128
H	0.684487	-5.261129	-1.256401	C	3.576947	0.166961	0.775783
H	1.402377	-1.435894	-2.295778	H	4.128315	-0.771077	0.712644
H	0.753573	5.297870	-1.126949	C	2.291587	0.245135	0.212869
H	0.339508	1.204628	-2.436655	C	3.999009	-2.966926	-1.313355
H	-2.828976	3.455739	-1.405482	C	2.000364	-3.808142	-2.135821
H	-0.138618	2.807585	1.911589	C	1.398057	-3.829191	-0.737819
H	2.270254	-2.944593	2.027017	H	0.311998	-3.660448	-0.786184
				H	1.581302	-4.816667	-0.288336
<b>3-ts(L6)</b>				C	2.074100	-2.738663	0.083524
Ni	-0.679196	-0.667844	-0.569471	C	2.309631	-1.449994	-2.261339

C	3.799313	-1.674952	-2.090858	O	5.307363	2.556552	1.242961
H	4.281644	-0.826106	-1.586462	O	6.001522	0.058245	1.161327
H	4.272084	-1.788951	-3.078365	O	2.899719	-3.588304	0.165008
C	-2.244020	-2.559724	1.346945	O	1.980331	-4.836760	-1.578519
C	-2.000417	-3.887666	1.731985	O	0.429377	-3.167663	-2.080172
H	-1.605390	-4.578336	0.983672	O	-2.000239	-1.920056	-0.233071
C	-2.263947	-4.308626	3.030798	C	-0.109370	2.853737	1.102870
H	-2.067847	-5.346668	3.311642	C	-1.535601	3.297175	0.845407
C	-2.781555	-3.411421	3.965656	H	-1.845535	4.029593	1.605324
H	-2.991423	-3.733237	4.988141	H	-2.230960	2.449716	0.881075
C	-3.032248	-2.096569	3.579963	C	-1.574886	3.963940	-0.519773
H	-3.438408	-1.383885	4.304416	C	0.618158	4.660371	-0.299337
C	-2.768297	-1.647197	2.282436	C	1.045455	3.811368	-1.487004
C	-3.033642	-0.230659	1.873831	H	0.943042	4.418682	-2.398905
H	-2.093613	0.192646	1.461243	H	2.097794	3.505524	-1.412286
H	-3.310491	0.368056	2.752942	C	0.115868	2.617113	-1.566108
C	-4.088361	-0.109608	0.813415	C	2.067903	1.082557	0.239618
C	-5.336278	0.453522	1.089812	C	3.033714	2.046386	0.586844
H	-5.559032	0.770184	2.113028	H	2.742370	3.090406	0.663369
C	-6.282618	0.640409	0.082863	C	4.342609	1.689223	0.892595
H	-7.249179	1.091176	0.321419	C	4.970507	3.920305	1.332255
C	-5.988339	0.264592	-1.228263	H	4.646619	4.329935	0.360626
H	-6.723560	0.413855	-2.022539	H	5.876640	4.448388	1.647662
C	-4.756130	-0.309328	-1.520694	H	4.178041	4.102851	2.076317
H	-4.500882	-0.610521	-2.539039	C	4.721385	0.321639	0.857562
C	-3.807042	-0.514673	-0.508140	C	6.419590	-1.287227	1.156108
C	-2.500460	-1.053600	-0.905502	H	5.873188	-1.890499	1.898700
O	-2.124907	-1.346147	-2.046701	H	7.483098	-1.285789	1.417225
H	1.609040	-4.617510	-2.766304	H	6.301609	-1.751956	0.163340
H	5.061507	-3.226473	-1.204757	C	3.767897	-0.637052	0.531392
H	2.093939	-0.625954	-2.957079	H	4.039781	-1.692470	0.529688
H	0.271515	1.719579	-2.707553	C	2.445442	-0.274576	0.220800
H	-0.028619	5.597196	-0.832468	C	2.952664	-3.887318	-1.220307
H	-1.135431	2.615110	1.639341	C	0.680562	-4.327837	-1.321497
H	1.818607	-2.805479	1.151650	C	0.541038	-4.100757	0.175817
H	-3.270071	3.502277	-2.012458	H	-0.460265	-3.712402	0.404846
				H	0.674320	-5.064755	0.688251
				C	1.623289	-3.125390	0.614455
<b>4(L6)</b>				C	1.363917	-2.119325	-1.866787
Ni	-0.838153	-0.378656	-0.194216	C	2.772636	-2.643730	-2.078776
P	0.299392	1.448241	-0.091234	H	3.531913	-1.884858	-1.841988
P	1.117985	-1.471916	-0.106671	H	2.903152	-2.928431	-3.133731
O	-0.708959	5.080668	-0.500245	C	-2.831936	-2.341187	0.682700
O	0.763697	3.973356	0.931635	C	-3.194114	-3.713883	0.704334
O	-1.238421	3.068849	-1.560776				

H	-2.779308	-4.356497	-0.077960	C	-1.409502	3.686469	0.536885
C	-4.058365	-4.227834	1.661589	H	-1.706834	4.494014	1.221786
H	-4.313796	-5.291645	1.638583	H	-2.200114	2.924680	0.541808
C	-4.599707	-3.399414	2.648851	C	-1.244081	4.270021	-0.857834
H	-5.273301	-3.799542	3.409998	C	0.994400	4.705045	-0.459015
C	-4.271630	-2.044763	2.634567	C	1.408281	3.715751	-1.538881
H	-4.700549	-1.376916	3.390571	H	1.491621	4.258481	-2.492542
C	-3.410223	-1.499215	1.678162	H	2.390853	3.274576	-1.319914
C	-3.142066	-0.021713	1.645919	C	0.327676	2.657177	-1.646831
H	-2.060182	0.167428	1.468532	C	1.914984	0.993333	0.270478
H	-3.378849	0.412816	2.629179	C	2.938922	1.780803	0.825244
C	-3.959892	0.690174	0.596411	H	2.744268	2.830145	1.042136
C	-5.212505	1.208614	0.952995	C	4.182241	1.236328	1.129974
H	-5.554307	1.094082	1.986229	C	5.005777	3.286919	1.957208
C	-6.021206	1.863273	0.029620	H	4.775872	3.872447	1.051321
H	-6.989431	2.261577	0.343683	H	5.944911	3.656239	2.382462
C	-5.595185	2.013401	-1.292271	H	4.199974	3.439638	2.693050
H	-6.226081	2.526735	-2.022088	C	4.422919	-0.142081	0.878369
C	-4.362343	1.500801	-1.668871	C	5.922441	-1.959049	0.986237
H	-3.993147	1.606268	-2.692018	H	5.257888	-2.615331	1.570706
C	-3.539277	0.837817	-0.742536	H	6.955066	-2.124139	1.311017
C	-2.216572	0.384268	-1.235164	H	5.842332	-2.226788	-0.080466
O	-1.934391	0.304716	-2.411647	C	3.408234	-0.923527	0.334883
H	3.931911	-4.362032	-1.376272	H	3.571901	-1.989712	0.182778
H	-0.028792	-5.079877	-1.691614	C	2.152568	-0.371506	0.025445
H	1.696008	-3.051194	1.709295	C	2.272347	-3.947292	-1.642911
H	1.225999	5.570477	-0.196776	C	-0.025147	-4.049999	-1.928551
H	0.238419	2.043440	-2.496154	C	-0.245064	-3.888418	-0.432054
H	-2.575301	4.341453	-0.770562	H	-1.215942	-3.427175	-0.209770
H	0.043201	2.505700	2.135308	H	-0.239681	-4.886727	0.030600
H	1.103791	-1.321171	-2.577458	C	0.904351	-3.064147	0.118364
				C	1.035983	-1.938997	-2.328122
				C	2.357071	-2.672371	-2.466428
<b>5-ts(L6)</b>				H	3.201253	-2.044337	-2.147022
P	0.230204	1.592924	-0.090484	H	2.523211	-2.945233	-3.519338
P	0.734219	-1.339133	-0.576400	Ni	-1.101768	-0.220910	-0.169034
O	-0.245264	5.270706	-0.814125	O	-0.912429	-0.906425	1.830647
O	0.941531	4.106165	0.823370	C	-1.945548	-1.630534	2.159513
O	-0.938489	3.285199	-1.824338	C	-1.826237	-2.995268	2.539547
O	5.203083	1.923002	1.667238	H	-0.821670	-3.427093	2.595475
O	5.642484	-0.596317	1.207128	C	-2.940745	-3.781767	2.813630
O	2.144758	-3.673683	-0.258717	H	-2.801430	-4.834532	3.081101
O	1.203607	-4.723974	-2.125202	C	-4.229387	-3.245937	2.749233
O	-0.047209	-2.817757	-2.629178	H	-5.104950	-3.864404	2.959404
C	-0.071973	3.106962	0.971538				

C	-4.371424	-1.892517	2.436247	C	-0.038019	3.662914	-1.824411
H	-5.371175	-1.442411	2.419201	H	0.077686	4.143788	-2.807220
C	-3.269869	-1.083152	2.160983	H	0.943068	3.665893	-1.329426
C	-3.424678	0.395319	1.936083	C	-0.571210	2.253235	-2.002401
H	-2.467852	0.866586	2.231224	C	1.001383	1.590758	0.422122
H	-4.196736	0.792353	2.612891	C	1.361870	2.696602	1.210467
C	-3.736551	0.872642	0.544014	H	0.642699	3.498803	1.367874
C	-4.791891	1.770995	0.339196	C	2.623994	2.783296	1.791992
H	-5.425576	2.036720	1.191416	C	2.133700	4.851337	2.819241
C	-5.036566	2.344083	-0.908593	H	1.829220	5.369145	1.894751
H	-5.873316	3.036440	-1.032588	H	2.657071	5.564496	3.464705
C	-4.214864	2.035304	-1.991694	H	1.231072	4.497059	3.342314
H	-4.390909	2.485186	-2.971770	C	3.570242	1.743148	1.580914
C	-3.165158	1.139855	-1.813679	C	5.732322	0.898924	1.995586
H	-2.528824	0.872530	-2.662632	H	5.404626	-0.072127	2.400457
C	-2.916541	0.555129	-0.563663	H	6.625267	1.223404	2.540017
C	-2.353898	-1.180980	-0.878577	H	5.994309	0.771634	0.932047
O	-3.057474	-2.008177	-1.310110	C	3.215445	0.648366	0.798550
H	1.705157	5.537410	-0.361639	H	3.918993	-0.172732	0.659192
H	-0.065058	2.819394	2.033260	C	1.937068	0.561192	0.220870
H	-2.162238	4.754998	-1.214839	C	4.102043	-2.211284	-1.620538
H	0.472510	2.006139	-2.522114	C	2.229796	-3.366926	-2.354654
H	3.177593	-4.563449	-1.735363	C	1.751568	-3.560821	-0.922774
H	-0.802905	-4.664521	-2.399995	H	0.657801	-3.646049	-0.858752
H	0.952017	-1.097628	-3.031819	H	2.183944	-4.494834	-0.534971
H	0.900723	-3.003366	1.215291	C	2.249236	-2.382945	-0.106002
				C	2.134603	-0.969963	-2.402247
				C	3.649405	-0.944649	-2.328063
<b>6(L6)</b>				H	4.011882	-0.047823	-1.804865
P	-0.634144	1.331396	-0.355893	H	4.073659	-0.935754	-3.343108
P	1.338455	-0.873716	-0.710238	Ni	-0.906620	-0.905679	-0.555960
O	-2.273808	4.454162	-1.733229	O	-0.260445	-1.704687	1.248801
O	-1.221169	3.939432	0.288708	C	-0.968125	-2.426043	2.074422
O	-1.890673	2.291469	-2.536779	C	-0.563523	-3.725844	2.469603
O	3.037475	3.801830	2.561636	H	0.350476	-4.139754	2.031399
O	4.760412	1.901384	2.179911	C	-1.295268	-4.460906	3.397243
O	3.663559	-2.244116	-0.274781	H	-0.951503	-5.459567	3.685086
O	3.642599	-3.326543	-2.347081	C	-2.461525	-3.938309	3.961046
O	1.690274	-2.205238	-2.964359	H	-3.035923	-4.515623	4.689522
C	-1.795776	2.630257	0.359865	C	-2.878852	-2.660273	3.581706
C	-3.088548	2.628011	-0.438360	H	-3.789172	-2.234468	4.020108
H	-3.802211	3.318391	0.034191	C	-2.154707	-1.901414	2.664441
H	-3.550853	1.636160	-0.478742	C	-2.582481	-0.532563	2.227506
C	-2.783363	3.138389	-1.835149	H	-1.673047	0.071120	2.057508
C	-1.059864	4.451230	-1.023447				

H	-3.164527	-0.043134	3.023197	C	0.773619	2.766204	1.368433
C	-3.408526	-0.563324	0.964239	H	-0.082767	3.411777	1.559190
C	-4.798885	-0.397703	1.078623	C	1.984912	3.019258	2.008479
H	-5.225811	-0.254184	2.077386	C	1.093987	4.826016	3.234097
C	-5.635883	-0.396022	-0.034066	H	0.700530	5.376844	2.364512
H	-6.713556	-0.261149	0.088875	H	1.459903	5.548445	3.971012
C	-5.080349	-0.559221	-1.300621	H	0.275843	4.241847	3.684677
H	-5.714024	-0.553498	-2.191792	C	3.111400	2.191999	1.741805
C	-3.701238	-0.730723	-1.431429	C	5.384253	1.727159	2.163174
H	-3.290708	-0.824810	-2.440837	H	5.232642	0.677730	2.462243
C	-2.849674	-0.749373	-0.316619	H	6.186525	2.154503	2.773675
C	-1.178388	-2.052105	-1.892924	H	5.691610	1.755889	1.104756
O	-1.424479	-2.818756	-2.716843	C	2.981035	1.122894	0.861560
H	-1.965529	2.429975	1.428392	H	3.824582	0.455647	0.685071
H	-0.767409	5.502028	-0.889867	C	1.750488	0.853876	0.238493
H	-3.683386	3.196332	-2.461363	C	4.396088	-1.362921	-1.690227
H	0.029132	1.673299	-2.718753	C	2.781141	-2.728702	-2.634749
H	2.061000	-2.493332	0.968500	C	2.266758	-3.133181	-1.263387
H	1.740176	-0.180159	-3.058457	H	1.193166	-3.365154	-1.284451
H	5.196457	-2.295292	-1.574574	H	2.807698	-4.033223	-0.936325
H	1.939024	-4.198394	-3.010223	C	2.542624	-1.988904	-0.301575
				C	2.276973	-0.395134	-2.467730
				C	3.761616	-0.125340	-2.305142
				H	3.947709	0.765633	-1.688515
				H	4.216703	0.049076	-3.291485
				Ni	-0.802963	-1.038350	-0.699682
				O	-0.149416	-2.412311	0.632325
				C	-2.675979	-1.286541	-0.234925
				C	-3.675776	-1.551215	-1.180042
				H	-3.433428	-1.622054	-2.243798
				C	-5.011049	-1.704040	-0.801332
				H	-5.769600	-1.906904	-1.562556
				C	-5.366711	-1.592299	0.540411
				H	-6.408742	-1.704845	0.850451
				C	-4.378119	-1.337329	1.487247
				H	-4.647813	-1.258969	2.546407
				C	-3.031285	-1.177815	1.124705
				C	-2.015849	-0.943224	2.218758
				H	-1.222838	-0.265246	1.855928
				H	-2.502300	-0.443078	3.070186
				C	-1.382839	-2.220923	2.683014
				C	-1.675802	-2.773535	3.929803
				H	-2.365518	-2.234977	4.590442
				C	-1.110397	-3.977237	4.355178
<b>10(L6)</b>							
P	-0.903698	1.168452	-0.348334				
P	1.418378	-0.589971	-0.808461				
O	-3.059410	3.950303	-1.714018				
O	-1.965168	3.609283	0.323462				
O	-2.257774	1.915533	-2.542006				
O	2.189459	4.009717	2.889141				
O	4.237510	2.512054	2.396781				
O	3.919148	-1.605121	-0.379208				
O	4.164563	-2.459102	-2.539922				
O	2.078492	-1.618685	-3.170587				
C	-2.290590	2.215801	0.362535				
C	-3.542354	1.980631	-0.467080				
H	-4.387316	2.510132	-0.003407				
H	-3.799396	0.917137	-0.530293				
C	-3.308646	2.566019	-1.849473				
C	-1.879873	4.165049	-0.977754				
C	-0.710766	3.599006	-1.765144				
H	-0.663979	4.111436	-2.737697				
H	0.241121	3.774275	-1.243975				
C	-0.966504	2.117833	-1.974360				
C	0.641721	1.683453	0.483186				

H	-1.348084	-4.386170	5.339924	H	-1.270584	6.279981	2.719637
C	-0.237539	-4.644219	3.492426	H	-1.839662	4.588315	2.746630
H	0.216322	-5.591788	3.799595	C	1.714531	3.474103	1.226091
C	0.061636	-4.120656	2.239982	C	3.957469	4.032068	1.690253
H	0.739456	-4.649156	1.562407	H	4.201790	3.080735	2.190258
C	-0.491355	-2.890967	1.793967	H	4.492315	4.842691	2.196714
C	-0.966590	-1.483572	-2.456178	H	4.302348	3.981125	0.644156
O	-1.092044	-1.522658	-3.600481	C	2.069976	2.305472	0.558284
H	-1.795718	5.249532	-0.823795	H	3.121949	2.034516	0.462632
H	-4.189208	2.465817	-2.497006	C	1.090705	1.448842	0.026557
H	-2.442841	1.968775	1.424201	C	4.416250	0.476884	-1.822701
H	-0.249623	1.673872	-2.682961	C	3.612988	-1.588462	-2.497980
H	1.777859	0.385177	-3.062950	C	3.377787	-2.003872	-1.052859
H	2.665834	-3.528987	-3.377492	H	2.531451	-2.703485	-0.988638
H	5.485997	-1.265976	-1.591391	H	4.278064	-2.513833	-0.678752
H	2.344191	-2.257210	0.743631	C	3.111806	-0.746531	-0.235857
				C	2.067660	0.224851	-2.514284
				C	3.246627	1.180343	-2.495236
<b>11-ts(L6)</b>				H	2.997927	2.116908	-1.976308
P	-1.457391	0.517036	-0.423075	H	3.537932	1.433711	-3.525737
P	1.422502	-0.150230	-0.781724	Ni	-0.448771	-1.424269	-0.622123
O	-4.842990	1.677760	-1.621807	O	0.139614	-2.980121	0.513451
O	-3.564985	2.193071	0.262263	C	-1.598225	-2.476612	0.691984
O	-3.185541	0.260937	-2.459863	C	-2.479438	-3.443294	0.180538
O	0.078565	4.958134	2.010919	H	-2.264285	-3.926366	-0.775881
O	2.585885	4.335890	1.777826	C	-3.645615	-3.741136	0.881012
O	4.158735	0.202554	-0.459087	H	-4.353071	-4.457757	0.454187
O	4.711188	-0.698962	-2.538947	C	-3.911980	-3.139307	2.114140
O	2.465664	-1.017935	-3.090962	H	-4.825693	-3.377498	2.662831
C	-3.101883	0.846319	0.418230	C	-2.970325	-2.262480	2.660030
C	-4.098869	-0.106821	-0.224876	H	-3.139766	-1.823730	3.649307
H	-5.052589	-0.077811	0.322403	C	-1.790918	-1.945002	1.984671
H	-3.730680	-1.142310	-0.210809	C	-0.707515	-1.100613	2.588192
C	-4.342361	0.353578	-1.653983	H	-0.599243	-0.148662	2.027729
C	-3.884710	2.548322	-1.070412	H	-0.978551	-0.808126	3.613860
C	-2.660082	2.560287	-1.970531	C	0.602290	-1.842367	2.611891
H	-2.964920	2.915302	-2.966722	C	1.520785	-1.677132	3.654969
H	-1.895360	3.250925	-1.587467	H	1.287027	-0.953286	4.442454
C	-2.132227	1.141035	-2.068903	C	2.703786	-2.410572	3.721900
C	-0.271690	1.776668	0.170137	H	3.404448	-2.252066	4.544567
C	-0.629886	2.966542	0.828426	C	2.965879	-3.370220	2.740936
H	-1.685425	3.215322	0.939735	H	3.873729	-3.977461	2.790632
C	0.340283	3.813338	1.357166	C	2.070121	-3.561861	1.696691
C	-1.269056	5.333342	2.168789	H	2.252773	-4.310141	0.922032
H	-1.770483	5.487444	1.198712				

C	0.907704	-2.775134	1.593109	H	-2.957718	5.687870	-0.568332
C	-0.781621	-2.009716	-2.314217	H	-3.082725	4.226119	0.449015
O	-0.990518	-2.102075	-3.446768	C	-1.386094	2.157093	-0.319274
H	5.330059	1.087644	-1.831047	H	-2.476143	2.155355	-0.326777
H	1.241307	0.599328	-3.137363	C	-0.701898	0.933491	-0.209903
H	3.878413	-2.442420	-3.135161	C	-4.348622	0.275673	1.088413
H	3.109134	-0.945897	0.846198	C	-4.198755	-2.021554	0.822158
H	-3.014214	0.679780	1.502832	C	-3.916307	-1.857275	-0.664567
H	-4.359661	3.537174	-1.001168	H	-3.279779	-2.675404	-1.030861
H	-1.351884	1.044245	-2.839391	H	-4.871241	-1.887328	-1.209516
H	-5.102083	-0.256043	-2.160763	C	-3.232285	-0.512627	-0.869156
				C	-2.243313	-0.896770	1.591772
				C	-3.121258	0.276216	1.985259
<b>12(L6)</b>				H	-2.579024	1.229680	1.911687
P	1.508898	-0.719963	-0.143087	H	-3.453522	0.160210	3.028425
P	-1.509851	-0.711957	-0.143727	Ni	-0.003057	-2.052336	-0.890349
O	5.007218	-0.964658	1.280785	C	-0.002057	-3.084793	-2.288864
O	4.028063	0.498622	-0.248769	O	0.000414	-3.706600	-3.275027
O	2.996280	-2.098551	1.621423	H	-4.751826	-2.945748	1.038155
O	1.309839	4.557113	-0.590799	H	-5.065174	1.062438	1.363778
O	-1.281041	4.568346	-0.547134	H	-3.155741	-0.247420	-1.933972
O	-4.022613	0.518223	-0.263573	H	3.173517	-0.276292	-1.921279
O	-5.022835	-0.952996	1.244870	H	1.403878	-1.047816	2.315631
O	-3.019241	-2.097689	1.595451	H	5.056858	1.051448	1.384534
C	3.238382	-0.533252	-0.853637	H	4.730304	-2.957744	1.086637
C	3.914664	-1.879241	-0.632072	H	-1.429809	-1.058844	2.313727
H	4.874557	-1.917819	-1.167787				
H	3.277960	-2.697498	-0.997825	<b>2(L7)</b>			
C	4.182746	-2.033124	0.858504	P	1.798625	0.778737	1.370153
C	4.339789	0.265490	1.108299	P	3.245029	-1.016066	-0.679106
C	3.103614	0.278446	1.992855	C	3.568528	0.346399	1.722774
H	3.424800	0.170495	3.040325	H	4.070995	1.136301	2.305705
H	2.566153	1.233381	1.905090	H	3.548222	-0.547572	2.369135
C	2.225082	-0.894552	1.600527	C	1.861595	2.590881	1.106930
C	0.709838	0.928710	-0.221210	C	3.682494	-2.707938	-0.129543
C	1.401405	2.146087	-0.350009	C	4.128621	-0.913926	-2.276440
H	2.491183	2.135211	-0.375519	C	1.014018	0.668178	3.014708
C	0.721259	3.354976	-0.461009	C	4.298209	0.048024	0.421837
C	2.715483	4.602460	-0.630930	H	5.284241	-0.413570	0.597903
H	3.168239	4.217167	0.298189	H	4.490932	0.981761	-0.133784
H	2.993309	5.656047	-0.743711	Ni	1.187433	-0.408581	-0.274547
H	3.124028	4.036068	-1.483484	O	-1.366292	-1.109190	0.599266
C	-0.698721	3.360847	-0.440252	C	-2.689530	-1.395194	0.395138
C	-2.685582	4.629067	-0.497972	C	-3.098372	-2.665325	-0.005585
H	-3.155065	4.087941	-1.335545				



H	-2.340937	-3.429030	-0.193731	C	-3.989845	1.849375	-1.477931
C	-4.460017	-2.928447	-0.157530	C	-0.720468	-2.280557	2.148021
H	-4.788156	-3.922318	-0.472750	C	-4.011080	-0.197329	0.512503
C	-5.398773	-1.926236	0.085308	H	-4.902513	0.232805	0.999815
H	-6.464923	-2.132788	-0.035825	H	-4.380619	-0.772138	-0.353848
C	-4.977253	-0.656430	0.486000	Ni	-0.993827	0.146482	-0.469653
H	-5.713494	0.130300	0.676731	O	0.769150	1.167246	-1.082185
C	-3.619791	-0.376397	0.647688	C	1.712439	1.834664	-0.366273
C	-3.069352	0.955727	1.065011	C	2.137944	3.069008	-0.874973
H	-2.429350	0.802283	1.952932	H	1.718613	3.409839	-1.824099
H	-3.884439	1.621344	1.382542	C	3.070274	3.833311	-0.180193
C	-2.273245	1.631847	-0.026721	H	3.393489	4.794167	-0.589011
C	-2.588753	2.954313	-0.367358	C	3.593471	3.372183	1.028995
H	-3.383061	3.459882	0.190879	H	4.325992	3.967531	1.578809
C	-1.939060	3.629859	-1.397163	C	3.174166	2.141469	1.528848
H	-2.211779	4.660877	-1.635425	H	3.577414	1.769056	2.475843
C	-0.955961	2.964978	-2.131234	C	2.233884	1.360617	0.851793
H	-0.447658	3.468300	-2.957922	C	1.780423	0.029398	1.361129
C	-0.627788	1.655036	-1.810558	H	0.668058	0.019483	1.346585
H	0.140095	1.121919	-2.377878	H	2.115330	-0.122495	2.396895
C	-1.254223	0.967779	-0.752093	C	2.261946	-1.083772	0.478966
C	-0.718475	-0.385915	-0.445858	C	3.243492	-1.981891	0.903547
O	-0.175785	-1.095242	-1.386052	H	3.668281	-1.867498	1.905527
H	3.160193	-3.446514	-0.753771	C	3.676071	-3.020650	0.079438
H	3.346670	-2.868671	0.904391	H	4.441321	-3.715173	0.434947
H	4.764793	-2.902007	-0.183711	C	3.125563	-3.172380	-1.193647
H	3.691171	-1.627415	-2.988581	H	3.459233	-3.984462	-1.844544
H	4.014324	0.089391	-2.709520	C	2.150927	-2.283449	-1.635186
H	5.202576	-1.133606	-2.175967	H	1.701270	-2.384667	-2.626003
H	2.379150	2.822668	0.165258	C	1.718004	-1.230595	-0.815422
H	0.841895	2.992336	1.018017	C	0.608914	-0.392580	-1.304657
H	2.370945	3.116089	1.929576	O	-0.034227	-0.558452	-2.355155
H	-0.005151	1.076298	2.961353	H	-0.989318	-3.398980	-0.700543
H	1.570968	1.219670	3.787813	H	-2.440915	-3.791929	0.264035
H	0.928209	-0.383558	3.320647	H	-2.550387	-2.719137	-1.164939
				H	-1.297673	-3.116997	2.572685
				H	0.261890	-2.667841	1.837933
				H	-0.553176	-1.538473	2.941365
				H	-2.508259	2.082227	2.031596
				H	-2.474037	3.330201	0.781706
				H	-4.044981	2.708070	1.362828
				H	-4.989635	2.114172	-1.100252
				H	-4.102745	1.134841	-2.304657
				H	-3.523711	2.754541	-1.891475
<b>3-ts(L7)</b>							
P	-1.574664	-1.514807	0.719064				
P	-2.917944	1.135282	-0.177897				
C	-3.229144	-1.100648	1.452454				
H	-3.791364	-2.014466	1.709191				
H	-3.029388	-0.584837	2.407359				
C	-1.930921	-2.995607	-0.300359				
C	-3.008603	2.429964	1.116905				

				H	-2.649517	-2.686147	-1.721530
				H	-3.779790	-1.331391	-1.579290
<b>4(L7)</b>				H	-4.081384	-2.832789	-0.649261
P	-2.268332	-1.473007	0.313440	H	-1.247785	1.957642	2.400657
P	-2.069105	1.578090	0.132217	H	-0.562935	3.119308	1.248292
C	-3.427898	-0.492801	1.364749	H	-2.233890	3.336746	1.840143
H	-4.366081	-1.044006	1.541196	H	-1.646039	3.374191	-1.420576
H	-2.942235	-0.382994	2.349402	H	-3.262259	3.565774	-0.685299
C	-3.303746	-2.148806	-1.020668	H	-2.984327	2.357537	-1.976529
C	-1.484497	2.591105	1.534352				
C	-2.545625	2.836174	-1.090693				
C	-1.857476	-2.933667	1.314662	<b>5-ts(L7)</b>			
C	-3.672418	0.867715	0.726802	P	-1.912333	0.957161	-1.138624
H	-4.191632	1.556906	1.412066	P	-2.038907	-1.456003	0.807072
H	-4.324992	0.765150	-0.156322	C	-3.367384	-0.177422	-1.252811
Ni	-0.760079	-0.181701	-0.455775	H	-4.257508	0.345036	-1.639502
O	0.541839	0.867560	-1.408641	H	-3.102808	-0.941216	-2.003520
C	1.358370	1.682006	-0.799748	C	-2.614161	2.568275	-0.657427
C	1.790398	2.867393	-1.449120	C	-1.849645	-3.114459	0.088123
H	1.419439	3.049412	-2.461911	C	-2.426623	-1.785257	2.552093
C	2.653526	3.765040	-0.833703	C	-1.406682	1.201170	-2.865795
H	2.961653	4.667415	-1.370968	C	-3.626844	-0.826191	0.097716
C	3.123899	3.527443	0.460759	H	-4.374120	-1.634459	0.034234
H	3.798040	4.233328	0.951277	H	-4.026209	-0.088224	0.813960
C	2.719826	2.362608	1.114392	Ni	-0.452073	-0.071532	0.228510
H	3.087368	2.156605	2.126491	O	0.342416	-1.166643	-1.372779
C	1.853933	1.440545	0.519873	C	1.545282	-1.528276	-1.016931
C	1.467369	0.175269	1.238066	C	1.885654	-2.879980	-0.747333
H	0.364028	0.031930	1.213237	H	1.113267	-3.641576	-0.892272
H	1.729248	0.279428	2.302720	C	3.151795	-3.237608	-0.293467
C	2.154359	-1.058471	0.699860	H	3.367763	-4.289655	-0.079013
C	3.421795	-1.366843	1.214981	C	4.145919	-2.274033	-0.107298
H	3.843945	-0.717131	1.987967	H	5.138823	-2.556005	0.250993
C	4.148768	-2.465107	0.770393	C	3.848879	-0.941937	-0.407618
H	5.132009	-2.676459	1.198646	H	4.624363	-0.175234	-0.293479
C	3.618060	-3.293272	-0.220874	C	2.588381	-0.557677	-0.861665
H	4.181965	-4.157682	-0.580527	C	2.288779	0.863399	-1.251160
C	2.368818	-3.001657	-0.747881	H	1.505616	0.821276	-2.030902
H	1.927527	-3.623420	-1.531152	H	3.174843	1.319129	-1.719452
C	1.623062	-1.893648	-0.307354	C	1.791756	1.804465	-0.184385
C	0.279207	-1.688428	-0.949469	C	2.279976	3.119291	-0.148837
O	-0.078986	-2.415965	-1.860712	H	3.062457	3.405751	-0.858832
H	-1.183506	-2.657144	2.137508	C	1.792717	4.063618	0.752762
H	-1.331525	-3.665957	0.686121	H	2.205841	5.075678	0.754841
H	-2.754748	-3.413214	1.733054	C	0.788019	3.712891	1.654069

H	0.403161	4.442511	2.370866	H	1.665658	0.436006	-2.117914
C	0.290475	2.414019	1.639329	H	3.389969	0.639099	-1.786640
H	-0.478848	2.119839	2.361066	C	2.111553	1.419874	-0.278236
C	0.770057	1.458388	0.728500	C	3.037749	2.458892	-0.084899
C	0.662313	-0.196950	1.537512	H	3.956906	2.451025	-0.680704
O	1.317604	-0.508339	2.456817	C	2.824682	3.486654	0.830998
H	-1.809039	3.316641	-0.617359	H	3.572049	4.274554	0.954761
H	-3.057064	2.509748	0.346821	C	1.654933	3.492281	1.585450
H	-3.380548	2.919408	-1.364309	H	1.466538	4.282756	2.317294
H	-2.256340	1.444343	-3.521024	C	0.724492	2.466209	1.408551
H	-0.676108	2.019924	-2.925904	H	-0.188068	2.476488	2.015859
H	-0.915152	0.283748	-3.216805	C	0.926764	1.428329	0.486805
H	-1.558229	-2.249294	3.040502	C	0.023365	-0.395695	2.032517
H	-3.289929	-2.458078	2.664185	O	0.337291	-0.643648	3.115091
H	-2.639611	-0.846031	3.080705	H	-1.680590	-3.456403	0.404036
H	-2.756114	-3.725648	0.211534	H	-1.808362	-2.757745	-1.218205
H	-1.009322	-3.624274	0.578928	H	-3.299032	-3.270417	-0.330177
H	-1.594647	-3.022327	-0.975840	H	-2.609660	-2.059562	2.712408
				H	-4.416081	-0.970711	-0.903171
<b>6(L7)</b>				H	-3.352309	-0.453166	2.593895
P	-1.505732	1.389607	-1.031850	H	-4.207228	-1.881186	1.944523
P	-2.388604	-1.156149	0.474992	H	0.249303	2.523785	-2.258367
C	-2.951372	0.451529	-1.690422	H	-0.248633	0.999515	-3.040499
H	-3.636333	1.110739	-2.247774	H	-1.265743	2.464907	-3.201979
H	-2.539261	-0.270442	-2.415011	H	-1.403860	3.614730	-0.089554
C	-2.215076	2.941796	-0.400496	H	-2.845234	2.754010	0.479725
C	-2.300657	-2.818163	-0.239684	H	-2.816763	3.454324	-1.165749
C	-3.221268	-1.410163	2.070790				
C	-0.612959	1.896508	-2.523346	<b>10(L7)</b>			
C	-3.644903	-0.267830	-0.549539	P	-1.943849	0.830058	-0.953328
H	-4.157364	0.449547	0.112866	P	-1.573861	-2.043089	-0.069209
Ni	-0.476177	0.037400	0.406129	C	-2.892011	-0.475160	-1.870506
O	0.119794	-1.199292	-1.191694	H	-3.827708	-0.057450	-2.276608
C	1.242272	-1.784004	-0.860667	H	-2.274772	-0.753940	-2.741036
C	1.313640	-3.156445	-0.506030	C	-3.243112	1.836160	-0.168359
H	0.393386	-3.746668	-0.535594	C	-0.534175	-2.956523	-1.241646
C	2.515156	-3.755253	-0.135971	C	-1.981068	-3.269743	1.199500
H	2.526063	-4.816064	0.135248	C	-1.358821	1.923972	-2.281957
C	3.700999	-3.018872	-0.109664	C	-3.134973	-1.679401	-0.975970
H	4.644439	-3.486130	0.182563	H	-3.495301	-2.553615	-1.541651
C	3.659664	-1.671975	-0.482380	H	-3.904123	-1.457815	-0.217077
H	4.585191	-1.083960	-0.491120	Ni	-0.646790	-0.091064	0.527541
C	2.469697	-1.052361	-0.859894	O	1.000076	-1.225432	0.802461
C	2.427328	0.374592	-1.323320	C	2.229752	-1.221568	0.380721

C	3.175792	-2.100893	0.973895	C	0.703349	-2.896946	-1.053567
H	2.826048	-2.738275	1.791424	C	-0.945904	-3.719557	1.098941
C	4.497046	-2.155412	0.546556	C	-1.929943	1.700024	-2.130639
H	5.190343	-2.847932	1.034722	C	-2.126228	-2.428244	-1.169395
C	4.945298	-1.335774	-0.492550	H	-2.054808	-3.338151	-1.788116
H	5.983340	-1.373541	-0.830799	H	-3.021899	-2.556520	-0.537788
C	4.032779	-0.463843	-1.090276	Ni	-0.680209	-0.110371	0.689073
H	4.363045	0.187846	-1.907992	O	1.198069	0.284074	1.303354
C	2.698661	-0.394607	-0.685784	C	2.264600	-0.176783	0.633565
C	1.738431	0.566380	-1.326947	C	3.202441	-0.927256	1.365704
H	0.813228	0.022853	-1.595227	H	3.017134	-1.085164	2.430604
H	2.175349	0.951288	-2.261852	C	4.326380	-1.457044	0.741522
C	1.366648	1.718055	-0.424110	H	5.037893	-2.046932	1.325598
C	2.125281	2.896663	-0.455627	C	4.549111	-1.230565	-0.618798
H	2.972245	2.962015	-1.147606	H	5.432794	-1.640862	-1.112479
C	1.819341	3.978501	0.367789	C	3.633861	-0.463889	-1.337817
H	2.418422	4.891423	0.319692	H	3.805908	-0.267977	-2.401262
C	0.746979	3.884197	1.252732	C	2.487082	0.067369	-0.740614
H	0.497670	4.720643	1.911782	C	1.487370	0.882518	-1.509370
C	-0.007489	2.709026	1.304182	H	0.643788	0.226107	-1.819049
H	-0.838977	2.653275	2.015666	H	1.940696	1.268991	-2.434644
C	0.288409	1.618757	0.476741	C	0.962813	1.998477	-0.657201
C	-1.504360	0.074765	2.161411	C	1.100759	3.346312	-0.985229
O	-2.346911	0.297770	2.920093	H	1.566409	3.605652	-1.942283
H	-0.548332	1.454952	-2.855213	C	0.669655	4.355419	-0.119647
H	-2.182779	2.162097	-2.970971	H	0.781334	5.406100	-0.395074
H	-0.976302	2.861864	-1.857101	C	0.131233	3.997495	1.121344
H	-2.780480	2.649990	0.407776	H	-0.184843	4.772330	1.825933
H	-3.837739	1.229012	0.527664	C	-0.005775	2.661092	1.484360
H	-3.918034	2.279000	-0.915548	H	-0.405715	2.386985	2.463784
H	-0.250423	-2.324891	-2.094244	C	0.330200	1.655627	0.559103
H	0.391804	-3.251516	-0.731071	C	-1.730260	-0.077333	2.169906
H	-1.041798	-3.856780	-1.618166	O	-2.642915	-0.118591	2.884870
H	-1.066124	-3.493966	1.765731	H	1.631202	-2.944066	-0.465526
H	-2.719976	-2.865979	1.904700	H	0.883130	-2.210230	-1.893120
H	-2.368631	-4.205301	0.770722	H	0.501200	-3.899153	-1.462566
				H	-0.072660	-3.835388	1.756464
				H	-1.815596	-3.530897	1.743996
				H	-1.101506	-4.666159	0.558910
				H	-4.126089	-0.282537	0.255154
				H	-3.852985	1.465253	0.282269
				H	-4.512382	0.695936	-1.188006
				H	-2.749309	1.691861	-2.865295
				H	-0.976597	1.652299	-2.673321
<b>11-ts(L7)</b>							
P	-2.087877	0.326736	-0.942799				
P	-0.680998	-2.299747	-0.016487				
C	-2.248950	-1.172243	-2.018274				
H	-3.192606	-1.153815	-2.589008				
H	-1.435011	-1.123555	-2.762125				
C	-3.802671	0.571306	-0.356129				

H	-1.956463	2.656889	-1.590199	H	-1.703657	-0.515032	2.998736
				H	-3.253247	0.297129	3.330818
<b>12(L7)</b>				H	-1.920894	1.199641	2.572108
P	1.647070	-0.134483	0.005881	C	-3.659191	-1.530686	1.268145
P	-1.381339	-0.799518	-0.063559	H	-4.411268	-1.535009	2.073015
C	1.086103	-1.686715	0.874281	H	-2.947894	-2.349036	1.457477
H	1.884323	-2.448522	0.872034	C	-4.376171	-1.749188	-0.062351
H	0.923320	-1.415650	1.931829	C	-5.173206	-3.021464	-0.108849
C	2.483964	-0.833345	-1.472342	H	-5.682602	-3.105613	-1.076513
C	-2.234580	-0.673577	1.554643	H	-5.927288	-3.029673	0.687298
C	-2.665676	-1.619798	-1.081136	H	-4.512968	-3.888125	0.017465
C	3.087684	0.342962	1.030559	C	-4.618945	0.579700	-0.326447
C	-0.201815	-2.210154	0.254496	C	-5.674096	1.647885	-0.397574
H	-0.667765	-2.994050	0.875644	H	-6.321906	1.486520	-1.267587
H	0.005325	-2.678069	-0.723955	H	-5.212904	2.640463	-0.481673
Ni	-0.179494	0.974335	-0.361745	H	-6.290393	1.622505	0.509335
C	-0.685835	2.607640	-0.094737	C	-3.712349	0.537720	-1.552034
O	-1.050646	3.681744	0.188797	H	-4.347058	0.374017	-2.438248
H	3.793087	-0.488586	1.184786	H	-3.192408	1.495274	-1.698288
H	2.748753	0.701320	2.012511	C	-2.726347	-0.611886	-1.443018
H	3.626577	1.172550	0.552159	C	-1.982317	-0.856105	-2.729043
H	3.215695	-1.614068	-1.212594	H	-1.294176	-1.707017	-2.635729
H	3.006466	-0.034408	-2.017387	H	-1.402011	0.033069	-3.014257
H	1.742418	-1.260946	-2.161680	H	-2.690453	-1.077808	-3.540895
H	-2.681762	-1.628344	1.874008	C	-0.703889	1.233246	-0.077262
H	-3.024713	0.088408	1.499645	C	-1.388638	2.462399	-0.025761
H	-1.525480	-0.342755	2.326475	H	-2.474374	2.462968	0.051728
H	-3.523548	-0.944959	-1.209794	C	-0.707446	3.674043	0.002440
H	-3.024429	-2.558711	-0.631162	C	-2.699267	4.934718	0.073752
H	-2.272313	-1.840582	-2.083443	H	-3.128788	4.510564	-0.849374
				H	-2.974569	5.993475	0.130946
<b>LiNi(CO)<sub>2</sub></b>				H	-3.131087	4.411463	0.942873
P	-1.529293	-0.403334	0.016574	C	0.711492	3.673571	-0.011397
P	1.529659	-0.406770	0.009162	C	2.704259	4.934692	0.011564
O	-5.283638	-0.668482	-0.241573	H	3.157128	4.420297	0.875304
O	-3.871200	0.832872	0.858696	H	2.980419	5.994020	0.051558
O	-3.454530	-1.813507	-1.147639	H	3.111203	4.501176	-0.917394
O	-1.293487	4.882815	0.065998	C	1.392034	2.461636	-0.049331
O	1.298835	4.882357	0.039278	H	2.478642	2.463739	0.012160
O	3.866969	0.836475	0.851768	C	0.706666	1.232165	-0.088046
O	5.286159	-0.672064	-0.229626	C	4.620355	0.574574	-0.327800
O	3.461365	-1.825994	-1.132413	C	5.674983	1.643020	-0.403392
C	-2.939156	-0.186016	1.258852	H	6.286321	1.627034	0.507083
C	-2.422063	0.221778	2.614687	H	5.213861	2.634451	-0.499905

H	6.327695	1.473576	-1.268178	C	-3.442203	-3.593135	0.058998
C	4.379176	-1.751993	-0.044580	H	-3.124663	-4.637328	0.111681
C	5.177596	-3.023843	-0.077307	C	-2.487910	-2.586501	-0.054132
H	4.517859	-3.890077	0.054345	H	-1.423890	-2.848926	-0.066720
H	5.928924	-3.024329	0.721512	C	-2.451281	1.571030	-0.631055
H	5.690570	-3.115866	-1.042359	C	-2.426020	2.661105	0.245800
C	3.656481	-1.523237	1.280962	H	-1.875987	2.580800	1.188234
H	2.946505	-2.341640	1.474715	C	-3.101988	3.841596	-0.065370
H	4.405214	-1.518772	2.088971	H	-3.076031	4.681093	0.633435
C	2.934327	-0.180209	1.256620	C	-3.804329	3.948800	-1.263663
C	2.410058	0.238515	2.606383	H	-4.332766	4.873184	-1.509492
H	1.689020	-0.494937	2.992042	C	-3.836997	2.868962	-2.147267
H	1.909570	1.216185	2.553378	H	-4.391372	2.945139	-3.086068
H	3.237146	0.319046	3.326663	C	-3.166994	1.689578	-1.833444
C	2.733932	-0.627535	-1.442561	H	-3.221197	0.845166	-2.527392
C	3.719633	0.521447	-1.557586	C	2.434238	-1.604280	-0.611185
H	3.199692	1.477277	-1.714721	C	3.284445	-1.703525	-1.724637
H	4.358869	0.350309	-2.439079	H	3.476571	-0.824288	-2.347673
C	1.996070	-0.887208	-2.729060	C	3.903787	-2.910564	-2.037097
H	2.708298	-1.111067	-3.536711	H	4.568637	-2.971559	-2.902188
H	1.409585	-0.005225	-3.023791	C	3.675029	-4.039693	-1.248214
H	1.314649	-1.742887	-2.629098	H	4.162136	-4.986492	-1.494438
Ni	-0.001684	-1.942311	0.368896	C	2.827094	-3.955218	-0.146515
C	0.007913	-2.514900	2.040971	H	2.643262	-4.835094	0.474537
O	0.016448	-2.933273	3.124038	C	2.211132	-2.743542	0.169235
C	-0.022122	-3.258419	-0.822708	H	1.549638	-2.676734	1.038021
O	-0.042944	-4.159495	-1.551089	C	2.903744	1.219253	-0.151893
<b>L2Ni(CO)2</b>				C	2.522966	2.571378	-0.138493
P	-1.554249	0.030237	-0.188737	H	1.461068	2.838153	-0.192316
P	1.575063	-0.037743	-0.186450	C	3.477967	3.577890	-0.031685
C	-0.655540	-0.374513	-1.767519	H	3.163616	4.624288	-0.025773
H	-0.512129	-1.467964	-1.786889	C	4.830641	3.251564	0.080519
H	-1.259782	-0.127358	-2.654156	H	5.580318	4.041231	0.170496
C	0.681584	0.341026	-1.774498	C	5.217358	1.913465	0.090226
H	0.538096	1.433636	-1.818231	H	6.273023	1.648469	0.189120
H	1.291696	0.069925	-2.650617	C	4.262437	0.903011	-0.024141
C	-2.873486	-1.238090	-0.131363	H	4.583360	-0.141441	-0.006351
C	-4.236816	-0.923861	-0.059789	Ni	0.010682	0.035611	1.388271
H	-4.562888	0.118652	-0.096573	C	0.250785	1.556080	2.269568
C	-5.190816	-1.933886	0.065798	O	0.471174	2.530573	2.857027
H	-6.250005	-1.670672	0.122221	C	-0.196302	-1.395516	2.414964
C	-4.799033	-3.269309	0.118405	O	-0.371776	-2.305111	3.111590
H	-5.548151	-4.058706	0.215111	<b>L3Ni(CO)2</b>			

Ni	-0.000283	0.001008	1.236493	H	2.929009	-1.635306	-2.620154
P	1.616844	0.009843	-0.349144	C	-3.934601	1.178837	0.683525
P	-1.617206	-0.010168	-0.349061	H	-4.571327	2.072247	0.785185
C	0.726089	-0.231626	-1.969559	H	-3.450246	1.009885	1.658343
H	1.280445	0.236069	-2.801427	H	-4.607072	0.333203	0.483713
H	0.769814	-1.314607	-2.162896	C	-3.609753	-1.731308	-1.593152
C	2.505270	1.691139	-0.546875	H	-3.915748	-2.776865	-1.764739
C	-2.504247	-1.692241	-0.545631	H	-3.293274	-1.331557	-2.568530
C	-2.915107	1.389032	-0.433146	H	-4.512782	-1.192422	-1.275103
C	2.914050	-1.389978	-0.432187	C	-1.415440	-2.687247	-0.941381
C	-0.726663	0.230737	-1.969595	H	-1.810134	-3.714788	-0.892008
H	-1.281103	-0.236967	-2.801404	H	-0.556168	-2.632868	-0.256681
H	-0.770424	1.313725	-2.162927	H	-1.055294	-2.535417	-1.970621
C	3.934327	-1.178390	0.683519	C	-3.066505	-2.128040	0.806050
H	4.571390	-2.071497	0.785676	H	-3.494718	-3.139776	0.719601
H	3.450701	-1.008489	1.658523	H	-3.865651	-1.472629	1.175189
H	4.606390	-0.332759	0.482234	H	-2.288387	-2.168149	1.580607
C	2.185961	-2.710278	-0.177195	C	0.078681	-1.436480	2.261958
H	2.924536	-3.526360	-0.128962	O	0.172892	-2.314567	3.017779
H	1.489907	-2.969506	-0.988209	C	-0.077960	1.439642	2.259903
H	1.627888	-2.721774	0.768137	O	-0.173165	2.319416	3.013442
C	3.068596	2.127102	0.804329				
H	3.497234	3.138605	0.717339				
H	3.867726	1.471400	1.173030	<b>L4Ni(CO)2</b>			
H	2.291140	2.167701	1.579488	P	-1.573164	0.037811	-0.043029
C	-2.187139	2.709821	-0.180453	P	1.533710	0.160409	-0.117757
H	-2.925693	3.526003	-0.133592	C	-0.707263	-0.236047	-1.671984
H	-1.491140	2.967618	-0.991994	H	-0.530770	-1.319935	-1.765893
H	-1.628898	2.722898	0.764741	H	-1.353427	0.050063	-2.516384
C	1.417382	2.687030	-0.942971	C	0.605234	0.524250	-1.677918
H	1.813175	3.714184	-0.894284	H	0.426114	1.612734	-1.666819
H	0.558242	2.633969	-0.257983	H	1.205093	0.329552	-2.580805
H	1.056841	2.534982	-1.972026	C	-2.756141	-1.360090	0.001489
C	3.610730	1.728208	-1.594447	C	-4.129252	-1.193352	0.211351
H	3.917528	2.773323	-1.767247	H	-4.591567	-0.207995	0.289746
H	3.294040	1.327440	-2.569345	C	-4.934396	-2.322013	0.327115
H	4.513290	1.188996	-1.275637	C	-4.432366	-3.613532	0.244704
C	-3.629656	1.523208	-1.778252	H	-5.081232	-4.483945	0.337130
H	-4.247774	2.436043	-1.768897	C	-3.062170	-3.746652	0.049323
H	-4.305939	0.693465	-2.008401	C	-2.216052	-2.653465	-0.064482
H	-2.931546	1.632546	-2.621255	H	-1.142829	-2.828843	-0.180672
C	3.627661	-1.525741	-1.777645	C	-2.621016	1.499211	-0.423709
H	4.245330	-2.438860	-1.767970	C	-2.509526	2.634691	0.381848
H	4.304192	-0.696412	-2.008763	H	-1.846691	2.655885	1.250041
				C	-3.262926	3.762282	0.067556

C	-4.126578	3.800128	-1.018046	H	-0.413841	1.144463	1.880038
H	-4.709272	4.691784	-1.248890	H	-1.260643	-0.220315	2.591641
C	-4.218562	2.653538	-1.799882	C	2.924041	-1.601213	0.122261
C	-3.483394	1.507267	-1.529773	C	4.247630	-1.230922	-0.130795
H	-3.603261	0.636868	-2.179030	H	4.519659	-0.180549	-0.258561
C	2.392989	-1.424661	-0.446215	C	5.252442	-2.207104	-0.239153
C	2.401860	-2.048688	-1.698737	C	4.944933	-3.563336	-0.087777
H	1.924289	-1.614254	-2.578345	H	5.725382	-4.320315	-0.168365
C	3.050398	-3.272120	-1.837062	C	3.617849	-3.935486	0.163780
C	3.702694	-3.896656	-0.783503	C	2.615484	-2.960243	0.258544
H	4.205096	-4.854828	-0.913591	H	1.584151	-3.282776	0.423630
C	3.682854	-3.249228	0.447108	C	2.385491	1.210501	0.424022
C	3.032013	-2.038458	0.640559	C	2.278092	2.220986	-0.533905
H	3.024748	-1.586418	1.635990	H	1.726196	2.037428	-1.460226
C	2.881884	1.399922	-0.185817	C	2.874620	3.475953	-0.323500
C	2.540970	2.720260	0.138999	C	3.580691	3.726526	0.858166
H	1.526341	2.990358	0.444580	H	4.041295	4.700191	1.028280
C	3.518016	3.703795	0.070724	C	3.695802	2.711715	1.818300
C	4.832737	3.423786	-0.284736	C	3.100834	1.458824	1.599952
H	5.590014	4.206550	-0.321638	H	3.216444	0.680475	2.359190
C	5.141074	2.104306	-0.586483	C	-2.916772	-1.256533	0.475003
C	4.195834	1.084814	-0.547365	C	-3.660121	-1.213460	1.658858
H	4.502182	0.069738	-0.806483	H	-3.462909	-0.452069	2.418033
Ni	0.022127	0.108998	1.489161	C	-4.685096	-2.145544	1.887597
F	-3.147301	4.848843	0.833037	C	-4.979295	-3.121131	0.926206
F	-5.047944	2.662613	-2.846724	H	-5.773434	-3.846744	1.103958
F	-6.245972	-2.157880	0.520409	C	-4.247599	-3.152699	-0.266194
F	-2.544439	-4.975446	-0.022895	C	-3.217343	-2.223473	-0.486017
F	3.191502	4.964436	0.362892	H	-2.646403	-2.259617	-1.418397
F	6.395602	1.806406	-0.935073	C	-2.379690	1.527825	-0.009167
F	3.050549	-3.867592	-3.032953	C	-1.556097	2.659025	-0.056442
F	4.307320	-3.821801	1.477530	H	-0.469242	2.545455	0.023584
C	0.053633	-1.463417	2.323021	C	-2.101647	3.939594	-0.214176
O	0.071348	-2.491855	2.850386	C	-3.486271	4.099709	-0.365238
C	0.126005	1.531785	2.547261	H	-3.916751	5.092764	-0.495865
O	0.253934	2.429518	3.266894	C	-4.307570	2.967217	-0.350217
				C	-3.757225	1.686165	-0.166461
				H	-4.426190	0.822592	-0.153609
<b>L5Ni(CO)2</b>				Ni	-0.033778	-0.558376	-1.420109
P	1.544276	-0.396557	0.108117	C	-1.236979	5.077608	-0.207665
P	-1.536927	-0.095157	0.120355	N	-0.513253	5.989459	-0.180654
C	0.663074	-0.725471	1.708474	C	-5.720761	3.111546	-0.511301
H	0.452247	-1.807109	1.731313	N	-6.872876	3.220308	-0.639413
H	1.291334	-0.511156	2.586879	C	2.756373	4.497123	-1.317117
C	-0.628181	0.072258	1.740003				



N	2.659670	5.323132	-2.131523	H	-3.144645	4.336417	1.165992
C	4.417104	2.949624	3.029411	C	0.708735	3.572259	0.253226
N	5.000755	3.127270	4.021093	C	2.698198	4.836852	0.280337
C	6.599810	-1.808395	-0.501520	H	3.143768	4.338884	1.156745
N	7.695723	-1.477693	-0.714375	H	2.972194	5.897098	0.301837
C	3.282020	-5.315712	0.324157	H	3.116018	4.383374	-0.634072
N	3.003337	-6.437570	0.463567	C	1.395071	2.362365	0.213370
C	-5.427516	-2.095380	3.108102	H	2.485153	2.358208	0.233703
N	-6.023945	-2.043656	4.106717	C	0.703616	1.138703	0.177175
C	-4.547942	-4.138906	-1.256404	C	4.358641	0.343797	-1.035241
N	-4.797583	-4.940786	-2.062572	C	4.148666	-1.934400	-0.660319
C	0.006233	-2.258953	-1.951758	C	3.858062	-1.692237	0.814096
O	0.091550	-3.363558	-2.277928	H	3.205144	-2.481008	1.214471
C	-0.157039	0.673867	-2.706660	H	4.808686	-1.712532	1.366562
O	-0.315401	1.472511	-3.525030	C	3.202533	-0.323984	0.947602

### L6Ni(CO)2

P	-1.493313	-0.512946	0.204483
P	1.493276	-0.511734	0.203632
O	-5.003264	-0.908273	-1.123165
O	-4.017007	0.656971	0.299918
O	-2.974039	-2.018211	-1.443738
O	-1.296504	4.781038	0.301335
O	1.292126	4.782084	0.298795
O	4.016010	0.660135	0.300270
O	5.004500	-0.905224	-1.121173
O	2.976232	-2.016753	-1.442466
C	-3.203269	-0.326920	0.947240
C	-3.857573	-1.695645	0.812412
H	-4.808545	-1.717055	1.364237
H	-3.204279	-2.484141	1.212725
C	-4.147020	-1.937141	-0.662335
C	-4.358348	0.341138	-1.036054
C	-3.143879	0.328647	-1.950318
H	-3.485557	0.149102	-2.981162
H	-2.625644	1.298060	-1.934140
C	-2.231189	-0.799502	-1.507425
C	-0.705086	1.138130	0.178211
C	-1.397586	2.361154	0.215625
H	-2.487638	2.355966	0.237306
C	-0.712252	3.571665	0.254553
C	-2.702681	4.834870	0.288050
H	-3.123613	4.381394	-0.624932
H	-2.977279	5.894933	0.310814

H	-3.144645	4.336417	1.165992
C	0.708735	3.572259	0.253226
C	2.698198	4.836852	0.280337
H	3.143768	4.338884	1.156745
H	2.972194	5.897098	0.301837
H	3.116018	4.383374	-0.634072
C	1.395071	2.362365	0.213370
H	2.485153	2.358208	0.233703
C	0.703616	1.138703	0.177175
C	4.358641	0.343797	-1.035241
C	4.148666	-1.934400	-0.660319
C	3.858062	-1.692237	0.814096
H	3.205144	-2.481008	1.214471
H	4.808686	-1.712532	1.366562
C	3.202533	-0.323984	0.947602
C	2.232646	-0.798585	-1.507579
C	3.144916	0.329902	-1.950463
H	2.625942	1.298941	-1.935366
H	3.487570	0.149943	-2.980913
Ni	0.000821	-1.967033	0.871054
C	0.002108	-2.186148	2.628894
O	0.003179	-2.319817	3.780511
H	4.680670	-2.880713	-0.826371
H	5.097749	1.100294	-1.334369
H	3.119861	-0.006001	1.997670
H	-3.121701	-0.009535	1.997577
H	-1.415671	-0.978202	-2.224108
H	-5.097740	1.097297	-1.335330
H	-4.678261	-2.883728	-0.829278
H	1.417848	-0.978326	-2.224819
C	0.001045	-3.399634	-0.185314
O	0.000697	-4.318606	-0.887845

### L7Ni(CO)2

P	-1.607388	-0.044826	0.016627
P	1.607179	-0.044797	-0.016431
C	-0.681389	1.556107	0.341293
H	-1.283728	2.435754	0.047747
H	-0.561036	1.623427	1.436861
C	-2.494039	0.391511	-1.549022
C	2.496496	0.387822	1.548787
C	3.015693	0.206145	-1.188216
C	-3.017373	0.203337	1.187021
C	0.680917	1.556940	-0.336721

H	1.283182	2.435980	-0.041311	H	1.949143	-2.571987	1.031270
H	0.560253	1.626798	-1.432083	H	3.459396	-2.211302	0.217350
Ni	-0.000040	-1.316141	-0.000955	C	-2.348089	-1.825087	-0.651947
H	-3.494915	1.191656	1.081404	H	-1.879575	-2.804253	-0.456144
H	-2.668998	0.098232	2.224966	H	-3.205607	-2.051901	-1.319227
H	-3.786980	-0.565804	1.024738	C	-2.517278	1.304011	-0.967413
H	-3.045348	1.343421	-1.476582	H	-3.460619	0.741448	-1.053385
H	-3.210079	-0.401526	-1.811538	H	-2.640825	2.156883	-1.652983
H	-1.778592	0.467341	-2.380788	C	-2.854436	-1.240911	0.666982
H	3.044702	1.341698	1.478863	H	-3.236586	-2.053276	1.304475
H	3.215903	-0.404078	1.805587	H	-3.722661	-0.587940	0.492637
H	1.783403	0.457632	2.383061	C	-2.342415	1.843843	0.454743
H	3.784731	-0.564452	-1.030305	H	-3.319257	2.176406	0.860566
H	3.494534	1.193544	-1.079732	H	-1.733287	2.762204	0.414269
H	2.665398	0.105498	-2.225948				

**<sup>32</sup>(L1)**

<b><sup>3</sup>Ni(COD)<sub>2</sub></b>				Ni	0.542944	-0.538434	0.087583
Ni	-0.021549	-0.114461	0.069154	P	-0.267176	1.475816	0.169916
C	-1.367365	0.443616	-1.449768	P	-1.502542	-1.316853	0.065357
H	-0.745165	0.886603	-2.236771	O	1.463725	4.817570	0.372534
C	-1.329657	-0.958300	-1.338770	O	-0.187980	3.965997	-1.040897
H	-0.706294	-1.486319	-2.070990	O	1.506092	2.831055	1.611654
C	-1.802670	-0.473129	1.430665	O	-5.026782	3.343938	-1.202346
H	-1.311276	-1.000849	2.256739	O	-6.090232	0.968762	-1.190855
C	-1.663260	0.894568	1.394562	O	-3.379508	-3.120380	-0.879006
H	-1.068011	1.356874	2.189436	O	-2.763325	-4.813097	0.612302
C	1.689558	-1.435390	-0.735377	O	-1.173059	-3.434578	1.632572
H	1.112314	-2.266705	-1.154227	O	3.719191	-1.282556	-1.867021
C	1.853371	-0.329359	-1.532424	C	0.422782	2.669425	-1.125231
H	1.290690	-0.298348	-2.472762	C	0.173671	2.155905	-2.520283
C	1.463137	0.312073	1.518971	H	0.626822	1.162282	-2.651890
H	0.927026	0.311643	2.476567	H	0.612342	2.839059	-3.262115
C	1.245008	1.435425	0.696740	H	-0.902419	2.071764	-2.730294
H	0.598447	2.222933	1.101424	C	1.906585	2.789222	-0.788471
C	2.782748	0.814696	-1.258354	H	2.421923	3.344134	-1.588985
H	3.698882	0.448522	-0.772170	H	2.361743	1.787381	-0.713553
H	3.122453	1.246496	-2.212549	C	2.083915	3.546915	0.525391
C	2.130820	1.918454	-0.420741	C	3.518577	3.795714	0.891856
H	2.911121	2.600444	-0.023657	H	3.565537	4.380194	1.819076
H	1.518914	2.551724	-1.085476	H	4.026087	4.355405	0.096559
C	2.675170	-0.590746	1.455679	H	4.037127	2.842910	1.052596
H	2.884980	-0.984083	2.462389	C	0.071870	4.713337	0.145374
H	3.575281	-0.012299	1.192851	C	-0.446968	6.101688	-0.106376
C	2.482671	-1.768434	0.498794	H	-0.246938	6.746513	0.757783

H	-1.528809	6.084628	-0.289657	C	-2.023776	-2.279321	1.610889
H	0.050940	6.529568	-0.985137	C	-3.468548	-2.736723	1.527413
C	-0.548279	4.042818	1.369332	H	-4.149589	-1.879428	1.421202
H	-0.339461	4.678665	2.245322	H	-3.734207	-3.249482	2.466376
H	-1.641065	3.970117	1.275658	C	-1.715880	-1.488429	2.854316
C	0.078234	2.679373	1.598776	H	-1.878334	-2.103924	3.751338
C	-0.300844	2.062605	2.919343	H	-2.363870	-0.602629	2.920919
H	0.201899	1.093445	3.050564	H	-0.668547	-1.150852	2.844154
H	-1.387689	1.907286	2.980303	C	5.057859	-1.518030	-1.667917
H	0.000496	2.719830	3.748370	C	5.639850	-2.567763	-2.378453
C	-2.066238	1.376127	-0.174811	H	5.003970	-3.184101	-3.016915
C	-2.868992	2.480661	-0.514144	C	7.007376	-2.807066	-2.262206
H	-2.417478	3.469040	-0.569807	H	7.462209	-3.631883	-2.816107
C	-4.211310	2.333227	-0.851813	C	7.788576	-1.998451	-1.437534
C	-4.484539	4.641327	-1.250259	H	8.860848	-2.183507	-1.340436
H	-4.134234	4.975699	-0.259206	C	7.196438	-0.946997	-0.739025
H	-5.290220	5.307803	-1.576441	H	7.805570	-0.304396	-0.096274
H	-3.652886	4.714992	-1.970463	C	5.828353	-0.683784	-0.846915
C	-4.789407	1.036686	-0.857597	C	5.156516	0.441187	-0.117092
C	-6.711056	-0.294229	-1.156728	H	4.633671	1.076088	-0.860399
H	-6.268638	-0.996349	-1.882614	H	5.911645	1.081679	0.360473
H	-7.762466	-0.135634	-1.419112	C	4.169514	-0.041915	0.906602
H	-6.663152	-0.743521	-0.150739	C	4.269965	0.348599	2.226349
C	-3.994383	-0.061741	-0.546809	H	5.100160	1.004011	2.510584
H	-4.414648	-1.064640	-0.616252	C	3.337531	-0.055070	3.214350
C	-2.637835	0.086036	-0.205313	H	3.453943	0.273782	4.249175
C	-3.647296	-3.729183	0.381042	C	2.285522	-0.883624	2.840058
C	-5.038142	-4.291474	0.287940	H	1.583920	-1.253061	3.595164
H	-5.092259	-5.008739	-0.539980	C	2.120071	-1.288797	1.513050
H	-5.764644	-3.489292	0.104925	H	1.434071	-2.122118	1.296520
H	-5.308711	-4.807029	1.217453	C	3.077129	-0.887880	0.491943
C	-1.400254	-4.407248	0.612676	C	2.797643	-1.292146	-0.839091
C	-0.569522	-5.603244	0.979903	O	1.638432	-1.692105	-1.190909
H	0.494543	-5.337192	0.994043				
H	-0.721609	-6.412783	0.256069	<sup>34</sup> (L1)			
H	-0.856157	-5.962678	1.975579	Ni	0.666216	-0.806036	-0.309643
C	-1.081570	-3.848208	-0.770756	P	0.566542	1.466585	-0.084580
H	-0.034018	-3.513408	-0.824222	P	-1.595573	-0.790239	0.267959
H	-1.221693	-4.652721	-1.510185	O	3.168218	4.170703	0.369821
C	-2.024798	-2.695598	-1.103167	O	1.315803	3.968483	-1.041694
C	-1.927414	-2.255716	-2.541363	O	2.709181	2.107254	1.374689
H	-0.900212	-1.939538	-2.772993	O	-3.418966	4.739698	-1.150989
H	-2.605208	-1.416119	-2.752148	O	-5.205122	2.860784	-0.907112
H	-2.194947	-3.085686	-3.211425	O	-4.065223	-1.808101	-0.482482

O	-4.040636	-3.545352	1.080461	C	-2.171869	0.909545	-0.079288
O	-1.993229	-2.817067	1.947938	C	-4.468066	-2.222024	0.820031
O	0.607525	-2.133329	-1.712787	C	-5.971380	-2.223197	0.817315
C	1.524651	2.571582	-1.291014	H	-6.340547	-2.902828	0.039710
C	1.101665	2.312816	-2.714935	H	-6.356906	-1.215674	0.615113
H	1.247702	1.255514	-2.978553	H	-6.355582	-2.558569	1.788077
H	1.697463	2.927410	-3.404910	C	-2.624591	-3.676814	1.002988
H	0.041379	2.557057	-2.870354	C	-2.275187	-5.079344	1.409718
C	2.996741	2.261272	-1.037684	H	-1.189161	-5.225215	1.366771
H	3.602243	2.771793	-1.803263	H	-2.758066	-5.802342	0.741565
H	3.197137	1.183977	-1.114992	H	-2.615165	-5.264473	2.435867
C	3.422284	2.772602	0.335320	C	-2.202659	-3.337201	-0.421723
C	4.880936	2.565989	0.624150	H	-1.111461	-3.411680	-0.533865
H	5.123452	2.969508	1.614755	H	-2.669808	-4.063612	-1.106135
H	5.496062	3.078105	-0.125518	C	-2.668462	-1.934279	-0.792897
H	5.120471	1.495376	0.612993	C	-2.524942	-1.626749	-2.260360
C	1.794234	4.468490	0.207387	H	-1.477752	-1.750976	-2.567108
C	1.659694	5.963538	0.139064	H	-2.850284	-0.601455	-2.489144
H	2.034478	6.424165	1.060833	H	-3.151675	-2.316257	-2.844833
H	0.609001	6.249818	0.003367	C	-2.346376	-1.434612	1.897464
H	2.240538	6.349208	-0.707523	C	-3.862608	-1.318752	1.888142
C	1.043181	3.838749	1.375125	H	-4.183461	-0.274650	1.761738
H	1.420852	4.293246	2.305204	H	-4.235497	-1.655199	2.869044
H	-0.033278	4.056677	1.321089	C	-1.730763	-0.775967	3.102406
C	1.299353	2.340667	1.436540	H	-2.145772	-1.222465	4.018096
C	0.808341	1.722695	2.717645	H	-1.961020	0.298718	3.114249
H	1.010607	0.644072	2.743678	H	-0.644733	-0.926451	3.107445
H	-0.272750	1.881237	2.832219	C	1.497561	-3.067963	-1.941990
H	1.314537	2.188791	3.575563	C	1.087496	-4.348021	-2.388794
C	-1.200105	1.924007	-0.231775	H	0.016141	-4.519063	-2.528075
C	-1.619215	3.221154	-0.587166	C	2.005073	-5.359157	-2.644979
H	-0.868997	3.993967	-0.744136	H	1.649821	-6.337216	-2.982721
C	-2.959090	3.527027	-0.799360	C	3.373346	-5.133416	-2.472782
C	-2.489966	5.792342	-1.252885	H	4.099470	-5.925790	-2.667678
H	-1.994842	5.989802	-0.287751	C	3.798640	-3.873258	-2.054095
H	-3.055372	6.683761	-1.544880	H	4.870036	-3.679600	-1.928796
H	-1.719841	5.597596	-2.017519	C	2.896801	-2.838929	-1.793101
C	-3.933158	2.505206	-0.661040	C	3.395127	-1.473515	-1.396515
C	-6.202124	1.876729	-0.763835	H	2.556067	-0.756285	-1.474712
H	-6.047853	1.027335	-1.449323	H	4.133462	-1.126939	-2.138829
H	-7.155503	2.356418	-1.009393	C	4.030407	-1.384342	-0.033487
H	-6.254320	1.498276	0.270585	C	5.427787	-1.323818	0.056497
C	-3.525493	1.224579	-0.304126	H	6.014808	-1.314123	-0.867434
H	-4.266370	0.429319	-0.253672	C	6.079942	-1.274892	1.286748

H	7.171058	-1.220294	1.322611	H	-0.626158	2.045273	-2.810441
C	5.335844	-1.290898	2.466543	H	-2.132214	1.671616	-3.685944
H	5.836814	-1.250002	3.437057	C	0.028903	2.181869	0.230430
C	3.950084	-1.365983	2.395702	C	-0.219520	3.484166	0.708192
H	3.342657	-1.391415	3.304139	H	-1.242272	3.764471	0.957368
C	3.281475	-1.409332	1.162216	C	0.805647	4.402085	0.906833
C	1.772061	-1.457342	1.197780	C	-0.661857	6.052996	1.733824
O	1.238847	-1.853057	2.223273	H	-1.322422	6.092271	0.852330
				H	-0.575099	7.062559	2.149515
<b><sup>36</sup>(L1)</b>				H	-1.116090	5.394581	2.492106
P	-1.307898	0.961771	-0.040150	C	2.139604	4.028332	0.598687
P	1.698261	0.026413	-0.317491	C	4.420293	4.621726	0.552133
O	-4.855000	2.170671	-0.498082	H	4.755251	3.774759	1.173924
O	-3.178077	2.714790	1.038956	H	5.024576	5.500357	0.801762
O	-3.435502	0.702504	-1.632459	H	4.582458	4.374056	-0.510302
O	0.640753	5.644260	1.389094	C	2.394221	2.740408	0.145524
O	3.079329	4.965511	0.807925	H	3.426952	2.434024	-0.006675
O	4.350419	0.409942	0.376406	C	1.363115	1.795736	-0.032790
O	5.164976	-1.248044	-1.057814	C	4.887242	0.134061	-0.914051
O	3.003246	-1.706765	-1.826915	C	6.195727	0.868450	-0.996452
C	-2.704524	1.364699	1.161674	H	6.855646	0.545476	-0.182130
C	-2.247844	1.178321	2.585127	H	6.037173	1.951076	-0.911421
H	-1.812461	0.176571	2.714264	H	6.691615	0.661371	-1.952580
H	-3.091931	1.303195	3.278765	C	4.010561	-2.052320	-0.869975
H	-1.476348	1.915331	2.850791	C	4.396929	-3.475182	-1.153855
C	-3.834465	0.424308	0.757030	H	3.539732	-4.143526	-1.008885
H	-4.637352	0.489853	1.508412	H	5.204812	-3.789061	-0.482021
H	-3.486291	-0.616149	0.715808	H	4.744528	-3.566795	-2.189902
C	-4.408864	0.824216	-0.598604	C	3.510862	-1.827418	0.552024
C	-5.576540	-0.018942	-1.020375	H	2.629088	-2.451388	0.759845
H	-5.957672	0.331703	-1.987241	H	4.305470	-2.130868	1.252586
H	-6.382340	0.044633	-0.279307	C	3.199306	-0.354433	0.771303
H	-5.264550	-1.065972	-1.122228	C	2.903060	-0.011775	2.208623
C	-3.796731	3.060771	-0.199246	H	1.952149	-0.473014	2.514659
C	-4.397994	4.424094	-0.003648	H	2.815425	1.074973	2.344616
H	-4.915544	4.748363	-0.914607	H	3.710093	-0.370779	2.864188
H	-3.620197	5.158395	0.240359	C	2.644870	-0.319825	-1.921387
H	-5.123009	4.392828	0.818789	C	3.905021	0.519051	-2.018973
C	-2.793753	2.992994	-1.348164	H	3.664375	1.592228	-1.986728
H	-3.310853	3.309563	-2.268468	H	4.392737	0.323354	-2.987921
H	-1.958130	3.689557	-1.190060	C	1.752868	-0.200225	-3.128046
C	-2.303188	1.566213	-1.545372	H	2.296959	-0.503644	-4.034333
C	-1.515327	1.398079	-2.817273	H	1.406690	0.833651	-3.262068
H	-1.195112	0.355272	-2.946790	H	0.874758	-0.856416	-3.029026

Ni	-0.303847	-1.316074	-0.131955	C	-4.036938	-0.357738	0.384312
O	-0.213759	-1.519776	1.862664	H	-4.879088	-0.419402	1.091862
C	-0.167862	-2.785005	2.213475	H	-3.575910	-1.350207	0.319236
C	1.014606	-3.361226	2.743251	C	-4.581924	0.061997	-0.972429
H	1.871102	-2.705142	2.921682	C	-5.602161	-0.883548	-1.535513
C	1.098150	-4.719371	3.030186	H	-5.971539	-0.502060	-2.495294
H	2.029917	-5.131539	3.429484	H	-6.449306	-0.983962	-0.846370
C	0.002394	-5.555829	2.808173	H	-5.154954	-1.872569	-1.690894
H	0.065924	-6.625612	3.020846	C	-4.309364	2.323848	-0.390672
C	-1.186749	-4.999786	2.332803	C	-5.101899	3.573184	-0.125715
H	-2.062080	-5.641710	2.182804	H	-5.635817	3.885974	-1.031073
C	-1.302125	-3.638145	2.051776	H	-4.441056	4.389835	0.192265
C	-2.600966	-3.042608	1.588811	H	-5.836513	3.386334	0.666962
H	-2.636687	-2.005277	1.963925	C	-3.256425	2.489905	-1.480547
H	-3.435954	-3.579584	2.064882	H	-3.773571	2.806663	-2.400745
C	-2.813344	-3.036248	0.090975	H	-2.534433	3.279377	-1.226244
C	-3.905856	-3.734052	-0.445897	C	-2.553767	1.169618	-1.753341
H	-4.579248	-4.272132	0.231123	C	-1.745958	1.208210	-3.021260
C	-4.145755	-3.759990	-1.819548	H	-1.262107	0.240565	-3.214345
H	-5.000977	-4.313274	-2.217624	H	-0.978173	1.991263	-2.977606
C	-3.280531	-3.083203	-2.675924	H	-2.408266	1.425308	-3.871930
H	-3.447212	-3.097693	-3.757160	C	-0.457889	2.020503	0.342123
C	-2.189820	-2.392760	-2.142023	C	-1.010980	3.186751	0.912735
H	-1.514816	-1.886813	-2.846543	H	-2.092351	3.284804	0.957715
C	-1.934288	-2.337021	-0.763710	C	-0.228106	4.183225	1.481321
C	0.588963	-3.067455	-0.566196	C	-2.102681	5.499967	2.040528
O	0.700018	-4.070118	-1.111172	H	-2.496474	5.561247	1.012153
				H	-2.288302	6.455439	2.543079
				H	-2.640119	4.705192	2.583845
<b><sup>3</sup>10(L1)</b>				C	1.181171	4.033155	1.494096
P	-1.515585	0.627749	-0.236020	C	3.283707	4.913548	2.091927
P	1.705810	0.363684	-0.336817	H	3.627774	4.004814	2.612561
O	-5.213388	1.326489	-0.820401	H	3.660544	5.790708	2.628417
O	-3.709714	1.960264	0.851553	H	3.698969	4.919770	1.070960
O	-3.530061	0.143763	-1.936506	C	1.739075	2.897419	0.921567
O	-0.709588	5.302544	2.049321	H	2.819046	2.763122	0.951589
O	1.879592	5.020198	2.078354	C	0.951640	1.883357	0.339396
O	4.223654	1.142603	0.587821	C	4.766959	1.458861	-0.691566
O	5.369545	0.323226	-1.284174	C	5.852294	2.469664	-0.449518
O	3.368425	-0.352045	-2.295103	H	6.607743	2.044955	0.222714
C	-3.055159	0.682069	0.903549	H	5.440205	3.374926	0.014299
C	-2.675233	0.452304	2.343565	H	6.337896	2.746023	-1.393249
H	-2.231963	-0.544879	2.467404	C	4.450592	-0.749036	-1.446324
H	-3.571245	0.507217	2.978351	C	5.163245	-1.855524	-2.168707
H	-1.956169	1.200132	2.706644				

H	4.484939	-2.703708	-2.323081	C	0.095549	-1.854587	-2.258405
H	6.029573	-2.194916	-1.588454	O	0.230960	-2.428562	-3.240386
H	5.511159	-1.499623	-3.146268				
C	3.946192	-1.150293	-0.069120	<b><sup>3</sup>12(L1)</b>			
H	3.219532	-1.970666	-0.143375	P	1.486657	-0.407472	-0.113391
H	4.805341	-1.490244	0.531123	P	-1.536676	-0.534616	-0.126650
C	3.302870	0.038739	0.633605	O	5.247760	-0.606891	0.151381
C	3.009198	-0.223236	2.088426	O	3.802291	0.906281	-0.893505
H	2.332664	-1.083036	2.188167	O	3.440946	-1.826388	1.001919
H	2.543036	0.648575	2.570212	O	1.052301	4.859779	0.071807
H	3.941325	-0.449425	2.626371	O	-1.548676	4.749066	0.078747
C	2.670025	0.835576	-1.912958	O	-3.961620	0.596980	-0.879209
C	3.676408	1.942880	-1.639408	O	-5.275021	-1.033394	0.158596
H	3.179499	2.843457	-1.250601	O	-3.374080	-2.118710	0.985060
H	4.153789	2.221047	-2.593144	C	2.904490	-0.120807	-1.342873
C	1.752603	1.194627	-3.049488	C	2.373981	0.313218	-2.684622
H	2.337344	1.356959	-3.966839	H	1.661721	-0.432328	-3.067206
H	1.207700	2.121732	-2.822931	H	3.195660	0.418242	-3.408116
H	1.025404	0.398597	-3.252261	H	1.852894	1.278951	-2.616521
Ni	-0.104093	-1.430331	-0.447772	C	3.653227	-1.446037	-1.398416
O	1.294843	-2.595669	0.363334	H	4.409455	-1.405541	-2.198624
C	-1.632025	-2.743765	-0.207245	H	2.956460	-2.267752	-1.628361
C	-2.525322	-3.154074	-1.206092	C	4.365904	-1.701300	-0.073762
H	-2.404294	-2.792437	-2.235755	C	5.188658	-2.957867	-0.069909
C	-3.609799	-3.992374	-0.932156	H	5.698812	-3.064429	0.895077
H	-4.286464	-4.296211	-1.737226	H	5.942872	-2.925971	-0.865444
C	-3.833203	-4.430525	0.372251	H	4.542383	-3.830319	-0.223536
H	-4.687141	-5.073256	0.603158	C	4.554749	0.621275	0.283455
C	-2.950411	-4.049025	1.381499	C	5.585339	1.709575	0.400588
H	-3.110400	-4.403760	2.406394	H	6.225872	1.536488	1.273604
C	-1.849545	-3.227142	1.100203	H	5.101431	2.688832	0.507826
C	-0.850405	-2.917311	2.191536	H	6.213279	1.725368	-0.498560
H	-0.476845	-1.880518	2.060633	C	3.644922	0.512564	1.502925
H	-1.326941	-2.967627	3.182999	H	4.280247	0.333343	2.386149
C	0.308430	-3.866811	2.127322	H	3.100461	1.451580	1.678096
C	0.408321	-4.965705	2.979829	C	2.686637	-0.654315	1.344118
H	-0.355882	-5.102733	3.752855	C	1.932101	-0.982359	2.604177
C	1.448752	-5.889338	2.865222	H	1.268548	-1.843115	2.436977
H	1.505789	-6.743674	3.543837	H	1.319389	-0.126855	2.923565
C	2.409433	-5.708503	1.866148	H	2.631795	-1.230118	3.415820
H	3.225570	-6.428892	1.757058	C	0.611049	1.187042	0.022959
C	2.336464	-4.619212	1.007263	C	1.245377	2.441016	0.033466
H	3.085924	-4.475326	0.223607	H	2.330621	2.489591	-0.034944
C	1.294873	-3.663259	1.115522	C	0.509969	3.626830	0.062325

C	2.454560	4.960300	0.079408
H	2.894243	4.498601	0.979562
H	2.694210	6.029222	0.084573
H	2.910297	4.503150	-0.814693
C	-0.903705	3.566681	0.064108
C	-2.954466	4.731437	0.096480
H	-3.376310	4.241150	-0.796674
H	-3.282751	5.776486	0.108308
H	-3.346515	4.230308	0.997547
C	-1.535964	2.322814	0.031986
H	-2.621296	2.278333	-0.038032
C	-0.797694	1.127381	0.019024
C	-4.678375	0.244412	0.300512
C	-5.788913	1.248705	0.435096
H	-6.424471	1.222333	-0.458362
H	-5.379491	2.261259	0.543974
H	-6.406496	1.022733	1.312588
C	-4.312203	-2.052407	-0.082786
C	-5.040916	-3.366330	-0.091350
H	-4.339892	-4.190397	-0.271188
H	-5.807053	-3.373765	-0.875860
H	-5.529055	-3.525400	0.877774
C	-3.623809	-1.729728	-1.405835
H	-2.861133	-2.491209	-1.636897
H	-4.378634	-1.747808	-2.208292
C	-2.983849	-0.348015	-1.340941
C	-2.500768	0.137940	-2.682919
H	-1.718502	-0.532995	-3.067006
H	-2.076790	1.149836	-2.613317
H	-3.329170	0.162816	-3.406114
C	-2.710217	-0.893232	1.336288
C	-3.755352	0.192398	1.514574
H	-3.284220	1.168909	1.698522
H	-4.370673	-0.045186	2.398346
C	-1.920829	-1.180354	2.584048
H	-2.588728	-1.499435	3.397567
H	-1.374691	-0.284968	2.914039
H	-1.191627	-1.981117	2.391441
Ni	0.039266	-1.993695	-0.474617
C	0.917536	-3.516347	-0.129903
O	1.538484	-4.486845	0.065576