

## Supporting Information for Manuscript

### Energetics of the Ruthenium-Halide Bond in Olefin Metathesis (Pre)catalysts

by

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#### *Computational details.*

**DFT calculations.** All the density functional theory (DFT) calculations were performed using the Gaussian09 package.<sup>[1]</sup> The BP86 GGA functional of Becke and Perdew was used.<sup>[2-4]</sup> Geometry optimizations were performed with the standard split-valence basis set with a polarization function of Ahlrichs and coworkers was used for H, C, N, O, and Cl atoms (SVP keyword in Gaussian)<sup>[5]</sup> while the quasi relativistic small-core Stuttgart effective core potential (ECP) was used for Ruthenium and Iodine (SDD keyword in Gaussian09).<sup>[6-8]</sup> The reported energies have been obtained via single point energy calculations with M06<sup>[9-10]</sup> functional with the triple- $\zeta$  basis set of Ahlrichs for H, C, and N atoms (TZVP keyword in Gaussian09), augmented with a diffuse d function for Cl atoms, and O atoms of anionic ligands.<sup>[11]</sup> Solvent effects, CH<sub>2</sub>Cl<sub>2</sub>, were included using the PCM method and considering also the non-electrostatic contributions.<sup>[12-13]</sup>

#### References.

- [S1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. Montgomery, J. A., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K.

- Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, B.1 ed., Gaussian, Inc., Pittsburgh PA,, **2003**.
- [S2] A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098.
- [S3] J. P. Perdew, *Phys. Rev. B* **1986**, *34*, 7406.
- [S4] J. P. Perdew, *Phys. Rev. B* **1986**, *33*, 8822.
- [S5] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
- [S6] U. Haeusermann, M. Dolg, H. Stoll, H. Preuss, *Mol. Phys.* **1993**, *78*, 1211.
- [S7] W. Kuechle, M. Dolg, H. Stoll, H. Preuss, *J. Chem. Phys.* **1994**, *100*, 7535.
- [S8] T. Leininger, A. Nicklass, H. Stoll, M. Dolg, P. Schwerdtfeger, *J. Chem. Phys.* **1996**, *105*, 1052.
- [S9] Y. Zhao, D. G. Truhlar, *J. Chem. Phys.* **2006**, *125*, 194101–194118.
- [S10] Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215–241.
- [S11] D. Rappoport, F. Furche, *J. Chem. Phys.* **2010**, *133*, 134105.
- [S12] J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.* **2005**, *105*, 2999.
- [S13] V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, *102*, 1995-2001.

**Table S1.** xyz coordinate data sets and M06 CH<sub>2</sub>Cl<sub>2</sub> energies (in a.u.) for DFT optimized complexes.

1-trans				1-cis			
-3357.46733663				-3357.47110508			
Ru	-0.024313	-0.033437	0.087756	Ru	-0.002268	0.392763	-1.159208
Cl	-0.028547	0.830184	2.370688	Cl	0.345723	-1.752956	-2.398996
Cl	-0.061126	-0.312494	-2.327031	P	2.102187	-0.008630	-0.040101
P	-2.439270	0.273670	0.007212	C	2.847783	1.594827	0.697542
P	2.352870	0.468778	0.025885	C	-0.137361	2.202135	-0.588403
C	-3.340708	-0.734778	-1.312942	H	0.844054	2.713138	-0.427043
C	-3.146936	-2.261183	-1.185153	C	-1.188185	3.222116	-0.475850
C	-3.669551	-2.984136	-2.441462	C	-0.889122	4.439560	0.204170
C	-5.143620	-2.646374	-2.721996	C	-2.496591	3.078667	-1.017739
C	-5.361838	-1.126343	-2.803862	C	-1.856219	5.438416	0.379029
C	-4.831546	-0.403439	-1.548004	H	0.127685	4.587038	0.604881
C	-3.277983	0.088881	1.694183	C	-3.454755	4.090108	-0.868024
C	-3.276742	-1.364217	2.216869	H	-2.715135	2.183070	-1.615223
C	-3.690706	-1.412837	3.699870	C	-3.146327	5.266806	-0.158115
C	-5.067590	-0.765044	3.919802	H	-1.600625	6.363399	0.920285
C	-5.106010	0.667105	3.361098	H	-4.452908	3.965746	-1.317911
C	-4.676572	0.721302	1.879446	H	-3.905119	6.056729	-0.038387
C	-2.863605	2.053427	-0.487924	P	-1.708837	-0.559259	0.146805
C	-2.256474	3.097185	0.476539	C	-2.054519	0.583387	1.644322
C	-2.716420	4.522905	0.117130	C	-3.477226	0.696390	2.240882
C	-2.394779	4.873833	-1.344742	C	-0.998165	0.414008	2.760864
C	-2.972796	3.826209	-2.309576	H	-1.853790	1.566888	1.172173
C	-2.515774	2.397928	-1.953651	C	-3.541879	1.834562	3.282294
C	2.598565	2.328198	-0.255280	H	-3.785195	-0.256854	2.723336
C	1.790054	2.819756	-1.477822	H	-4.214652	0.907585	1.441045
C	2.088989	4.297334	-1.791826	C	-1.080826	1.554113	3.793562
C	1.840462	5.198923	-0.571426	H	-1.141864	-0.551316	3.292401
C	2.614952	4.699555	0.658924	H	0.014936	0.375591	2.312652
C	2.315349	3.220400	0.973714	C	-2.492108	1.670082	4.391466
C	3.288702	-0.312377	-1.426172	H	-4.564737	1.881107	3.715425
C	4.528293	0.424164	-1.985455	H	-3.377998	2.806591	2.763606
C	5.043829	-0.268910	-3.264582	H	-0.326828	1.391970	4.594636
C	5.349548	-1.757794	-3.033501	H	-0.814136	2.517102	3.300838
C	4.131187	-2.488276	-2.446054	H	-2.544231	2.520530	5.105361
C	3.623614	-1.798455	-1.165857	H	-2.718467	0.752605	4.983018
C	3.282398	0.168759	1.644607	C	-3.334981	-0.603660	-0.861879
C	3.098289	-1.237786	2.251752	C	-3.205107	-1.154099	-2.303622
C	3.689894	-1.301513	3.672883	C	-4.566911	-1.278603	-0.198335
C	5.170937	-0.887481	3.693957	H	-3.555380	0.485859	-0.944027
C	5.367237	0.500507	3.063223	C	-4.471120	-0.831773	-3.119282
C	4.774420	0.572578	1.640459	H	-3.064935	-2.255249	-2.268975
H	-2.760339	-0.428884	-2.215346	H	-2.315112	-0.736595	-2.809265
H	-2.077825	-2.497615	-1.025392	C	-5.849190	-0.951299	-0.994200
H	-3.697271	-2.641075	-0.296460	H	-4.421632	-2.380534	-0.201037
H	-3.046089	-2.683896	-3.314313	H	-4.703158	-0.981270	0.857160
H	-3.537282	-4.081780	-2.325921	C	-5.742402	-1.392701	-2.462318
H	-5.776679	-3.061320	-1.903277	H	-4.356598	-1.230403	-4.150192
H	-5.486593	-3.137851	-3.658453	H	-4.560716	0.273972	-3.226958
H	-6.439864	-0.893099	-2.945813	H	-6.722569	-1.433414	-0.502194
H	-4.834570	-0.726661	-3.700529	H	-6.034015	0.147249	-0.947025
H	-5.428208	-0.729685	-0.666766	H	-6.650186	-1.085631	-3.026513

H	-4.996935	0.689511	-1.652142	H	-5.712918	-2.506270	-2.502769
H	-2.550427	0.648229	2.329128	C	-1.495685	-2.326229	0.860050
H	-2.274831	-1.820440	2.083038	C	-2.389430	-2.681625	2.078999
H	-3.991393	-1.978329	1.624279	C	-1.631819	-3.444690	-0.202229
H	-2.924237	-0.878324	4.305499	H	-0.437718	-2.316336	1.206949
H	-3.695973	-2.465853	4.056775	C	-2.014768	-4.060273	2.663124
H	-5.332079	-0.765688	4.999665	H	-3.454004	-2.708268	1.765787
H	-5.846094	-1.377843	3.408255	H	-2.318573	-1.920606	2.878957
H	-6.122891	1.102993	3.473322	C	-1.273774	-4.828894	0.371483
H	-4.421223	1.311893	3.958204	H	-2.685687	-3.477139	-0.554211
H	-5.426403	0.176679	1.262992	H	-1.005226	-3.213131	-1.086581
H	-4.691214	1.776068	1.534340	C	-2.112152	-5.174995	1.610788
H	-3.972645	2.104980	-0.387624	H	-2.670344	-4.282121	3.533648
H	-1.146673	3.037974	0.426940	H	-0.974296	-4.017697	3.061305
H	-2.513118	2.865908	1.530860	H	-1.408065	-5.598749	-0.418937
H	-3.816046	4.606512	0.281702	H	-0.194079	-4.849149	0.638911
H	-2.244310	5.254959	0.807922	H	-1.794250	-6.148454	2.043984
H	-2.775470	5.887644	-1.595952	H	-3.178507	-5.300749	1.311256
H	-1.288792	4.915973	-1.473408	Cl	-0.938163	1.169743	-3.257580
H	-4.086366	3.872925	-2.275692	C	4.388762	1.712948	0.794355
H	-2.685533	4.060077	-3.357719	H	2.549677	2.327428	-0.088457
H	-1.419681	2.295901	-2.111299	C	4.817509	3.131395	1.222533
H	-2.983287	1.674960	-2.652905	H	4.798232	0.978529	1.518130
H	3.680348	2.435996	-0.500685	H	4.850088	1.481487	-0.183917
H	1.979398	2.186185	-2.369002	C	4.160979	3.558644	2.543431
H	0.704129	2.701971	-1.260605	H	5.925512	3.173844	1.302241
H	1.475039	4.630169	-2.656947	H	4.536432	3.855846	0.423318
H	3.152688	4.394473	-2.111757	C	2.631943	3.458704	2.439778
H	0.750866	5.203331	-0.338026	H	4.520717	2.898169	3.366265
H	2.112157	6.251850	-0.802714	H	4.466812	4.591609	2.817155
H	2.379009	5.325054	1.547090	C	2.170588	2.053075	2.007240
H	3.708253	4.821341	0.475894	H	2.150748	3.730229	3.404239
H	2.926369	2.901611	1.843379	H	2.272290	4.203703	1.692201
H	1.256747	3.096718	1.290311	H	2.396260	1.330740	2.824157
H	2.496232	-0.291029	-2.211754	H	1.069660	2.047109	1.881669
H	4.294898	1.482799	-2.221354	C	3.205043	-0.410923	-1.534283
H	5.341950	0.439371	-1.226546	C	4.653790	-0.928316	-1.372799
H	4.270714	-0.173810	-4.061175	H	2.606505	-1.245694	-1.967417
H	5.946070	0.261568	-3.640158	C	5.200160	-1.389056	-2.741464
H	6.208126	-1.851437	-2.328342	H	5.327709	-0.143606	-0.969035
H	5.673654	-2.238153	-3.982331	H	4.697579	-1.772932	-0.655734
H	4.378422	-3.550252	-2.229435	C	5.137217	-0.263151	-3.787719
H	3.309754	-2.503948	-3.198022	H	6.244040	-1.754131	-2.623808
H	4.413684	-1.868934	-0.384592	H	4.601142	-2.257578	-3.098392
H	2.736317	-2.333879	-0.771602	C	3.710400	0.294207	-3.926114
H	2.725264	0.859469	2.319297	H	5.827119	0.558015	-3.481543
H	3.592144	-2.004189	1.616292	H	5.507202	-0.628016	-4.770498
H	2.019617	-1.486437	2.282801	C	3.138016	0.739343	-2.567765
H	3.106135	-0.623391	4.336309	H	3.689915	1.145247	-4.640500
H	3.566379	-2.326126	4.086256	H	3.041016	-0.487964	-4.348166
H	5.565754	-0.898976	4.733191	H	3.702925	1.626828	-2.198406
H	5.770030	-1.635812	3.124665	H	2.084058	1.073951	-2.712053
H	4.870274	1.267191	3.701174	C	2.362520	-1.406484	1.228045
H	6.445898	0.769406	3.035169	C	3.611494	-1.323078	2.137748
H	5.344958	-0.115413	0.976678	H	1.467944	-1.292226	1.886063
H	4.914820	1.594268	1.228781	C	3.642241	-2.470122	3.168270

C	0.024952	-1.748611	0.787744	H	4.532735	-1.370915	1.516963
H	-0.133871	-1.774431	1.895679	H	3.642663	-0.353734	2.674108
C	0.425935	-5.503181	0.797608	C	3.555698	-3.847040	2.493720
C	0.596689	-5.803869	-0.565999	H	4.563385	-2.390602	3.785784
C	0.584173	-4.763939	-1.516891	H	2.785496	-2.351847	3.871872
C	0.409172	-3.432622	-1.116305	C	2.311207	-3.934767	1.596907
C	0.232242	-3.106365	0.256738	H	4.468453	-4.012424	1.875744
C	0.243019	-4.172974	1.201613	H	3.545898	-4.655242	3.256797
H	0.433059	-6.309512	1.548431	C	2.269006	-2.799317	0.556822
H	0.737621	-6.848001	-0.888711	H	2.271458	-4.916468	1.077397
H	0.713608	-4.996557	-2.586051	H	1.400162	-3.885889	2.237201
H	0.390589	-2.615291	-1.855211	H	3.126915	-2.929045	-0.137890
H	0.103924	-3.936941	2.269745	H	1.364853	-2.863657	-0.083190

<b>1-trans<sup>+</sup></b>	<b>1-cis<sup>+</sup>c</b>
-2897.03940908	-2897.05626563

Ru	-0.030813	-0.038379	0.051761	Ru	0.008615	0.017346	0.220381
Cl	-0.042049	0.008732	-2.261964	Cl	-0.006355	-1.300470	2.121725
P	-2.418703	0.414702	0.047569	P	2.429086	-0.308302	0.009253
P	2.384264	0.391875	0.077483	P	-2.402160	-0.356040	0.039391
C	-3.423124	-0.341918	-1.354163	C	3.319292	1.085433	-0.922556
C	-3.210714	-1.860699	-1.546722	C	3.527381	2.354439	-0.064099
C	-3.883644	-2.339907	-2.847863	C	4.023442	3.531336	-0.926698
C	-5.379147	-1.986069	-2.880976	C	5.320834	3.175223	-1.669665
C	-5.602192	-0.481296	-2.657044	C	5.156150	1.886480	-2.490250
C	-4.928715	0.011838	-1.359260	C	4.646137	0.710071	-1.631330
C	-3.161326	-0.011192	1.744692	C	3.304266	-0.689602	1.635826
C	-3.397462	-1.526095	1.941277	C	3.076564	0.351676	2.756324
C	-3.763277	-1.850333	3.402806	C	3.619406	-0.175392	4.099744
C	-4.995042	-1.054552	3.863486	C	5.103676	-0.564793	4.004277
C	-4.801343	0.452120	3.632670	C	5.345373	-1.568540	2.865703
C	-4.426650	0.775842	2.171065	C	4.804331	-1.047849	1.517572
C	-2.725178	2.269575	-0.123642	C	2.747759	-1.832391	-1.055347
C	-1.984301	3.079797	0.964883	C	2.274007	-3.155515	-0.412131
C	-2.365669	4.571196	0.901019	C	2.660547	-4.360305	-1.292898
C	-2.117665	5.163092	-0.496034	C	2.121216	-4.222069	-2.725619
C	-2.810219	4.336844	-1.591503	C	2.547130	-2.889179	-3.362934
C	-2.424960	2.845223	-1.525869	C	2.165202	-1.684009	-2.480745
C	2.724029	2.242767	-0.122238	C	-2.735515	-2.041731	-0.746750
C	2.144760	2.830775	-1.429415	C	-1.993829	-2.191613	-2.094680
C	2.596046	4.291816	-1.618514	C	-2.360765	-3.514479	-2.794695
C	2.213009	5.165394	-0.413253	C	-2.112396	-4.729154	-1.885717
C	2.733519	4.568616	0.903781	C	-2.824336	-4.571162	-0.533352
C	2.298890	3.100831	1.090781	C	-2.445627	-3.252108	0.169157
C	3.314650	-0.409420	-1.360096	C	-3.242222	0.877486	-1.142117
C	4.637422	0.253702	-1.816175	C	-4.497742	0.364622	-1.892934
C	5.157316	-0.412480	-3.107715	C	-5.002255	1.411549	-2.907747
C	5.330824	-1.930892	-2.947538	C	-5.278626	2.771498	-2.249584
C	4.031651	-2.590064	-2.457282	C	-4.043204	3.275111	-1.487673
C	3.517325	-1.929894	-1.163264	C	-3.543304	2.235516	-0.466149
C	3.227390	0.004448	1.733625	C	-3.317745	-0.437932	1.686887
C	3.045374	-1.430199	2.279209	C	-3.039136	0.735054	2.653786
C	3.593903	-1.546982	3.716380	C	-3.663024	0.460626	4.036835
C	5.070618	-1.127478	3.797716	C	-5.170396	0.175899	3.939206
C	5.276791	0.282478	3.224923	C	-5.453969	-0.975316	2.961706
C	4.722297	0.406163	1.791583	C	-4.836028	-0.714084	1.572226
H	-2.943623	0.150741	-2.232627	H	2.581597	1.343997	-1.720100
H	-2.128623	-2.095077	-1.569538	H	2.594837	2.632520	0.467445
H	-3.643292	-2.420335	-0.689575	H	4.287846	2.141092	0.718587
H	-3.369998	-1.868317	-3.716676	H	3.232021	3.802985	-1.662124
H	-3.740235	-3.435997	-2.958694	H	4.172895	4.425905	-0.285379
H	-5.910870	-2.558584	-2.086288	H	6.141598	3.037728	-0.929070
H	-5.831885	-2.302495	-3.844508	H	5.635591	4.013627	-2.326644
H	-6.687409	-0.245933	-2.623972	H	6.117076	1.601985	-2.969609
H	-5.186596	0.087773	-3.519889	H	4.436288	2.065515	-3.322111
H	-5.422960	-0.473120	-0.488005	H	5.413708	0.450723	-0.870220
H	-5.088882	1.104908	-1.245911	H	4.525512	-0.184430	-2.274988
H	-2.339605	0.290933	2.439505	H	2.750049	-1.604279	1.950155
H	-2.510266	-2.114673	1.626453	H	1.995813	0.578957	2.849979
H	-4.232926	-1.848262	1.281718	H	3.594033	1.301915	2.504275
H	-2.896402	-1.609918	4.061241	H	3.019590	-1.061952	4.407311
H	-3.941192	-2.941819	3.508651	H	3.467678	0.591840	4.888862

H	-5.210901	-1.257372	4.933789		H	5.456723	-0.985552	4.969632
H	-5.888283	-1.402004	3.295758		H	5.714452	0.349575	3.823270
H	-5.721091	1.010952	3.907883		H	6.428127	-1.797092	2.767210
H	-3.997101	0.830456	4.305064		H	4.843995	-2.533249	3.108494
H	-5.273918	0.505537	1.504013		H	5.380235	-0.142451	1.222302
H	-4.279069	1.869875	2.067403		H	4.981005	-1.807360	0.726799
H	-3.820235	2.381130	0.051997		H	3.856880	-1.880728	-1.145744
H	-0.885774	2.967469	0.810113		H	1.168456	-3.129478	-0.278537
H	-2.193748	2.679592	1.979502		H	2.701754	-3.280664	0.604003
H	-3.442847	4.679453	1.164746		H	3.770799	-4.447046	-1.322209
H	-1.801779	5.137165	1.673108		H	2.291153	-5.297740	-0.825262
H	-2.457780	6.219494	-0.534083		H	2.460159	-5.074592	-3.351307
H	-1.021091	5.184588	-0.692128		H	1.008587	-4.278075	-2.704500
H	-3.914923	4.430853	-1.481406		H	3.650695	-2.887396	-3.516381
H	-2.565833	4.739784	-2.597270		H	2.096086	-2.774268	-4.371747
H	-1.343930	2.719750	-1.758623		H	1.054501	-1.611618	-2.413528
H	-2.974132	2.285940	-2.310909		H	2.508667	-0.742805	-2.959783
H	3.834675	2.295338	-0.193535		H	-3.830007	-2.033494	-0.953770
H	2.437814	2.222015	-2.309377		H	-2.207178	-1.334372	-2.768557
H	1.033115	2.787072	-1.391742		H	-0.895547	-2.167387	-1.901912
H	2.157217	4.700805	-2.553498		H	-1.788971	-3.608304	-3.742782
H	3.701052	4.317158	-1.759700		H	-3.435914	-3.482138	-3.084991
H	1.103026	5.249279	-0.363731		H	-1.017127	-4.838362	-1.711602
H	2.594132	6.200022	-0.545345		H	-2.439341	-5.662424	-2.390885
H	2.390582	5.172753	1.770794		H	-2.588628	-5.427054	0.134103
H	3.846550	4.617145	0.916165		H	-3.926912	-4.596995	-0.691655
H	2.732525	2.710052	2.034483		H	-3.005575	-3.170143	1.123136
H	1.191903	3.047959	1.208861		H	-1.368118	-3.263010	0.445880
H	2.569709	-0.281412	-2.180537		H	-2.449808	1.057745	-1.908236
H	4.503864	1.339302	-1.999157		H	-4.288011	-0.583838	-2.427610
H	5.406919	0.158221	-1.018928		H	-5.304028	0.144439	-1.159747
H	4.438996	-0.207372	-3.934193		H	-4.238695	1.536413	-3.710075
H	6.116726	0.061380	-3.406281		H	-5.915125	1.024810	-3.408828
H	6.144990	-2.133448	-2.214137		H	-6.132934	2.671909	-1.541383
H	5.658868	-2.385020	-3.906566		H	-5.594775	3.513732	-3.012872
H	4.185042	-3.677060	-2.285900		H	-4.266008	4.229591	-0.964871
H	3.249621	-2.503767	-3.245902		H	-3.225101	3.499962	-2.209801
H	4.263975	-2.101354	-0.356035		H	-4.328869	2.086008	0.306226
H	2.576078	-2.416147	-0.832972		H	-2.647977	2.621041	0.062222
H	2.667646	0.680575	2.423214		H	-2.829835	-1.332074	2.139185
H	3.579791	-2.153358	1.627526		H	-3.460443	1.678509	2.245375
H	1.976694	-1.725839	2.258120		H	-1.946114	0.883598	2.758544
H	2.988223	-0.901416	4.393722		H	-3.148615	-0.412900	4.498435
H	3.463141	-2.588657	4.079749		H	-3.471313	1.324576	4.708540
H	5.429680	-1.176292	4.847464		H	-5.586536	-0.058527	4.941857
H	5.690818	-1.852936	3.223157		H	-5.698247	1.093608	3.590958
H	4.767361	1.027655	3.878282		H	-5.034830	-1.922108	3.372909
H	6.354023	0.553767	3.228165		H	-6.547392	-1.140424	2.854818
H	5.301325	-0.262361	1.117284		H	-5.337238	0.166767	1.112642
H	4.881771	1.440183	1.423142		H	-5.042723	-1.578656	0.906117
C	-0.065643	-1.737131	0.694909		C	0.015440	1.706610	0.950644
H	-0.159749	-1.580225	1.818620		H	0.036731	1.833883	2.055985
C	-0.058039	-5.503170	0.848776		C	-0.120879	5.372178	-0.009776
C	0.061405	-5.839947	-0.512551		C	-0.097988	5.287996	-1.413897
C	0.148404	-4.825557	-1.488399		C	-0.031800	4.028968	-2.048971
C	0.114528	-3.478557	-1.111966		C	0.009384	2.864148	-1.276097

C	-0.012119	-3.121504	0.260649	C	-0.016029	2.927741	0.146966
C	-0.094991	-4.156937	1.235236	C	-0.079017	4.204363	0.767121
H	-0.123117	-6.295082	1.610861	H	-0.170711	6.356108	0.481974
H	0.088821	-6.898240	-0.816161	H	-0.129639	6.206172	-2.020977
H	0.244082	-5.093430	-2.552113	H	-0.010584	3.966898	-3.148130
H	0.184384	-2.676658	-1.863530	H	0.065736	1.878509	-1.779454
H	-0.190277	-3.892964	2.301119	H	-0.097140	4.269423	1.866996

2-trans	2-cis
-3379.22534264	-3379.21104354

Ru	0.161925	0.072910	0.040957	Ru	-0.020166	0.687113	-0.945476
Cl	0.241399	1.244118	2.128130	Cl	-1.617907	1.029761	-2.699234
Cl	0.127117	0.109695	-2.331846	P	-1.768873	-0.620184	-0.036642
P	2.552719	0.069397	-0.002711	C	-0.358991	3.404460	0.238769
C	-0.686202	-2.851532	0.256653	C	-0.154004	1.964822	0.415525
C	0.181068	-1.712877	0.563576	H	-0.071634	1.691138	1.494196
H	1.007792	-1.995550	1.260743	P	1.884587	-0.248585	0.061120
P	-2.230726	0.558204	0.035610	C	-3.470277	0.150538	-0.015168
C	3.346518	-0.662743	-1.512505	C	-3.655702	1.533531	-0.212752
C	2.839446	-1.877202	-2.025480	C	-4.587392	-0.653645	0.309876
C	4.465345	-0.066414	-2.132761	C	-4.937200	2.101056	-0.093882
C	3.451712	-2.490988	-3.130008	H	-2.798611	2.166467	-0.479309
H	1.952505	-2.338440	-1.564226	C	-5.868131	-0.086478	0.411826
C	5.070653	-0.679377	-3.244740	H	-4.458603	-1.732751	0.491000
H	4.867341	0.882909	-1.746170	C	-6.045932	1.294448	0.211414
C	4.567016	-1.892727	-3.743785	H	-5.065652	3.183395	-0.253070
H	3.044267	-3.436268	-3.522259	H	-6.730139	-0.727505	0.656836
H	5.941525	-0.202677	-3.722625	H	-7.049916	1.740514	0.295455
H	5.040392	-2.370564	-4.616464	C	-1.952995	-2.134665	-1.088677
C	3.167905	1.814302	0.006979	C	-0.987657	-3.164791	-0.995570
C	4.086467	2.302606	0.958881	C	-2.964174	-2.231912	-2.070552
C	2.650839	2.692144	-0.975596	C	-1.055333	-4.285769	-1.840633
C	4.484428	3.651588	0.927813	H	-0.170481	-3.091793	-0.261000
H	4.492067	1.629812	1.729930	C	-3.021419	-3.350387	-2.919498
C	3.058597	4.035493	-1.005475	H	-3.698504	-1.421506	-2.184001
H	1.929056	2.316755	-1.720834	C	-2.074334	-4.382689	-2.804143
C	3.973914	4.519338	-0.052471	H	-0.300068	-5.082539	-1.748985
H	5.200187	4.024371	1.677910	H	-3.812821	-3.409118	-3.683514
H	2.653673	4.708957	-1.777636	H	-2.124664	-5.257903	-3.471290
H	4.288187	5.575113	-0.073643	C	-1.822561	-1.240056	1.728270
C	3.476440	-0.784936	1.371163	C	-1.908922	-2.598904	2.096093
C	4.619657	-1.576530	1.112846	C	-1.908428	-0.256551	2.742897
C	3.018061	-0.655904	2.704159	C	-2.070008	-2.963689	3.445680
C	5.293027	-2.218987	2.166663	H	-1.871004	-3.385687	1.328912
H	4.987713	-1.694685	0.082840	C	-2.070607	-0.622543	4.087844
C	3.699078	-1.298318	3.752524	H	-1.885711	0.811679	2.474874
H	2.125163	-0.043593	2.912333	C	-2.151305	-1.980911	4.444999
C	4.836498	-2.081430	3.488700	H	-2.141298	-4.030438	3.711756
H	6.181956	-2.832362	1.948423	H	-2.147942	0.159555	4.860158
H	3.331463	-1.185464	4.785122	H	-2.287750	-2.270445	5.499178
H	5.366059	-2.586393	4.312563	C	1.763316	-1.544118	1.396392
C	-3.055886	0.508450	1.699108	C	1.384369	-1.157868	2.703351
C	-2.741560	-0.545638	2.584775	C	2.081189	-2.898924	1.154325
C	-4.008279	1.474276	2.089316	C	1.345668	-2.099268	3.743528
C	-3.380352	-0.639317	3.832252	H	1.144310	-0.105295	2.921000
H	-1.985762	-1.292287	2.297792	C	2.024805	-3.844298	2.195730
C	-4.637642	1.383609	3.343420	H	2.401719	-3.216263	0.150256
H	-4.256821	2.307484	1.414070	C	1.664446	-3.446504	3.493096
C	-4.327636	0.326517	4.216171	H	1.061280	-1.777335	4.757179
H	-3.125660	-1.466460	4.513869	H	2.283358	-4.895391	1.989548
H	-5.373578	2.148323	3.639439	H	1.634522	-4.183597	4.311197
H	-4.820044	0.258579	5.199488	C	3.113476	0.922009	0.845961
C	-3.437830	-0.371483	-1.032524	C	3.149791	2.275430	0.444096
C	-3.267945	-0.363019	-2.439174	C	4.037132	0.473092	1.820363
C	-4.514934	-1.098251	-0.478303	C	4.083831	3.160174	1.010584
C	-4.162022	-1.062963	-3.265522	H	2.462949	2.624892	-0.342127

H	-2.418916	0.180867	-2.880936	C	4.971243	1.361678	2.381169
C	-5.404446	-1.799845	-1.311704	H	4.027816	-0.575686	2.153279
H	-4.665310	-1.117858	0.611299	C	4.995347	2.708670	1.980178
C	-5.233409	-1.783726	-2.706010	H	4.096573	4.212241	0.684276
H	-4.017720	-1.043823	-4.357770	H	5.682427	0.995396	3.138962
H	-6.239907	-2.360326	-0.862430	H	5.725701	3.404880	2.422967
H	-5.934594	-2.330084	-3.357150	C	2.870088	-1.139721	-1.243008
C	-2.486390	2.319967	-0.521480	C	4.278437	-1.213565	-1.201708
C	-3.595352	2.707876	-1.307333	C	2.179523	-1.774822	-2.298822
C	-1.548838	3.303948	-0.130272	C	4.980826	-1.916485	-2.196358
C	-3.756866	4.048408	-1.700147	H	4.835980	-0.707308	-0.399242
H	-4.340246	1.960443	-1.618199	C	2.883437	-2.482758	-3.286984
C	-1.715807	4.642190	-0.524856	H	1.081709	-1.704645	-2.363824
H	-0.694014	3.025108	0.506714	C	4.286641	-2.554657	-3.238694
C	-2.816689	5.018653	-1.313761	H	6.081220	-1.956688	-2.158243
H	-4.626584	4.332977	-2.313996	H	2.328899	-2.965291	-4.107174
H	-0.974689	5.394285	-0.210711	H	4.840329	-3.099212	-4.020181
H	-2.943083	6.067653	-1.626258	C	-0.396927	4.221562	1.407390
C	-0.738072	-3.937868	1.178940	C	-0.583256	5.606434	1.317690
C	-1.525053	-5.066384	0.917249	C	-0.739608	6.210749	0.055164
C	-2.247696	-5.156629	-0.289054	C	-0.709182	5.421082	-1.110476
C	-2.177757	-4.110036	-1.227219	C	-0.520941	4.034957	-1.029070
C	-1.415783	-2.964282	-0.957239	H	-0.271436	3.745411	2.394349
H	-0.149577	-3.877767	2.109665	H	-0.606672	6.219701	2.232616
H	-1.566408	-5.888821	1.649393	H	-0.886756	7.300314	-0.019546
H	-2.855778	-6.050577	-0.501608	H	-0.833024	5.893164	-2.098036
H	-2.725152	-4.184659	-2.179910	H	-0.499723	3.417036	-1.939257
H	-1.340212	-2.151610	-1.693812	Cl	1.541763	1.671232	-2.466809

2-trans <sup>+</sup>	2-cis <sup>+</sup> c
-2918.80104350	-2918.81412383

Ru	-0.027310	0.127695	-0.108847	Ru	-0.043552	-0.251774	-1.274089
Cl	-0.105548	0.302570	-2.418603	Cl	-0.463634	0.165459	-3.503759
P	-2.371634	-0.291606	0.010300	P	1.958191	-0.223922	-0.093824
C	0.249070	3.176652	0.246819	C	-1.561987	-2.853627	-0.691568
C	0.077842	1.794259	0.647999	C	-0.363240	-2.030885	-0.788924
H	-0.016690	1.629483	1.762577	H	0.561965	-2.644274	-0.664116
P	2.291607	-0.503261	-0.019257	P	-1.444904	0.817144	0.201185
C	-3.588263	0.731647	-0.909117	C	3.189059	-0.369899	-1.471844
C	-3.293219	2.089501	-1.162816	C	2.974996	-1.363010	-2.459319
C	-4.819997	0.187696	-1.339706	C	4.325588	0.464795	-1.566269
C	-4.229177	2.898351	-1.828275	C	3.877803	-1.511036	-3.523603
H	-2.326340	2.510948	-0.848668	H	2.099450	-2.029833	-2.405435
C	-5.749086	1.002900	-2.007512	C	5.226411	0.310032	-2.634433
H	-5.053958	-0.872892	-1.158184	H	4.516467	1.231886	-0.801502
C	-5.456032	2.356745	-2.251109	C	5.003162	-0.672193	-3.614911
H	-3.993307	3.955440	-2.026617	H	3.697440	-2.283263	-4.287306
H	-6.707139	0.575238	-2.342074	H	6.110804	0.963173	-2.697356
H	-6.185230	2.990760	-2.779456	H	5.708683	-0.786185	-4.452640
C	-2.714032	-2.036567	-0.484381	C	2.467507	1.282942	0.841481
C	-3.320124	-2.958129	0.399856	C	2.936719	1.202659	2.172421
C	-2.382359	-2.440044	-1.800462	C	2.407170	2.542978	0.200446
C	-3.592697	-4.268291	-0.031444	C	3.334915	2.368953	2.849289
H	-3.591596	-2.652737	1.421770	H	3.000663	0.228499	2.679586
C	-2.664495	-3.749140	-2.222661	C	2.809004	3.702890	0.881708
H	-1.902781	-1.727955	-2.491486	H	2.059849	2.621509	-0.841154
C	-3.267347	-4.665016	-1.340470	C	3.270614	3.618345	2.208185
H	-4.070773	-4.979539	0.660239	H	3.707067	2.296599	3.883304
H	-2.410352	-4.054619	-3.249726	H	2.763140	4.677272	0.371445
H	-3.487360	-5.690766	-1.675882	H	3.587780	4.528736	2.740526
C	-2.807743	-0.164882	1.795952	C	2.374750	-1.637098	1.030702
C	-3.909594	0.590169	2.252247	C	3.655006	-2.234062	0.971972
C	-1.956985	-0.797558	2.736636	C	1.433974	-2.101486	1.978210
C	-4.157995	0.704887	3.631705	C	3.986277	-3.280996	1.849801
H	-4.574499	1.087873	1.529624	H	4.397145	-1.887188	0.237101
C	-2.212820	-0.680568	4.112765	C	1.775158	-3.145204	2.855394
H	-1.096395	-1.396859	2.390488	H	0.430846	-1.651635	2.034092
C	-3.313626	0.072357	4.561438	C	3.049247	-3.737705	2.792361
H	-5.022069	1.291581	3.980921	H	4.984260	-3.742825	1.791523
H	-1.551291	-1.181436	4.836736	H	1.036334	-3.498125	3.591648
H	-3.515157	0.164053	5.640170	H	3.310946	-4.559415	3.477294
C	2.760746	-0.706025	1.758425	C	-1.392259	0.312981	1.970232
C	2.838660	0.446001	2.578270	C	-2.123372	-0.831095	2.376181
C	3.006822	-1.976563	2.324934	C	-0.557509	0.966343	2.906393
C	3.163216	0.326286	3.938409	C	-2.044069	-1.287150	3.702503
H	2.661394	1.444628	2.146124	H	-2.758023	-1.369476	1.655744
C	3.322803	-2.090196	3.690883	C	-0.485081	0.503597	4.231903
H	2.961054	-2.879956	1.697797	H	0.044385	1.836178	2.606185
C	3.401215	-0.943180	4.498791	C	-1.231456	-0.616938	4.635299
H	3.234085	1.229307	4.564941	H	-2.626105	-2.170588	4.008197
H	3.517505	-3.084699	4.122034	H	0.160722	1.027531	4.953594
H	3.653708	-1.035822	5.566677	H	-1.178359	-0.970592	5.676840
C	3.614527	0.533676	-0.768742	C	-3.240516	0.802730	-0.282282
C	3.369813	1.143615	-2.021278	C	-3.578794	0.886715	-1.652610
C	4.872673	0.693183	-0.143790	C	-4.263690	0.881593	0.690197
C	4.378459	1.901806	-2.638471	C	-4.920858	1.025882	-2.041744
H	2.391685	1.015141	-2.511517	H	-2.792876	0.839865	-2.424054

C	5.872959	1.458035	-0.768524	C	-5.605160	1.017964	0.291439
H	5.077066	0.220947	0.829385	H	-4.024538	0.848515	1.763260
C	5.628454	2.062320	-2.014236	C	-5.937822	1.086384	-1.071854
H	4.183961	2.371861	-3.615265	H	-5.170853	1.088498	-3.112389
H	6.851237	1.578445	-0.277176	H	-6.393800	1.075897	1.057994
H	6.415490	2.660089	-2.500185	H	-6.989771	1.193948	-1.379281
C	2.456896	-2.171707	-0.780483	C	-1.112963	2.637365	0.089638
C	3.611679	-2.546920	-1.500920	C	-1.461293	3.528003	1.130570
C	1.389510	-3.089926	-0.645241	C	-0.654959	3.157209	-1.142973
C	3.696989	-3.829438	-2.069478	C	-1.317419	4.913656	0.947234
H	4.443933	-1.836686	-1.621972	H	-1.865418	3.151189	2.081977
C	1.481776	-4.370783	-1.213514	C	-0.519339	4.544638	-1.320958
H	0.477314	-2.804465	-0.091941	H	-0.427177	2.481644	-1.985687
C	2.636289	-4.741277	-1.926385	C	-0.842958	5.424745	-0.274037
H	4.600189	-4.116068	-2.630452	H	-1.592347	5.599312	1.764052
H	0.645176	-5.077840	-1.103667	H	-0.168523	4.936679	-2.288473
H	2.707852	-5.744133	-2.375754	H	-0.741348	6.512267	-0.414616
C	0.278006	4.176872	1.264173	C	-1.435974	-4.129338	-0.062524
C	0.435686	5.527750	0.931714	C	-2.544614	-4.972492	0.078925
C	0.564760	5.907342	-0.417796	C	-3.796829	-4.579361	-0.431763
C	0.537349	4.930935	-1.435090	C	-3.932545	-3.339644	-1.087834
C	0.384114	3.578494	-1.113645	C	-2.832460	-2.483418	-1.213677
H	0.171282	3.877877	2.319634	H	-0.452352	-4.443485	0.322715
H	0.456163	6.290323	1.725555	H	-2.431945	-5.948960	0.575298
H	0.687452	6.970139	-0.679558	H	-4.665505	-5.249608	-0.335505
H	0.638842	5.233474	-2.488954	H	-4.903891	-3.045170	-1.514255
H	0.357567	2.807988	-1.899102	H	-2.937523	-1.532229	-1.751334

3-trans

3-cis

-3257.37438753				-3257.35887501		
Ru	0.097372	-0.337987	0.071594	Ru	0.251108	-0.236128
P	-1.112980	1.824864	0.151823	Cl	0.971112	-1.745984
Cl	-0.127285	-0.335289	-2.346215	C	0.166915	-2.011311
Cl	-0.150295	-0.407039	2.503126	N	1.230238	-2.750406
C	-0.778192	2.879373	1.684808	N	-0.879056	-2.915488
C	0.711732	3.154347	1.979631	C	0.894409	-4.171753
C	0.884036	3.787322	3.373593	C	-0.415311	-4.317120
C	0.051978	5.071825	3.527740	C	2.513280	-2.325779
C	-1.428377	4.817113	3.199477	C	-2.305627	-2.709465
C	-1.603408	4.181234	1.804860	C	2.598972	-1.739153
H	-1.112298	2.172286	2.479432	C	3.869675	-1.441641
H	1.281105	2.205895	1.927566	C	5.056061	-1.737958
H	1.140504	3.836201	1.213551	C	4.939189	-2.348771
H	1.959675	3.997166	3.561530	C	3.692521	-2.658848
H	0.570391	3.047091	4.144614	C	1.356045	-1.463366
H	0.449333	5.851824	2.837087	H	3.931594	-0.980945
H	0.155575	5.484588	4.554979	H	5.853452	-2.595929
H	-2.010291	5.763042	3.257764	C	3.633375	-3.346077
H	-1.863257	4.134938	3.965875	C	-3.004384	-2.694990
H	-2.681345	3.997643	1.611062	C	-4.412086	-2.591742
H	-1.264319	4.909224	1.033804	C	-5.148127	-2.533932
C	-2.979156	1.535274	0.271916	C	-4.434380	-2.629601
C	-3.501478	0.631138	-0.867762	C	-3.031149	-2.747408
C	-5.041863	0.602013	-0.871755	C	-2.313873	-2.876343
C	-5.605378	0.153091	0.487144	H	-4.950653	-2.574967
C	-5.033405	0.988064	1.644899	H	-4.987845	-2.644388
C	-3.491325	1.020280	1.634430	C	-2.348336	-3.037511
H	-3.417758	2.549201	0.124978	C	6.412909	-1.397284
H	-3.118207	0.963427	-1.854726	C	-6.652588	-2.380944
H	-3.108268	-0.401230	-0.727775	H	-0.255145	-4.731465
H	-5.425450	1.620650	-1.115072	H	1.695927	-4.831797
H	-5.403905	-0.066496	-1.682867	C	1.906787	0.256053
H	-5.336119	-0.914272	0.647661	H	2.042027	0.339338
H	-6.716360	0.204273	0.484831	C	3.127655	0.634677
H	-5.394874	0.595745	2.620529	C	4.268035	0.997780
H	-5.416809	2.032776	1.570547	C	3.239016	0.692304
H	-3.133463	1.660957	2.466442	C	5.464330	1.397833
H	-3.079403	0.006714	1.830599	H	4.198491	0.953062
C	-0.964396	2.880726	-1.417485	C	4.440427	1.091917
C	0.380465	3.638377	-1.484680	H	2.367132	0.421060
C	0.599435	4.263728	-2.875124	C	5.554318	1.445505
C	-0.560317	5.193680	-3.265600	H	6.331558	1.676668
C	-1.910402	4.465661	-3.166434	H	4.506734	1.130807
C	-2.130045	3.831827	-1.776377	H	6.493378	1.762201
H	-0.923857	2.077842	-2.192062	P	-0.781493	1.596327
H	0.389533	4.448804	-0.721254	C	0.274376	3.161060
H	1.220903	2.958920	-1.239810	C	-0.456315	4.509150
H	0.689383	3.446757	-3.626884	C	1.461136	3.339443
H	1.565368	4.813679	-2.893534	H	0.694247	2.887164
H	-0.411585	5.595579	-4.291667	C	0.523153	5.585300
H	-0.568191	6.076436	-2.584290	H	-0.911253	4.857282
H	-2.747033	5.160949	-3.397573	H	-1.282824	4.400935
H	-1.950022	3.662031	-3.937315	C	2.440956	4.411966
H	-2.215905	4.640056	-1.015655	H	1.094307	3.647633
H	-3.101962	3.297440	-1.778813	H	2.004397	2.384967

C	1.811636	0.323666	0.317400	C	1.734539	5.755763	0.115965
C	2.863460	0.948489	-0.505262	H	-0.013468	6.551512	-0.937943
C	2.861388	1.060690	-1.922426	H	0.876203	5.291582	-1.829326
C	3.925936	1.677109	-2.593936	H	3.277564	4.535745	1.078939
C	5.013232	2.214373	-1.877051	H	2.898001	4.054283	-0.592803
C	5.032493	2.122144	-0.473702	H	2.446110	6.499122	-0.304985
C	3.977617	1.489359	0.199513	H	1.392304	6.171645	1.092652
H	2.130706	0.289182	1.387863	C	-2.453656	1.996643	-0.602391
H	2.001547	0.657094	-2.478777	C	-3.190697	0.734884	-1.098374
H	3.904845	1.747838	-3.693493	C	-3.439120	2.928699	0.137097
H	5.841602	2.706685	-2.411871	H	-2.091465	2.518431	-1.517749
H	5.874298	2.544315	0.098556	C	-4.376626	1.109414	-2.006689
H	3.999558	1.406366	1.298148	H	-3.554972	0.131012	-0.238034
C	0.481410	-2.361638	0.149188	H	-2.489196	0.089718	-1.666810
N	-0.471318	-3.347226	0.120912	C	-4.620424	3.312216	-0.778166
N	1.680566	-2.976146	0.393540	H	-3.838576	2.409977	1.037005
C	1.578955	-4.450005	0.479267	H	-2.936346	3.847242	0.497767
C	0.065264	-4.688078	0.445933	C	-5.353691	2.071629	-1.312013
H	2.057094	-4.820251	1.409747	H	-4.903234	0.186133	-2.330476
H	2.110952	-4.919137	-0.378766	H	-3.980860	1.586902	-2.931730
H	-0.333440	-5.033780	1.424729	H	-5.322141	3.976694	-0.227811
H	-0.245879	-5.425845	-0.323027	H	-4.232964	3.908358	-1.636143
C	3.007575	-2.427528	0.397581	H	-6.169042	2.370893	-2.006315
C	3.696722	-2.281181	-0.836929	H	-5.845811	1.546315	-0.460228
C	5.041255	-1.869828	-0.802095	C	-1.019017	1.531948	2.096337
C	5.714680	-1.615420	0.410522	C	-1.393251	2.840980	2.837093
C	5.002920	-1.781098	1.614079	C	-1.986705	0.403724	2.506389
C	3.654486	-2.194114	1.638501	H	0.001647	1.238160	2.442646
C	3.001376	-2.547528	-2.150003	C	-1.388902	2.632325	4.364816
C	7.159331	-1.168997	0.406706	H	-2.406996	3.169738	2.529442
C	2.927326	-2.381770	2.948722	H	-0.703082	3.665580	2.572137
H	5.578966	-1.742731	-1.756527	C	-2.021999	0.201082	4.033390
H	5.513790	-1.591956	2.573509	H	-3.011548	0.651905	2.150475
H	2.134727	-1.866670	-2.296923	H	-1.703965	-0.534080	1.989151
H	2.600091	-3.582848	-2.202947	C	-2.346884	1.505082	4.780490
H	3.697054	-2.414280	-3.001075	H	-1.661264	3.582754	4.873457
H	7.798300	-1.866788	-0.175188	H	-0.355400	2.384453	4.701498
H	7.572347	-1.103600	1.433095	H	-2.761751	-0.586339	4.294562
H	7.264019	-0.168299	-0.065670	H	-1.031854	-0.177632	4.375945
H	3.549088	-2.036182	3.798070	H	-2.309297	1.343305	5.879765
H	1.963605	-1.825939	2.963900	H	-3.392523	1.811530	4.545870
H	2.684997	-3.451770	3.135021	H	0.785566	-4.370780	1.794779
C	-1.880342	-3.268043	-0.171574	H	-1.163993	-4.947055	0.454181
C	-2.303928	-3.444106	-1.518219	Cl	-0.106961	1.317555	-2.881359
C	-3.687316	-3.521714	-1.777805	H	7.143754	-2.215162	2.491403
C	-4.647691	-3.477513	-0.748970	H	6.834113	-0.487585	2.177943
C	-4.189577	-3.348778	0.577579	H	6.360996	-1.200770	3.749662
C	-2.819419	-3.250314	0.896713	H	4.591482	-3.230632	-1.643063
C	-1.312329	-3.583645	-2.645926	H	3.456943	-4.439971	-0.985040
C	-6.125981	-3.562539	-1.056154	H	2.812662	-2.939313	-1.727524
C	-2.383755	-3.182259	2.341135	H	1.591535	-0.866798	3.969118
H	-4.019544	-3.654996	-2.821145	H	0.594438	-0.920968	2.470696
H	-4.920451	-3.349179	1.403989	H	0.879025	-2.407298	3.410039
H	-0.784254	-2.620579	-2.823356	H	-7.116020	-2.805106	0.655843
H	-0.533194	-4.341627	-2.418069	H	-6.944714	-1.308471	-0.305733
H	-1.819896	-3.885783	-3.582854	H	-7.106679	-2.878631	-1.139053

H	-6.316073	-4.088508	-2.013508	H	-2.940909	-2.652974	3.165419
H	-6.573975	-2.548072	-1.144793	H	-2.247767	-4.135895	2.464491
H	-6.680941	-4.090932	-0.254093	H	-1.330738	-2.609204	2.373950
H	-3.256560	-3.032929	3.007052	H	-2.940471	-2.488589	-3.628207
H	-1.891432	-4.127203	2.662244	H	-1.318720	-2.391634	-2.851703
H	-1.658329	-2.358893	2.520040	H	-2.146865	-3.958740	-3.000635

3-trans <sup>+</sup>				3-cis <sup>+</sup> c			
-2796.95303728				-2796.96555843			
Ru	0.146468	-0.338306	-0.097092	Ru	-0.102211	-0.616309	-0.765600
Cl	0.129803	-0.203872	-2.436571	C	0.319459	-1.688516	0.918316
C	0.966509	-2.229074	-0.272260	N	1.405899	-1.945379	1.706165
N	2.263988	-2.629810	-0.211973	N	-0.660307	-2.595201	1.264321
N	0.191146	-3.325160	-0.502041	C	1.127053	-3.000289	2.716920
C	2.421887	-4.082780	-0.485249	C	-0.180029	-3.627641	2.210780
C	0.968775	-4.587261	-0.515361	C	2.747226	-1.417588	1.643270
C	3.443109	-1.838325	0.016402	C	-1.776907	-2.825056	0.394577
C	-1.249790	-3.365138	-0.474188	C	3.156094	-0.402531	2.547540
C	3.906317	-1.677326	1.348055	C	4.498250	0.028293	2.517410
C	5.116679	-0.986399	1.554862	C	5.452413	-0.548572	1.658061
C	5.877230	-0.477939	0.482777	C	5.024852	-1.589272	0.807800
C	5.387065	-0.664555	-0.826766	C	3.693847	-2.046575	0.785307
C	4.181466	-1.341467	-1.090335	C	2.219346	0.178713	3.578498
C	3.135886	-2.243501	2.519558	H	4.810338	0.826573	3.211657
H	5.484835	-0.857867	2.586461	H	5.757085	-2.074052	0.141144
H	5.966708	-0.272562	-1.678914	C	3.318023	-3.181752	-0.137670
C	3.700402	-1.535407	-2.508824	C	-1.543882	-3.022648	-1.004347
C	-1.965477	-3.444302	-1.701062	C	-2.654606	-3.236722	-1.847407
C	-3.368799	-3.557058	-1.641613	C	-3.967957	-3.318817	-1.347314
C	-4.071041	-3.617051	-0.420493	C	-4.154043	-3.169321	0.042256
C	-3.325925	-3.566212	0.774596	C	-3.089784	-2.914013	0.928961
C	-1.920120	-3.466091	0.776346	C	-0.151334	-3.161402	-1.586540
C	-1.253525	-3.443003	-3.031683	H	-2.477288	-3.375764	-2.925815
H	-3.930982	-3.615090	-2.588287	H	-5.174572	-3.238553	0.454048
H	-3.852491	-3.641489	1.741140	C	-3.365263	-2.750574	2.405910
C	-1.165702	-3.575828	2.083270	C	6.898033	-0.109556	1.684481
C	7.193718	0.225575	0.718117	C	-5.129505	-3.588226	-2.274840
C	-5.571814	-3.795715	-0.393060	H	-0.017091	-4.589367	1.673496
H	0.733357	-5.184842	-1.419165	H	1.969347	-3.718776	2.766729
H	2.946062	-4.227820	-1.454041	C	1.653691	0.012517	-0.920007
C	1.629122	0.661230	0.407875	H	2.090941	0.587525	-0.076533
H	1.858315	0.556112	1.501123	C	2.598416	-0.119115	-2.026392
C	2.537547	1.623098	-0.212405	C	3.917207	0.394576	-1.831290
C	3.471260	2.273312	0.649573	C	2.282671	-0.681479	-3.299119
C	2.541221	1.978030	-1.591141	C	4.875327	0.335873	-2.849831
C	4.358236	3.241508	0.160542	H	4.175729	0.841434	-0.858222
H	3.489228	2.006086	1.718635	C	3.244436	-0.732949	-4.315633
C	3.436789	2.938279	-2.076036	H	1.256939	-1.025634	-3.497780
H	1.830106	1.480664	-2.266763	C	4.542096	-0.231319	-4.095206
C	4.344202	3.576324	-1.205773	H	5.885600	0.739439	-2.679310
H	5.064188	3.736385	0.845577	H	2.978755	-1.156770	-5.296660
H	3.428024	3.198483	-3.146213	H	5.292820	-0.272408	-4.900267
H	5.040261	4.336346	-1.594821	P	-0.878744	1.476806	0.049065
P	-1.399240	1.512501	0.322320	C	0.067405	2.853869	-0.878270
C	-1.154277	1.458237	2.191941	C	-0.735825	4.095231	-1.336304
C	-2.209693	2.030587	3.161789	C	1.379455	3.307916	-0.191133
C	-0.873869	-0.024174	2.544162	H	0.338883	2.298351	-1.804253
H	-0.204522	2.027999	2.328395	C	0.112952	4.962429	-2.290096
C	-1.754384	1.872908	4.627055	H	-1.035236	4.706547	-0.455795
H	-3.173164	1.491739	3.019211	H	-1.666959	3.794304	-1.856651
H	-2.407824	3.098240	2.937612	C	2.230961	4.168009	-1.146463
C	-0.407923	-0.197310	4.002183	H	1.141460	3.910947	0.711320
H	-1.788153	-0.630357	2.364486	H	1.976751	2.445333	0.166576

H	-0.066517	-0.513685	1.891884	C	1.446363	5.387342	-1.656147
C	-1.440204	0.408328	4.973259	H	-0.474718	5.853640	-2.597681
H	-2.536220	2.270378	5.308123	H	0.310979	4.383968	-3.221050
H	-0.848181	2.497959	4.797360	H	3.159758	4.490133	-0.628289
H	-0.243955	-1.271915	4.228506	H	2.553373	3.542244	-2.009810
H	0.573316	0.311594	4.136515	H	2.055276	5.964110	-2.384325
H	-1.068480	0.323832	6.016220	H	1.246389	6.076720	-0.803664
H	-2.378007	-0.190804	4.927965	C	-2.690296	1.646500	-0.505727
C	-0.903013	3.219265	-0.288162	C	-3.515869	0.343381	-0.407992
C	-1.193649	3.384257	-1.799399	C	-3.502759	2.819220	0.093404
C	-1.385390	4.445438	0.521601	H	-2.536149	1.835614	-1.592722
H	0.205100	3.164413	-0.174252	C	-4.866216	0.499551	-1.135697
C	-0.574974	4.688309	-2.338740	H	-3.698248	0.087473	0.658724
H	-2.294391	3.413570	-1.960525	H	-2.960364	-0.505017	-0.856033
H	-0.811554	2.505503	-2.360584	C	-4.842264	2.986210	-0.653935
C	-0.759010	5.740992	-0.036095	H	-3.720975	2.609991	1.164056
H	-2.492368	4.524220	0.473041	H	-2.936281	3.769275	0.063682
H	-1.117995	4.338542	1.594239	C	-5.675456	1.696521	-0.612322
C	-1.041376	5.915041	-1.537472	H	-5.449886	-0.440189	-1.034581
H	-0.829415	4.802936	-3.414018	H	-4.669344	0.629438	-2.223952
H	0.535029	4.611500	-2.286802	H	-5.408506	3.833912	-0.212149
H	-1.139446	6.612713	0.538093	H	-4.637765	3.265120	-1.712737
H	0.342143	5.714094	0.131654	H	-6.611100	1.818987	-1.198393
H	-0.549732	6.835816	-1.917152	H	-5.990634	1.499156	0.438404
H	-2.135215	6.062519	-1.691346	C	-0.772028	1.818734	1.905328
C	-3.214070	1.136006	-0.013186	C	-1.042421	3.275723	2.364725
C	-4.201831	2.301214	0.241276	C	-1.656303	0.834074	2.709851
C	-3.443501	0.518727	-1.415747	H	0.294129	1.583407	2.126016
H	-3.425407	0.332540	0.733902	C	-0.835637	3.426565	3.885133
C	-5.662232	1.840329	0.064085	H	-2.086919	3.558234	2.124458
H	-3.994892	3.115507	-0.487370	H	-0.392985	3.993941	1.826947
H	-4.061033	2.736480	1.250949	C	-1.507063	1.012867	4.235153
C	-4.909336	0.081890	-1.597406	H	-2.721339	1.003935	2.438118
H	-3.179477	1.263187	-2.198472	H	-1.424988	-0.211373	2.416600
H	-2.764883	-0.344531	-1.574818	C	-1.739826	2.466757	4.672959
C	-5.896554	1.228472	-1.325619	H	-1.032689	4.479274	4.179996
H	-6.344640	2.700131	0.235156	H	0.231299	3.228302	4.139006
H	-5.907791	1.088190	0.849123	H	-2.212744	0.330471	4.756613
H	-5.049668	-0.321041	-2.623137	H	-0.486485	0.699490	4.550013
H	-5.122743	-0.759985	-0.900154	H	-1.568231	2.573811	5.765077
H	-6.943630	0.869768	-1.419459	H	-2.805367	2.740710	4.497468
H	-5.769162	2.018602	-2.100702	H	1.014672	-2.538363	3.722547
H	3.642168	-2.015450	3.477361	H	-0.909478	-3.811182	3.022887
H	2.104188	-1.834673	2.573573	Cl	-1.001933	0.046182	-2.891782
H	3.033699	-3.348103	2.454198	H	7.363251	-0.165378	0.679718
H	4.307620	-0.938283	-3.216112	H	7.007764	0.926164	2.062667
H	3.784434	-2.597433	-2.828765	H	7.495580	-0.767447	2.353028
H	2.636506	-1.240880	-2.628144	H	2.343367	1.277319	3.664495
H	7.248802	1.179467	0.153713	H	1.160325	-0.033797	3.345909
H	7.357724	0.447781	1.790894	H	2.433629	-0.241511	4.585689
H	8.044837	-0.400483	0.372969	H	-6.101454	-3.515826	-1.749295
H	-1.774946	-3.206146	2.931685	H	-5.141447	-2.873779	-3.123852
H	-0.929347	-4.639439	2.308912	H	-5.059431	-4.606809	-2.713270
H	-0.205281	-3.025304	2.073978	H	-4.402402	-2.402293	2.578691
H	-1.978710	-3.466300	-3.867659	H	-3.260245	-3.714849	2.950879
H	-0.614648	-2.542683	-3.146438	H	-2.673695	-2.024693	2.877301

H	-0.594936	-4.331625	-3.142145	H	4.208685	-3.783607	-0.402551
H	-6.027294	-3.324982	0.501343	H	2.569996	-3.863447	0.314707
H	-6.054345	-3.371154	-1.295760	H	2.887944	-2.801610	-1.089335
H	-5.836969	-4.875502	-0.360718	H	-0.209547	-3.563832	-2.616812
H	3.036381	-4.561562	0.304231	H	0.480827	-2.222390	-1.755069
H	0.707129	-5.201373	0.374058	H	0.493020	-3.823699	-0.976225

3-cis <sup>+</sup> t			
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Ru	0.216820	-0.294857	-0.910742
Cl	0.580124	-1.368951	-2.967947
C	0.250813	-2.051551	0.033021
N	1.373113	-2.734312	0.447012
N	-0.800501	-2.936566	0.084955
C	1.119670	-4.178393	0.652119
C	-0.407779	-4.265310	0.611101
C	2.727492	-2.290679	0.663109
C	-2.219789	-2.730750	-0.086040
C	3.078656	-1.835800	1.967433
C	4.414165	-1.484054	2.222287
C	5.417650	-1.595843	1.233016
C	5.044886	-2.092008	-0.028045
C	3.718520	-2.467833	-0.336938
C	2.037896	-1.735786	3.058292
H	4.686008	-1.126168	3.229707
H	5.815719	-2.208505	-0.807829
C	3.417345	-3.091981	-1.677570
C	-2.841518	-3.119011	-1.309388
C	-4.247612	-3.082524	-1.381165
C	-5.055034	-2.734116	-0.278732
C	-4.410749	-2.405731	0.928218
C	-3.005683	-2.413489	1.055079
C	-2.050528	-3.652923	-2.478320
H	-4.729707	-3.379096	-2.327594
H	-5.020214	-2.164395	1.815437
C	-2.393519	-2.194653	2.420603
C	6.849073	-1.225818	1.544581
C	-6.561899	-2.748853	-0.392849
H	-0.781518	-5.068214	-0.055697
H	1.603637	-4.761649	-0.161322
C	1.829028	0.321831	-0.195060
H	2.036592	0.149788	0.882590
C	2.893552	1.088189	-0.842685
C	3.795943	1.814565	-0.009949
C	3.105312	1.114229	-2.250789
C	4.832898	2.575208	-0.564558
H	3.668707	1.772762	1.084028
C	4.162803	1.852166	-2.796827
H	2.453506	0.508748	-2.900735
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H	5.510573	3.143454	0.091581
H	4.327262	1.846492	-3.885729
H	5.844878	3.179610	-2.396345
P	-0.871694	1.439326	0.384785
C	-0.185482	1.936532	2.077280
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H	0.885933	1.646412	1.966338
C	0.515106	3.698192	3.774024
H	-1.253378	3.803829	2.510223
H	0.282544	4.038995	1.636084

C	-0.059519	1.361422	4.561759
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H	-0.711532	0.006876	2.970361
C	-0.076523	2.856549	4.915254
H	0.465539	4.780717	4.017817
H	1.596853	3.455994	3.658835
H	-0.533338	0.761108	5.367529
H	0.995716	1.011322	4.492161
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H	-1.125657	3.179322	5.106588
C	-0.389263	2.836532	-0.806837
C	-0.264950	2.243021	-2.233342
C	-1.201636	4.150782	-0.850847
H	0.645442	3.079523	-0.465261
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H	-1.258783	1.918590	-2.606566
H	0.392242	1.323588	-2.257717
C	-0.568962	5.156320	-1.834768
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H	-1.282919	4.605678	0.156290
C	-0.437902	4.563973	-3.247315
H	0.388948	2.791080	-4.240983
H	1.407581	3.446919	-2.932723
H	-1.177259	6.085361	-1.856917
H	0.437731	5.452844	-1.460589
H	0.052036	5.289839	-3.930162
H	-1.453412	4.380331	-3.666641
C	-2.752380	1.319814	0.483588
C	-3.475326	2.474811	1.220526
C	-3.357354	1.088845	-0.924928
H	-2.907505	0.382743	1.067149
C	-5.000778	2.249690	1.258329
H	-3.268008	3.437959	0.709243
H	-3.091819	2.580606	2.255583
C	-4.886276	0.904021	-0.876473
H	-3.133290	1.965026	-1.572027
H	-2.883738	0.204271	-1.407012
C	-5.581647	2.065890	-0.151681
H	-5.484493	3.104870	1.776756
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H	-5.273574	0.795212	-1.911972
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H	-6.676964	1.889481	-0.100547
H	-5.445844	3.007408	-0.732255
H	1.554164	-4.516507	1.614897
H	-0.859466	-4.424118	1.615193
H	4.083004	-2.682668	-2.462998
H	3.604008	-4.188627	-1.645128
H	2.372263	-2.926321	-1.999550
H	2.488035	-1.388713	4.008328
H	1.220973	-1.032554	2.789122
H	1.552829	-2.715250	3.257608
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H	-1.237647	-2.968468	-2.791986
H	-1.568619	-4.622599	-2.223821
H	-7.051856	-2.482379	0.564087
H	-6.914897	-2.036228	-1.168406
H	-6.929218	-3.752649	-0.694203
H	7.492572	-1.276923	0.644870
H	6.921493	-0.199440	1.961546
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4-trans				4-cis			
-7485.11751475				-7485.10496335			
Ru	0.107292	-0.302193	0.073516	Ru	0.245547	-0.227712	-0.850556
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Br	-0.186967	-0.333168	-2.473910	C	0.227978	-1.987431	0.205131
Br	-0.158959	-0.392101	2.645541	N	1.305308	-2.677650	0.736676
C	-0.787674	2.935814	1.673817	N	-0.787574	-2.929395	0.067206
C	0.702596	3.211344	1.968884	C	1.012649	-4.104157	0.994388
C	0.873787	3.845670	3.362316	C	-0.278117	-4.311140	0.209935
C	0.040621	5.129740	3.514645	C	2.556831	-2.198415	1.261323
C	-1.439318	4.874397	3.184822	C	-2.220088	-2.779311	-0.024852
C	-1.612386	4.238435	1.789853	C	2.573747	-1.555733	2.530200
H	-1.124826	2.236090	2.473748	C	3.811474	-1.193966	3.095823
H	1.273670	2.263142	1.917441	C	5.034689	-1.481406	2.458953
H	1.131271	3.892178	1.201980	C	4.988100	-2.160327	1.226920
H	1.949143	4.056733	3.550522	C	3.776505	-2.539546	0.613376
H	0.560409	3.105659	4.133577	C	1.295777	-1.304145	3.292564
H	0.438312	5.909730	2.824134	H	3.817281	-0.689802	4.077328
H	0.142825	5.543031	4.541819	H	5.932159	-2.411716	0.714877
H	-2.021354	5.820346	3.241817	C	3.808762	-3.326144	-0.673934
H	-1.875168	4.192632	3.950960	C	-2.898141	-2.753518	-1.275008
H	-2.690124	4.054774	1.594541	C	-4.309386	-2.737373	-1.270621
H	-1.271848	4.967038	1.020188	C	-5.068870	-2.758543	-0.086514
C	-2.983532	1.571659	0.261435	C	-4.371828	-2.843148	1.133450
C	-3.502504	0.680020	-0.889745	C	-2.965088	-2.885408	1.186524
C	-5.042214	0.632468	-0.889140	C	-2.176676	-2.770433	-2.598382
C	-5.593678	0.152379	0.463747	H	-4.831360	-2.726064	-2.242378
C	-5.031010	0.980701	1.630724	H	-4.939428	-2.912082	2.077169
C	-3.489654	1.035374	1.617455	C	-2.292593	-3.154286	2.515050
H	-3.425793	2.585820	0.128440	C	6.354525	-1.065447	3.068631
H	-3.126666	1.030604	-1.873322	C	-6.579395	-2.697531	-0.124399
H	-3.096309	-0.349960	-0.769349	H	-0.086231	-4.743502	-0.798052
H	-5.440026	1.650164	-1.112720	H	1.841038	-4.745554	0.634924
H	-5.398375	-0.026054	-1.710945	C	1.857814	0.366785	-0.135378
H	-5.305574	-0.912909	0.606036	H	1.948664	0.458340	0.971667
H	-6.705381	0.184575	0.466329	C	3.090360	0.802908	-0.801311
H	-5.383598	0.571182	2.602529	C	4.181471	1.193650	0.031421
H	-5.430602	2.020254	1.570121	C	3.266668	0.886063	-2.211670
H	-3.138536	1.670280	2.456823	C	5.391247	1.640049	-0.514278
H	-3.062444	0.025563	1.801475	H	4.062755	1.130362	1.125627
C	-0.981262	2.949735	-1.415145	C	4.480373	1.334449	-2.752325
C	0.361062	3.711409	-1.485158	H	2.435524	0.597613	-2.870138
C	0.568426	4.348755	-2.872063	C	5.544944	1.711160	-1.912575
C	-0.596892	5.278182	-3.246753	H	6.218875	1.937225	0.149781
C	-1.943995	4.545130	-3.144142	H	4.595382	1.392058	-3.846483
C	-2.152521	3.900827	-1.757080	H	6.494448	2.064742	-2.346481
H	-0.947888	2.160534	-2.203379	P	-0.906219	1.575451	0.392275
H	0.373440	4.515625	-0.715403	C	0.101714	3.180334	0.107879
H	1.205493	3.032800	-1.251441	C	-0.672995	4.497232	-0.129897
H	0.655412	3.538344	-3.631273	C	1.245369	3.415594	1.124201
H	1.532449	4.902019	-2.892505	H	0.572886	2.922395	-0.866401
H	-0.456522	5.688752	-4.270561	C	0.281316	5.604347	-0.622816
H	-0.602812	6.155469	-2.558383	H	-1.169667	4.836259	0.807345
H	-2.784294	5.239504	-3.364429	H	-1.470451	4.351514	-0.886021
H	-1.986213	3.747181	-3.920697	C	2.200444	4.520415	0.628984

H	-2.236076	4.703730	-0.991100	H	0.831736	3.720982	2.110573
H	-3.122684	3.363442	-1.757027	H	1.819752	2.485012	1.300998
C	1.827756	0.358182	0.307945	C	1.451055	5.833001	0.347567
C	2.872896	1.011419	-0.502483	H	-0.287675	6.547216	-0.777310
C	2.874773	1.160375	-1.915953	H	0.680688	5.312209	-1.620454
C	3.933818	1.805174	-2.569232	H	3.005352	4.683850	1.378612
C	5.012709	2.337207	-1.836349	H	2.704952	4.171668	-0.299874
C	5.030060	2.207960	-0.435898	H	2.147609	6.599487	-0.056639
C	3.981667	1.544669	0.217681	H	1.057928	6.244690	1.306636
H	2.165593	0.295582	1.370525	C	-2.588848	1.926599	-0.426886
H	2.023527	0.762628	-2.489440	C	-3.291357	0.642864	-0.915546
H	3.914524	1.902382	-3.666772	C	-3.602577	2.835131	0.303670
H	5.836232	2.853043	-2.356237	H	-2.242879	2.453683	-1.345430
H	5.865726	2.623924	0.149689	C	-4.481725	0.980237	-1.832981
H	4.004489	1.431417	1.313583	H	-3.643829	0.036083	-0.052451
C	0.508820	-2.330870	0.192167	H	-2.566875	0.015049	-1.473540
N	-0.433423	-3.331151	0.206892	C	-4.786990	3.184801	-0.621336
N	1.715399	-2.922461	0.468872	H	-3.995541	2.308457	1.201733
C	1.624923	-4.394055	0.601715	H	-3.128067	3.768087	0.664783
C	0.114146	-4.633021	0.650189	C	-5.486454	1.923664	-1.151717
H	2.150083	-4.738002	1.515899	H	-4.984058	0.041941	-2.152446
H	2.113243	-4.884410	-0.271273	H	-4.092211	1.459961	-2.759558
H	-0.245503	-4.867748	1.676215	H	-5.508069	3.834721	-0.078689
H	-0.225043	-5.446188	-0.024214	H	-4.409034	3.785825	-1.480083
C	3.044560	-2.378864	0.396503	H	-6.303484	2.198153	-1.854187
C	3.677570	-2.267899	-0.872009	H	-5.972447	1.392606	-0.299948
C	5.026246	-1.869031	-0.910273	C	-1.176780	1.494369	2.273375
C	5.759118	-1.591670	0.261448	C	-1.609159	2.787399	3.011185
C	5.105292	-1.729437	1.500619	C	-2.117385	0.335315	2.661526
C	3.757174	-2.132209	1.599148	H	-0.155289	1.233540	2.640798
C	2.928574	-2.562208	-2.147832	C	-1.621713	2.573608	4.537983
C	7.201784	-1.146781	0.179282	H	-2.629164	3.080981	2.690118
C	3.104795	-2.302001	2.950199	H	-0.945269	3.636503	2.757885
H	5.519963	-1.775826	-1.892028	C	-2.177809	0.125937	4.187153
H	5.663922	-1.527672	2.430358	H	-3.141836	0.554539	2.286437
H	2.096303	-1.841334	-2.307249	H	-1.798830	-0.592899	2.147666
H	2.467093	-3.572693	-2.135687	C	-2.552708	1.416842	4.933498
H	3.603190	-2.510806	-3.024435	H	-1.930964	3.513404	5.045279
H	7.788892	-1.793161	-0.506458	H	-0.586852	2.355627	4.890673
H	7.694688	-1.162399	1.171957	H	-2.901876	-0.681938	4.429198
H	7.273079	-0.109976	-0.216152	H	-1.185615	-0.228717	4.548790
H	3.764179	-1.925606	3.757019	H	-2.528690	1.251224	6.032572
H	2.132257	-1.765151	3.006262	H	-3.602834	1.694031	4.682964
H	2.893800	-3.371619	3.173386	H	0.893525	-4.282176	2.089421
C	-1.831588	-3.299622	-0.145439	H	-1.013453	-4.955633	0.729745
C	-2.189934	-3.539812	-1.502074	Br	-0.203076	1.347221	-2.851790
C	-3.558509	-3.621837	-1.829128	H	7.122961	-1.858413	2.958871
C	-4.569831	-3.531875	-0.854027	H	6.757200	-0.157824	2.567317
C	-4.176441	-3.373370	0.489374	H	6.253531	-0.830509	4.147321
C	-2.823655	-3.268152	0.873982	H	4.739944	-3.119031	-1.237517
C	-1.146776	-3.759926	-2.568947	H	3.794487	-4.421555	-0.471028
C	-6.032417	-3.611749	-1.229791	H	2.944898	-3.083634	-1.326862
C	-2.471108	-3.211313	2.341623	H	1.476002	-0.651000	4.168965
H	-3.837659	-3.796781	-2.881749	H	0.521157	-0.835367	2.654557
H	-4.946790	-3.355496	1.279001	H	0.862304	-2.254398	3.675472
H	-0.616359	-2.811083	-2.803820	H	-7.033397	-3.193638	0.757381

H -0.377343 -4.492591 -2.246146	H -6.935359 -1.643607 -0.126302
H -1.610755 -4.138110 -3.500891	H -6.984718 -3.177260 -1.038486
H -6.174976 -4.066474 -2.230594	H -2.918098 -2.803647 3.359093
H -6.492130 -2.599155 -1.258198	H -2.141421 -4.247110 2.664600
H -6.611923 -4.206358 -0.493544	H -1.298529 -2.676189 2.595938
H -3.336547 -2.865237 2.941065	H -2.847859 -3.132221 -3.402226
H -2.202943 -4.222420 2.723068	H -1.818641 -1.759992 -2.892303
H -1.617440 -2.532757 2.546587	H -1.265978 -3.398018 -2.577320

4-trans <sup>+</sup>				4-cis <sup>+</sup> c			
-4910.82598547				-4910.83787977			
Ru	0.327329	-0.267167	-0.158244	Ru	-0.080981	-0.629899	-0.637972
Br	0.243175	-0.715665	-2.566969	C	0.371034	-1.664249	1.066006
C	1.478935	-1.979487	-0.015215	N	1.480368	-1.900862	1.828011
N	2.809605	-2.191384	-0.187704	N	-0.599548	-2.557547	1.465573
N	0.866124	-3.183669	0.148245	C	1.228698	-2.924535	2.877423
C	3.147329	-3.639315	-0.224063	C	-0.092354	-3.564116	2.426421
C	1.819055	-4.319281	0.158996	C	2.820872	-1.380489	1.708175
C	3.872297	-1.223633	-0.287039	C	-1.741874	-2.813733	0.636783
C	-0.516376	-3.368833	0.509416	C	3.259713	-0.336624	2.565543
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C	5.519709	0.171620	0.827715	C	5.526459	-0.520215	1.609888
C	6.062718	0.565253	-0.414146	C	5.071756	-1.589181	0.811519
C	5.496576	0.023886	-1.583732	C	3.739538	-2.043474	0.846467
C	4.416351	-0.884238	-1.552677	C	2.356749	0.278708	3.606639
C	3.916308	-1.160833	2.265244	H	4.935712	0.909620	3.135152
H	5.957797	0.567478	1.758993	H	5.782416	-2.098555	0.140106
H	5.917341	0.303898	-2.563909	C	3.332654	-3.212463	-0.019109
C	3.910415	-1.496315	-2.837370	C	-1.548478	-3.059482	-0.760111
C	-1.429431	-3.891397	-0.448252	C	-2.682409	-3.300377	-1.563652
C	-2.752825	-4.140230	-0.032036	C	-3.981853	-3.359382	-1.024534
C	-3.186535	-3.907919	1.289582	C	-4.128391	-3.161689	0.363553
C	-2.247124	-3.413362	2.216961	C	-3.038542	-2.881053	1.211045
C	-0.909564	-3.152759	1.859930	C	-0.171718	-3.220431	-1.372271
C	-1.000904	-4.222159	-1.857712	H	-2.535423	-3.477254	-2.641085
H	-3.463996	-4.552422	-0.767139	H	-5.136918	-3.213472	0.806339
H	-2.555956	-3.255686	3.263715	C	-3.272029	-2.672213	2.689539
C	0.087427	-2.725274	2.914322	C	6.971436	-0.079263	1.577954
C	7.241357	1.509443	-0.475224	C	-5.169729	-3.651228	-1.910925
C	-4.614463	-4.189582	1.696005	H	0.055313	-4.539886	1.910507
H	1.508986	-5.098926	-0.565220	H	2.071070	-3.642941	2.925990
H	3.491131	-3.916859	-1.242970	C	1.673808	-0.008048	-0.845255
C	1.622434	1.039591	-0.288134	H	2.105954	0.624005	-0.041149
H	2.034024	1.244477	-1.302643	C	2.623648	-0.191465	-1.940008
C	2.159639	1.900525	0.766934	C	3.916585	0.397771	-1.791230
C	3.001392	2.987060	0.399703	C	2.339793	-0.871302	-3.160899
C	1.864087	1.717937	2.146869	C	4.876352	0.307183	-2.805835
C	3.512453	3.861217	1.369650	H	4.153170	0.933131	-0.857934
H	3.247739	3.135842	-0.663699	C	3.303472	-0.960042	-4.172886
C	2.384209	2.584726	3.115624	H	1.336023	-1.288732	-3.325749
H	1.229062	0.871833	2.460426	C	4.573034	-0.374774	-4.000111
C	3.206359	3.662620	2.728520	H	5.864572	0.774146	-2.671838
H	4.156884	4.701035	1.066298	H	3.060571	-1.478125	-5.113700
H	2.152844	2.424747	4.180338	H	5.324810	-0.442291	-4.802383
H	3.611120	4.346133	3.491310	P	-0.834493	1.481765	0.153588
P	-1.641149	1.246982	-0.119129	C	0.090990	2.848719	-0.813860
C	-1.692837	1.812570	1.689067	C	-0.728405	4.076576	-1.279875
C	-2.608087	2.992145	2.096430	C	1.413856	3.322445	-0.160449
C	-1.871771	0.599590	2.632639	H	0.352072	2.281161	-1.735445
H	-0.645941	2.178072	1.820195	C	0.097244	4.931842	-2.264404
C	-2.404339	3.358489	3.581127	H	-1.016761	4.702274	-0.405908
H	-3.675157	2.732999	1.928272	H	-1.666578	3.759865	-1.777740
H	-2.394130	3.881602	1.469540	C	2.241391	4.169309	-1.148305
C	-1.695863	0.985396	4.113420	H	1.193388	3.941705	0.735276
H	-2.882678	0.157058	2.490504	H	2.022810	2.469412	0.201035

H	-1.156192	-0.209546	2.353019	C	1.439615	5.375263	-1.662967
C	-2.618456	2.150842	4.506626	H	-0.501427	5.814264	-2.576089
H	-3.091415	4.187367	3.854334	H	0.281219	4.338516	-3.188785
H	-1.371590	3.752409	3.722001	H	3.178412	4.505671	-0.654462
H	-1.885997	0.100106	4.757432	H	2.550113	3.530623	-2.007176
H	-0.636987	1.281968	4.294292	H	2.030941	5.943736	-2.411845
H	-2.447335	2.437225	5.565944	H	1.251149	6.077120	-0.818082
H	-3.680109	1.818726	4.442882	C	-2.663750	1.644228	-0.348066
C	-1.585982	2.869025	-1.098424	C	-3.481054	0.339930	-0.203501
C	-0.834467	2.777656	-2.446216	C	-3.461982	2.823593	0.256869
C	-2.948051	3.579606	-1.295664	H	-2.545966	1.817440	-1.442916
H	-0.962167	3.498202	-0.417282	C	-4.855545	0.479223	-0.887891
C	-0.656984	4.171129	-3.080282	H	-3.624074	0.098060	0.872393
H	-1.397726	2.119683	-3.143404	H	-2.936981	-0.513252	-0.658327
H	0.153668	2.296787	-2.306689	C	-4.824957	2.973783	-0.449767
C	-2.760068	4.976234	-1.922531	H	-3.645157	2.631484	1.337242
H	-3.580241	2.966306	-1.974266	H	-2.900285	3.774773	0.192704
H	-3.502665	3.666077	-0.340976	C	-5.652186	1.682640	-0.359778
C	-1.997864	4.901428	-3.254020	H	-5.431574	-0.460628	-0.750653
H	-0.137386	4.068987	-4.056891	H	-4.695818	0.590228	-1.984333
H	0.013245	4.783423	-2.433183	H	-5.379472	3.827102	-0.003920
H	-3.753184	5.453751	-2.063833	H	-4.655951	3.235915	-1.519050
H	-2.201340	5.625644	-1.209663	H	-6.606132	1.791993	-0.918302
H	-1.835967	5.919915	-3.666495	H	-5.933790	1.502568	0.703518
H	-2.618671	4.357607	-4.002313	C	-0.671895	1.868922	2.000076
C	-3.207684	0.250437	-0.500044	C	-0.946987	3.335178	2.424342
C	-4.539402	0.757459	0.107921	C	-1.513532	0.897937	2.864636
C	-3.369638	-0.016686	-2.017503	H	0.404793	1.654572	2.188561
H	-2.970956	-0.728620	-0.014814	C	-0.690648	3.538225	3.930923
C	-5.693252	-0.223571	-0.184847	H	-2.003228	3.595426	2.214119
H	-4.790532	1.751634	-0.318612	H	-0.328768	4.044151	1.840406
H	-4.448305	0.895734	1.204113	C	-1.325066	1.132248	4.378957
C	-4.525842	-0.996579	-2.292643	H	-2.588858	1.037818	2.617131
H	-3.583223	0.944013	-2.536199	H	-1.269388	-0.153224	2.603859
H	-2.425109	-0.405145	-2.449528	C	-1.561315	2.596916	4.776217
C	-5.849241	-0.503679	-1.687111	H	-0.888086	4.598345	4.197643
H	-6.636582	0.180769	0.240742	H	0.385563	3.356876	4.156689
H	-5.497071	-1.181791	0.349328	H	-2.007843	0.459828	4.942220
H	-4.627827	-1.149454	-3.388291	H	-0.292699	0.840705	4.675692
H	-4.268129	-1.990805	-1.860547	H	-1.359134	2.740440	5.858861
H	-6.659251	-1.243865	-1.860808	H	-2.634227	2.855352	4.623346
H	-6.167065	0.430106	-2.205176	H	1.144833	-2.432146	3.871269
H	4.460180	-0.656526	3.086667	H	-0.798712	-3.724740	3.263425
H	2.837253	-0.931161	2.381982	Br	-1.043810	-0.014133	-2.905224
H	4.027544	-2.256740	2.413919	H	7.461347	-0.341723	0.619428
H	4.165589	-0.858928	-3.706567	H	7.070858	1.013991	1.733743
H	4.385297	-2.486293	-3.019722	H	7.551148	-0.574570	2.387539
H	2.811767	-1.640079	-2.828973	H	2.480573	1.379797	3.651084
H	7.410381	1.892394	-1.500780	H	1.291262	0.056290	3.417294
H	7.102283	2.377761	0.201398	H	2.606080	-0.106621	4.619694
H	8.174842	0.999083	-0.152618	H	-6.123536	-3.603381	-1.350581
H	-0.415815	-2.521471	3.878817	H	-5.228555	-2.931556	-2.753908
H	0.847749	-3.515020	3.099204	H	-5.092047	-4.664517	-2.359614
H	0.650759	-1.814071	2.622531	H	-4.299134	-2.303584	2.879469
H	-1.880620	-4.375663	-2.512279	H	-3.167220	-3.623301	3.257298
H	-0.376816	-3.417400	-2.297147	H	-2.557954	-1.944808	3.123148

H	-0.409268	-5.163787	-1.889759	H	4.217244	-3.808900	-0.314423
H	-4.725944	-4.246551	2.796651	H	2.622638	-3.890876	0.495640
H	-5.297278	-3.389936	1.333577	H	2.843602	-2.869965	-0.956264
H	-4.979695	-5.142327	1.261378	H	-0.254888	-3.662572	-2.384603
H	3.972616	-3.860555	0.483043	H	0.449670	-2.285842	-1.594235
H	1.843924	-4.785334	1.168478	H	0.489800	-3.857735	-0.753945

4-cis <sup>+</sup> t			
-4910.82913806			
Ru	0.176553	-0.337064	-0.758826
Br	0.494435	-1.675286	-2.809246
C	0.243288	-1.971340	0.384130
N	1.364455	-2.587378	0.900549
N	-0.803531	-2.849989	0.547783
C	1.111588	-3.990796	1.300358
C	-0.414291	-4.088394	1.260389
C	2.722829	-2.130175	1.056136
C	-2.216226	-2.696729	0.293559
C	3.084845	-1.531626	2.298123
C	4.421771	-1.151125	2.500401
C	5.418060	-1.373313	1.522676
C	5.035307	-2.008628	0.329109
C	3.706540	-2.416405	0.075021
C	2.055603	-1.316260	3.382954
H	4.700101	-0.678653	3.457468
H	5.799381	-2.212324	-0.439689
C	3.408765	-3.181605	-1.192057
C	-2.791101	-3.265937	-0.875114
C	-4.198702	-3.260642	-0.997319
C	-5.044812	-2.773144	0.012865
C	-4.443175	-2.262682	1.183896
C	-3.047945	-2.225540	1.352013
C	-1.980729	-3.954467	-1.947111
H	-4.645727	-3.700317	-1.904639
H	-5.084324	-1.911471	2.010253
C	-2.469453	-1.791557	2.679592
C	6.855122	-0.984207	1.780532
C	-6.548186	-2.808552	-0.132376
H	-0.781818	-4.977721	0.709568
H	1.605590	-4.678094	0.578561
C	1.807535	0.353613	-0.162965
H	2.053869	0.251901	0.915441
C	2.843595	1.092383	-0.886434
C	3.753086	1.879393	-0.118360
C	3.025053	1.041599	-2.297794
C	4.766029	2.621800	-0.737970
H	3.650668	1.897289	0.978836
C	4.060423	1.760530	-2.908417
H	2.368819	0.394243	-2.901141
C	4.923772	2.562583	-2.135872
H	5.448698	3.235892	-0.130093
H	4.201395	1.693829	-3.998622
H	5.730577	3.132128	-2.623643
P	-0.892351	1.547883	0.356883
C	-0.151267	2.233279	1.960576
C	-0.160048	3.770602	2.144798
C	-0.698377	1.519291	3.217055
H	0.915434	1.930019	1.846456
C	0.605669	4.176416	3.421309
H	-1.204634	4.142880	2.217825
H	0.298821	4.272762	1.268702

C	0.059682	1.947137	4.488727
H	-1.777184	1.759850	3.343577
H	-0.641369	0.418345	3.088915
C	0.052406	3.472962	4.670053
H	0.563462	5.279934	3.540448
H	1.683110	3.918855	3.298564
H	-0.384313	1.443270	5.373693
H	1.112812	1.590428	4.422519
H	0.639101	3.758658	5.568616
H	-0.989973	3.818800	4.857586
C	-0.450712	2.803181	-0.994745
C	-0.363980	2.056460	-2.348245
C	-1.270810	4.102492	-1.159395
H	0.591792	3.083918	-0.711511
C	0.218238	2.944206	-3.465756
H	-1.366206	1.688936	-2.652628
H	0.296779	1.141686	-2.284650
C	-0.671692	4.995408	-2.265165
H	-2.316194	3.846277	-1.437419
H	-1.326237	4.663790	-0.205803
C	-0.581238	4.251366	-3.607213
H	0.226970	2.381566	-4.422998
H	1.278269	3.181231	-3.224925
H	-1.284013	5.916073	-2.369820
H	0.344948	5.330774	-1.956527
H	-0.115952	4.897995	-4.380880
H	-1.608141	4.020418	-3.971735
C	-2.769849	1.451536	0.540507
C	-3.460062	2.696263	1.152610
C	-3.437061	1.040780	-0.797856
H	-2.900281	0.603186	1.251119
C	-4.982222	2.490603	1.287822
H	-3.276279	3.582356	0.511406
H	-3.028948	2.931086	2.146605
C	-4.961822	0.875618	-0.652220
H	-3.239200	1.820874	-1.565708
H	-2.991656	0.094681	-1.179005
C	-5.625484	2.126254	-0.058814
H	-5.439910	3.410667	1.709830
H	-5.181278	1.678166	2.023938
H	-5.399394	0.625577	-1.642105
H	-5.161472	0.005130	0.008895
H	-6.717208	1.962889	0.064106
H	-5.518385	2.981756	-0.764964
H	1.539804	-4.193911	2.302946
H	-0.873623	-4.105358	2.273406
H	3.873824	-2.690195	-2.070370
H	3.841660	-4.204209	-1.133407
H	2.327478	-3.269546	-1.400983
H	2.494301	-0.785995	4.250020
H	1.187112	-0.728194	3.020299
H	1.645487	-2.278676	3.758771
H	-3.110832	-1.035169	3.174351
H	-2.401243	-2.650787	3.383416
H	-1.450832	-1.372462	2.573414
H	-2.030511	-3.399692	-2.906969

H	-0.910409	-4.036504	-1.687385
H	-2.383893	-4.971199	-2.136239
H	-7.033644	-3.214303	0.779249
H	-6.960090	-1.787445	-0.287331
H	-6.862855	-3.427879	-0.994903
H	7.431607	-0.892536	0.839050
H	6.927398	-0.022474	2.328159
H	7.364255	-1.749613	2.406417

5-trans				5-cis			
-2359.78445577				-2359.77311329			
Ru	0.130419	-0.268419	0.101709	Ru	0.253122	-0.203768	-0.681780
P	-1.250735	1.850743	0.164720	I	1.452050	-1.869376	-2.624246
I	-0.589332	-0.622972	-2.571355	C	0.307075	-1.941617	0.407190
I	0.161761	-0.233277	2.937607	N	1.396105	-2.563770	1.004407
C	-0.841005	3.056134	1.573930	N	-0.656812	-2.938409	0.254296
C	0.655329	3.414675	1.715563	C	1.169307	-4.003140	1.263313
C	0.909753	4.191007	3.022044	C	-0.072798	-4.286981	0.425972
C	0.037164	5.453147	3.121100	C	2.585967	-2.014377	1.605101
C	-1.451550	5.110310	2.949720	C	-2.099021	-2.872832	0.169824
C	-1.712879	4.332235	1.643447	C	2.484125	-1.337377	2.854479
H	-1.082667	2.429827	2.462953	C	3.656989	-0.899915	3.497149
H	1.264343	2.488086	1.710682	C	4.938201	-1.146280	2.963725
H	0.991105	4.028697	0.852569	C	5.012410	-1.867480	1.759784
H	1.986863	4.456416	3.097474	C	3.867630	-2.322930	1.071099
H	0.691770	3.521502	3.885246	C	1.150986	-1.142076	3.532616
H	0.339942	6.174561	2.326620	H	3.563615	-0.369140	4.459996
H	0.206234	5.970316	4.090819	H	6.001904	-2.097025	1.329751
H	-2.071097	6.033785	2.966647	C	4.054987	-3.168829	-0.164088
H	-1.788545	4.492464	3.813707	C	-2.789272	-2.882843	-1.074474
H	-2.793692	4.087260	1.569553	C	-4.198718	-2.951675	-1.059646
H	-1.479512	4.992506	0.778583	C	-4.947337	-3.025160	0.129146
C	-3.087771	1.488026	0.492629	C	-4.236473	-3.073817	1.342473
C	-3.691191	0.507356	-0.538037	C	-2.829026	-3.030017	1.385481
C	-5.216175	0.382882	-0.358341	C	-2.082908	-2.854580	-2.405123
C	-5.587560	-0.036151	1.073396	H	-4.726743	-2.967225	-2.028053
C	-4.955768	0.904134	2.112293	H	-4.790927	-3.181686	2.290237
C	-3.430096	1.027293	1.926327	C	-2.136709	-3.261854	2.710735
H	-3.577559	2.477488	0.343661	C	6.184148	-0.641603	3.655669
H	-3.452360	0.814017	-1.577553	C	-6.458750	-3.059259	0.099732
H	-3.220737	-0.493313	-0.412179	H	0.187400	-4.707889	-0.571609
H	-5.695703	1.362143	-0.592756	H	2.045804	-4.600141	0.943948
H	-5.620880	-0.344749	-1.094797	C	1.803380	0.489784	0.082458
H	-5.219264	-1.072103	1.249479	H	1.834695	0.560917	1.194295
H	-6.692084	-0.069367	1.197948	C	3.044820	1.015294	-0.499892
H	-5.177900	0.551314	3.143032	C	4.074654	1.399328	0.410438
H	-5.419553	1.914444	2.024463	C	3.289829	1.192586	-1.890516
H	-3.022358	1.728498	2.683265	C	5.290494	1.925457	-0.042696
H	-2.947713	0.047021	2.129196	H	3.903517	1.263653	1.490845
C	-1.322084	2.857650	-1.453916	C	4.506833	1.725045	-2.339275
C	-0.057336	3.717457	-1.677365	H	2.506381	0.923446	-2.611285
C	-0.015902	4.284562	-3.109327	C	5.511026	2.090721	-1.423701
C	-1.277746	5.101511	-3.429351	H	6.070182	2.212579	0.680960
C	-2.548252	4.275622	-3.173111	H	4.671847	1.856622	-3.420404
C	-2.589540	3.697974	-1.742068	H	6.464460	2.509091	-1.785093
H	-1.291291	2.043178	-2.213475	P	-1.057538	1.540095	0.543338
H	-0.049047	4.566956	-0.958380	C	-0.140661	3.207039	0.293529
H	0.858371	3.125183	-1.480717	C	-0.992911	4.479798	0.078412
H	0.072578	3.440204	-3.830366	C	0.988799	3.487030	1.315079
H	0.896851	4.905522	-3.240536	H	0.351750	3.003864	-0.682394
H	-1.255112	5.462279	-4.480829	C	-0.104746	5.650712	-0.389185
H	-1.296847	6.013438	-2.787804	H	-1.511480	4.770510	1.019834
H	-3.456944	4.891254	-3.352275	H	-1.777279	4.301553	-0.684507

H	-2.592457	3.434667	-3.902628	C	1.874719	4.657653	0.843586
H	-2.673917	4.536717	-1.015822	H	0.562762	3.745296	2.309237
H	-3.509826	3.089238	-1.632496	H	1.617061	2.587905	1.468289
C	1.807019	0.536701	0.079681	C	1.046524	5.928122	0.590406
C	2.691382	1.231336	-0.876371	H	-0.728540	6.560864	-0.526611
C	2.542031	1.280650	-2.288012	H	0.314046	5.402976	-1.390911
C	3.464020	1.971640	-3.086202	H	2.668535	4.852526	1.597314
C	4.549894	2.652448	-2.502703	H	2.398826	4.360623	-0.092528
C	4.715932	2.623962	-1.105980	H	1.695457	6.745242	0.206867
C	3.808396	1.912675	-0.308747	H	0.626847	6.291748	1.557627
H	2.285711	0.551492	1.087877	C	-2.765784	1.801422	-0.262919
H	1.687966	0.765875	-2.751489	C	-3.400670	0.482777	-0.753201
H	3.329337	1.986990	-4.179742	C	-3.823460	2.641670	0.489423
H	5.264271	3.203822	-3.135191	H	-2.472106	2.362798	-1.178741
H	5.559399	3.155336	-0.636421	C	-4.619245	0.759668	-1.653615
H	3.951414	1.874562	0.783325	H	-3.709918	-0.145664	0.111030
C	0.732130	-2.240834	0.325957	H	-2.651230	-0.105155	-1.321705
N	-0.126007	-3.312331	0.461024	C	-5.038272	2.930357	-0.416959
N	1.995552	-2.711771	0.603203	H	-4.176487	2.084378	1.385558
C	2.021532	-4.169066	0.864484	H	-3.400649	3.597234	0.854990
C	0.540011	-4.497136	1.048285	C	-5.669279	1.634846	-0.949598
H	2.629059	-4.395342	1.762738	H	-5.068708	-0.203145	-1.978629
H	2.481464	-4.700463	-0.000580	H	-4.270132	1.271786	-2.579049
H	0.260075	-4.595425	2.121064	H	-5.787989	3.530698	0.143700
H	0.226164	-5.422227	0.524285	H	-4.710244	3.561824	-1.274225
C	3.277946	-2.077432	0.437935	H	-6.511099	1.865997	-1.638151
C	3.819620	-1.931736	-0.871262	H	-6.110166	1.067797	-0.096449
C	5.119272	-1.409996	-1.005111	C	-1.344592	1.425647	2.424091
C	5.904387	-1.051626	0.108923	C	-1.825340	2.696996	3.170384
C	5.359695	-1.256482	1.389522	C	-2.259648	0.237979	2.789143
C	4.064943	-1.782977	1.583843	H	-0.321309	1.193167	2.801828
C	3.044577	-2.348299	-2.095643	C	-1.848607	2.466218	4.694466
C	7.283146	-0.459636	-0.075221	H	-2.850289	2.962727	2.842521
C	3.586115	-2.075094	2.986024	H	-1.186166	3.568455	2.933076
H	5.532892	-1.285847	-2.019882	C	-2.345711	0.012113	4.311865
H	5.965405	-1.013025	2.278975	H	-3.282003	0.435525	2.398502
H	2.114310	-1.754886	-2.221337	H	-1.914116	-0.679783	2.273901
H	2.734270	-3.413689	-2.040352	C	-2.759632	1.286195	5.066012
H	3.655240	-2.224307	-3.010785	H	-2.183306	3.393723	5.208080
H	7.857209	-0.997451	-0.858245	H	-0.813318	2.266317	5.056548
H	7.871578	-0.486213	0.863722	H	-3.059975	-0.811518	4.528591
H	7.215417	0.602150	-0.399214	H	-1.355929	-0.328875	4.691189
H	4.066655	-1.396090	3.718421	H	-2.746649	1.108860	6.163415
H	2.488985	-1.960778	3.085068	H	-3.812016	1.543798	4.804545
H	3.856247	-3.112710	3.288623	H	1.014613	-4.178527	2.353974
C	-1.477517	-3.482938	-0.019437	H	-0.790667	-4.972357	0.916513
C	-1.654274	-3.967576	-1.347074	I	-0.333506	1.409211	-2.963264
C	-2.961730	-4.202218	-1.810603	H	7.057578	-1.293666	3.452462
C	-4.091910	-4.018018	-0.990106	H	6.451771	0.378566	3.301531
C	-3.875898	-3.623878	0.343201	H	6.046752	-0.578459	4.754416
C	-2.586696	-3.367222	0.859027	H	4.909304	-2.800987	-0.767177
C	-0.474789	-4.310314	-2.226488	H	4.289730	-4.221036	0.115661
C	-5.488015	-4.239739	-1.526927	H	3.160536	-3.162708	-0.815085
C	-2.421738	-3.073976	2.330523	H	1.221612	-0.387179	4.340038
H	-3.097392	-4.554477	-2.846873	H	0.367292	-0.826762	2.818486
H	-4.738553	-3.532184	1.024718	H	0.800528	-2.087983	4.002673

H 0.268159 -3.491387 -2.260643	H -6.878339 -3.508593 1.022361
H 0.041647 -5.226705 -1.861252	H -6.879344 -2.033237 0.012341
H -0.802734 -4.510499 -3.265024	H -6.836577 -3.636465 -0.769016
H -5.508483 -5.038904 -2.295916	H -2.790191 -2.975960 3.557768
H -5.878846 -3.316596 -2.009185	H -1.895231 -4.340054 2.846099
H -6.199449 -4.514569 -0.722037	H -1.186693 -2.703736 2.801797
H -3.383982 -2.763004 2.783499	H -2.743327 -3.244476 -3.204632
H -2.088020 -3.983886 2.878077	H -1.783697 -1.824986 -2.699537
H -1.670594 -2.284087 2.530849	H -1.144175 -3.439180 -2.398950

5-trans <sup>+</sup>				5-cis <sup>+</sup> c			
-2348.15901175				-2348.17272679			
Ru	0.211919	-0.282613	0.041005	Ru	-0.068131	-0.678980	-0.443964
I	0.098813	-0.458622	-2.625354	C	0.416617	-1.482538	1.373775
C	0.994665	-2.199990	0.046192	N	1.546946	-1.606341	2.131866
N	2.294088	-2.593153	0.151701	N	-0.540991	-2.307508	1.920690
N	0.218137	-3.317364	-0.054077	C	1.326429	-2.469806	3.322936
C	2.452545	-4.067110	0.045076	C	-0.011725	-3.156883	3.012735
C	0.999350	-4.573233	0.047832	C	2.887524	-1.127905	1.891963
C	3.466150	-1.790458	0.382244	C	-1.711657	-2.674641	1.176876
C	-1.219928	-3.364516	0.026292	C	3.371851	0.015316	2.581028
C	3.816499	-1.469613	1.720555	C	4.711664	0.406040	2.383208
C	5.009565	-0.755502	1.946379	C	5.596200	-0.329935	1.572102
C	5.864670	-0.377009	0.892441	C	5.100877	-1.494887	0.951919
C	5.495075	-0.735024	-0.420471	C	3.767274	-1.920092	1.100319
C	4.313067	-1.445237	-0.704244	C	2.526161	0.776352	3.572383
C	2.955324	-1.900766	2.886384	H	5.080635	1.304006	2.906919
H	5.288855	-0.504646	2.983311	H	5.780315	-2.104877	0.334071
H	6.153848	-0.455959	-1.259631	C	3.320777	-3.195831	0.426974
C	3.984895	-1.842294	-2.124153	C	-1.563178	-3.122334	-0.173882
C	-1.977318	-3.690644	-1.133835	C	-2.721617	-3.466727	-0.900218
C	-3.377104	-3.782143	-1.009099	C	-4.004508	-3.437390	-0.319955
C	-4.040502	-3.595307	0.221293	C	-4.106688	-3.040595	1.028700
C	-3.255308	-3.322550	1.358332	C	-2.989893	-2.649295	1.794101
C	-1.849383	-3.228460	1.295494	C	-0.208142	-3.378403	-0.800298
C	-1.322549	-4.018900	-2.454760	H	-2.607435	-3.798329	-1.944697
H	-3.968255	-4.026884	-1.907464	H	-5.100763	-3.021341	1.505556
H	-3.748792	-3.214264	2.338856	C	-3.179414	-2.232616	3.234564
C	-1.060516	-3.117272	2.582072	C	7.042665	0.079541	1.419997
C	7.150249	0.373347	1.151606	C	-5.220589	-3.840785	-1.119910
C	-5.541848	-3.739477	0.317362	H	0.111627	-4.203513	2.653497
H	0.772627	-5.243397	-0.805800	H	2.168020	-3.180590	3.444644
H	2.991299	-4.320346	-0.892668	C	1.681534	-0.111362	-0.807136
C	1.655199	0.762110	0.472562	H	2.114803	0.676196	-0.155206
H	1.719777	0.706250	1.601346	C	2.632422	-0.494561	-1.849206
C	2.644232	1.673760	-0.087387	C	3.898675	0.167072	-1.843487
C	3.413629	2.448437	0.830089	C	2.386607	-1.442259	-2.886007
C	2.877703	1.853069	-1.479150	C	4.863932	-0.099153	-2.821436
C	4.354122	3.382369	0.375410	H	4.109437	0.903292	-1.051702
H	3.257440	2.311547	1.912442	C	3.357113	-1.711308	-3.858675
C	3.825941	2.779774	-1.927250	H	1.409671	-1.942172	-2.946030
H	2.306770	1.247521	-2.197794	C	4.596515	-1.042278	-3.832020
C	4.561831	3.551940	-1.005824	H	5.828418	0.431816	-2.801897
H	4.929635	3.979176	1.100081	H	3.142505	-2.439370	-4.656375
H	3.994696	2.906400	-3.008148	H	5.352090	-1.251403	-4.605757
H	5.300652	4.284952	-1.366517	P	-0.768147	1.524309	0.122313
P	-1.414933	1.543981	0.379894	C	0.171382	2.767026	-0.991188
C	-1.101703	1.834536	2.226182	C	-0.641735	3.934184	-1.601506
C	-1.882192	2.894106	3.033380	C	1.491820	3.312568	-0.389417
C	-1.086088	0.471373	2.950329	H	0.438796	2.095690	-1.838665
H	-0.044050	2.190310	2.178796	C	0.189583	4.665745	-2.676605
C	-1.320702	3.002032	4.466734	H	-0.929262	4.658098	-0.806544
H	-2.959269	2.629594	3.081300	H	-1.579230	3.563962	-2.062698
H	-1.819837	3.883339	2.536132	C	2.327350	4.027232	-1.471712
C	-0.542389	0.583683	4.384368	H	1.267293	4.041151	0.418650
H	-2.113253	0.042528	2.966206	H	2.095298	2.510525	0.083828

H	-0.483864	-0.274243	2.356537	C	1.534200	5.167981	-2.128846
C	-1.316324	1.644264	5.188919	H	-0.403960	5.509942	-3.087875
H	-1.910947	3.745894	5.042568	H	0.369290	3.969173	-3.526643
H	-0.280558	3.399652	4.423204	H	3.267005	4.414163	-1.021796
H	-0.589895	-0.404094	4.890587	H	2.628887	3.287804	-2.248041
H	0.534873	0.866740	4.344913	H	2.131066	5.637684	-2.939244
H	-0.879815	1.745792	6.205025	H	1.350917	5.967912	-1.375123
H	-2.365453	1.299660	5.335531	C	-2.610876	1.674237	-0.342942
C	-1.233089	3.266592	-0.376838	C	-3.442002	0.412015	-0.014136
C	-0.703171	3.260998	-1.828820	C	-3.370334	2.932456	0.138897
C	-2.460547	4.203168	-0.255331	H	-2.537577	1.720739	-1.453735
H	-0.418775	3.684567	0.264242	C	-4.834711	0.490078	-0.671068
C	-0.364889	4.689107	-2.299171	H	-3.555204	0.308932	1.087326
H	-1.468716	2.819168	-2.503744	H	-2.921406	-0.502191	-0.368977
H	0.190252	2.610842	-1.908346	C	-4.751417	3.020262	-0.543022
C	-2.110709	5.631787	-0.721134	H	-3.524282	2.878184	1.238892
H	-3.282510	3.812168	-0.894150	H	-2.795587	3.857094	-0.058984
H	-2.852980	4.228434	0.781113	C	-5.594966	1.765045	-0.272293
C	-1.561359	5.643279	-2.156426	H	-5.420932	-0.414497	-0.401969
H	-0.013589	4.658137	-3.352633	H	-4.706904	0.462379	-1.777029
H	0.490273	5.075851	-1.698144	H	-5.280003	3.931594	-0.190248
H	-3.011192	6.277551	-0.640287	H	-4.609973	3.146346	-1.640618
H	-1.353571	6.067186	-0.028898	H	-6.563488	1.823261	-0.813101
H	-1.274153	6.674696	-2.452127	H	-5.847355	1.722009	0.812526
H	-2.366953	5.331703	-2.860153	C	-0.574226	2.102710	1.917253
C	-3.144603	0.830599	0.093074	C	-0.823563	3.606857	2.207381
C	-4.303251	1.377657	0.961599	C	-1.416409	1.237185	2.884633
C	-3.511168	0.855745	-1.411526	H	0.502046	1.897591	2.115165
H	-3.001346	-0.240886	0.376095	C	-0.511535	3.942128	3.679924
C	-5.616802	0.623069	0.670574	H	-1.884697	3.858288	2.012776
H	-4.449901	2.460490	0.760168	H	-0.222071	4.251697	1.538154
H	-4.061599	1.284707	2.040100	C	-1.172958	1.595160	4.365040
C	-4.829896	0.107057	-1.679801	H	-2.494093	1.392655	2.658298
H	-3.621372	1.910967	-1.745319	H	-1.215123	0.160595	2.707339
H	-2.691259	0.415384	-2.016269	C	-1.363414	3.095502	4.638326
C	-5.981533	0.653576	-0.821550	H	-0.687309	5.024800	3.855556
H	-6.434355	1.057637	1.284826	H	0.569911	3.766528	3.883733
H	-5.507136	-0.435464	1.000852	H	-1.852909	0.993837	5.006806
H	-5.078627	0.174304	-2.760460	H	-0.138840	1.303372	4.655224
H	-4.680852	-0.974720	-1.459745	H	-1.115724	3.330172	5.695291
H	-6.912955	0.076170	-1.003864	H	-2.436791	3.362590	4.504445
H	-6.203928	1.702300	-1.125595	H	1.279496	-1.841220	4.239300
H	3.407949	-1.594593	3.849216	H	-0.695328	-3.175337	3.883296
H	1.935471	-1.462272	2.838757	I	-1.126800	-0.373203	-2.991747
H	2.821688	-3.003213	2.919206	H	7.451602	-0.216447	0.433294
H	4.585915	-1.257491	-2.847170	H	7.175785	1.173191	1.540377
H	4.217061	-2.914513	-2.309518	H	7.673430	-0.412302	2.192755
H	2.912518	-1.690947	-2.363335	H	2.652355	1.872076	3.457184
H	7.173500	1.332305	0.592167	H	1.452201	0.537937	3.474374
H	7.286151	0.600590	2.227048	H	2.830957	0.532971	4.613873
H	8.030926	-0.214347	0.815621	H	-6.153097	-3.737763	-0.531780
H	-1.638403	-2.583979	3.362107	H	-5.320415	-3.221644	-2.035773
H	-0.841414	-4.129776	2.988381	H	-5.145546	-4.897339	-1.454239
H	-0.090580	-2.600683	2.455555	H	-4.197216	-1.827294	3.397933
H	-1.979611	-3.746926	-3.304333	H	-3.067135	-3.096609	3.926491
H	-0.356861	-3.496347	-2.588840	H	-2.447314	-1.460872	3.542785

H	-1.137332	-5.113641	-2.532884	H	4.185396	-3.858557	0.229906
H	-5.923673	-3.439791	1.312988	H	2.589907	-3.763565	1.036861
H	-6.060059	-3.128445	-0.450651	H	2.842620	-2.985191	-0.553540
H	-5.849012	-4.793533	0.144908	H	-0.325844	-3.913393	-1.762620
H	3.053817	-4.453341	0.893487	H	0.434939	-2.485252	-1.107346
H	0.728583	-5.111502	0.982526	H	0.453056	-3.968629	-0.134912

5-cis <sup>+</sup> t			
-2348.16479073			
Ru	0.335122	-0.168419	-0.700808
I	1.162791	-1.278892	-3.015625
C	0.384725	-1.908688	0.263544
N	1.511511	-2.546906	0.744532
N	-0.634309	-2.842244	0.263911
C	1.254812	-3.954191	1.125021
C	-0.134952	-4.210980	0.542430
C	2.816123	-2.034942	1.093064
C	-2.070975	-2.692183	0.233716
C	2.995546	-1.450771	2.381647
C	4.280381	-1.023583	2.756473
C	5.400250	-1.185455	1.910793
C	5.200564	-1.828667	0.677610
C	3.932190	-2.283552	0.253088
C	1.842344	-1.310937	3.349895
H	4.417079	-0.566410	3.750895
H	6.066649	-2.006071	0.018307
C	3.836779	-3.073927	-1.029545
C	-2.801617	-2.894668	-0.971041
C	-4.208109	-2.956433	-0.896811
C	-4.912043	-2.840700	0.319062
C	-4.159754	-2.664927	1.495385
C	-2.750553	-2.620500	1.483743
C	-2.128875	-3.095106	-2.307893
H	-4.771792	-3.133842	-1.827998
H	-4.682485	-2.609700	2.465081
C	-2.012367	-2.632516	2.803773
C	6.763916	-0.686137	2.327000
C	-6.420345	-2.927834	0.352179
H	-0.099482	-4.797604	-0.402405
H	2.033807	-4.613866	0.693702
C	1.756124	0.615860	0.223290
H	1.847002	0.370803	1.301582
C	2.774854	1.579521	-0.194634
C	3.438198	2.320911	0.829528
C	3.176244	1.794932	-1.543361
C	4.416544	3.271964	0.514643
H	3.170273	2.136815	1.882650
C	4.178113	2.724233	-1.849962
H	2.722993	1.188393	-2.342626
C	4.790282	3.475857	-0.827618
H	4.904623	3.845885	1.317841
H	4.491635	2.862334	-2.896550
H	5.572491	4.210369	-1.076234
P	-1.154946	1.415961	0.377379
C	-0.819182	1.920307	2.172261
C	-1.096346	3.396231	2.543503
C	-1.469503	0.953899	3.186542
H	0.284648	1.770481	2.233355
C	-0.664118	3.693168	3.994787
H	-2.179259	3.620723	2.433032
H	-0.555494	4.077558	1.855901

C	-1.036695	1.272054	4.631507
H	-2.576965	1.030721	3.119604
H	-1.218345	-0.094649	2.932070
C	-1.323060	2.735884	4.999528
H	-0.904968	4.749074	4.241281
H	0.443891	3.602507	4.071456
H	-1.550927	0.582301	5.334448
H	0.053741	1.070986	4.740106
H	-0.970507	2.952636	6.030019
H	-2.424106	2.906265	5.006014
C	-0.660611	2.909186	-0.685037
C	-0.246656	2.397033	-2.085722
C	-1.609860	4.122153	-0.819017
H	0.271407	3.251035	-0.174242
C	0.386023	3.504393	-2.949735
H	-1.122945	1.971001	-2.616617
H	0.503879	1.556619	-2.012648
C	-0.960688	5.234272	-1.667965
H	-2.553061	3.801827	-1.312693
H	-1.895075	4.522076	0.174016
C	-0.549233	4.721752	-3.057811
H	0.625899	3.099735	-3.955776
H	1.351160	3.817646	-2.493579
H	-1.665407	6.087782	-1.760596
H	-0.064600	5.627476	-1.135410
H	-0.055446	5.528528	-3.639606
H	-1.461343	4.439481	-3.631581
C	-2.999558	1.073404	0.157057
C	-3.964384	2.086400	0.825190
C	-3.346831	0.887750	-1.342845
H	-3.129119	0.086614	0.659791
C	-5.436129	1.681598	0.606533
H	-3.806302	3.100704	0.401573
H	-3.760935	2.163861	1.912124
C	-4.828914	0.528438	-1.558740
H	-3.135033	1.833768	-1.887086
H	-2.695265	0.108044	-1.796776
C	-5.768636	1.540648	-0.886292
H	-6.098284	2.431548	1.089458
H	-5.629718	0.713407	1.122108
H	-5.034613	0.462656	-2.648581
H	-5.015955	-0.483897	-1.140930
H	-6.827372	1.233083	-1.021422
H	-5.670094	2.533385	-1.383084
H	1.293126	-4.066304	2.232179
H	-0.813994	-4.737236	1.241344
H	4.328774	-2.539184	-1.867148
H	4.364230	-4.046414	-0.918399
H	2.793592	-3.272119	-1.333113
H	2.161516	-0.790392	4.273452
H	0.989951	-0.746657	2.915548
H	1.440609	-2.301123	3.655549
H	-2.569970	-2.073814	3.580944
H	-1.909460	-3.674311	3.182113
H	-0.992723	-2.210584	2.732595
H	-2.773624	-3.688229	-2.985498

H	-1.921086	-2.129389	-2.816173
H	-1.151530	-3.606291	-2.218680
H	-6.808333	-2.961561	1.388889
H	-6.885890	-2.054522	-0.154121
H	-6.782610	-3.832249	-0.179535
H	7.575159	-1.190262	1.765759
H	6.859391	0.405090	2.135140
H	6.942965	-0.841110	3.410500

6-trans				6-cis			
	-3493.11093038			-3493.09576731			
Ru	-0.029658	-0.020586	0.033295	Ru	0.267911	0.059106	-0.940439
P	2.456230	-0.092436	0.057708	Cl	1.655463	-1.241258	-2.430781
Cl	0.009269	-0.101290	-2.388687	C	0.586926	-1.577499	0.256530
Cl	0.052909	0.524946	2.410395	N	1.759062	-1.954448	0.899913
C	3.229308	-0.663512	1.686643	N	-0.141579	-2.762150	0.102676
C	2.690633	-2.007744	2.222016	C	1.780478	-3.401790	1.223399
C	3.208062	-2.277886	3.648062	C	0.741954	-3.938888	0.259865
C	4.743623	-2.237268	3.716950	C	2.916211	-1.204442	1.334192
C	5.286908	-0.907089	3.171076	C	-1.523554	-3.039336	-0.234827
C	4.774117	-0.622089	1.743945	C	2.851484	-0.425942	2.532379
H	2.826076	0.111050	2.379456	C	4.037654	0.157255	3.023664
H	1.583227	-1.980934	2.223800	C	5.265731	-0.023735	2.375733
H	2.998736	-2.844456	1.559517	C	5.320090	-0.797874	1.213674
H	2.829037	-3.260273	4.005293	C	4.168526	-1.408362	0.672513
H	2.785329	-1.510760	4.336499	C	1.559289	-0.251453	3.334381
H	5.161315	-3.077836	3.115048	H	4.001156	0.756338	3.945551
H	5.093103	-2.398852	4.760088	H	6.285865	-0.941046	0.704516
H	6.398986	-0.904310	3.178848	C	4.349407	-2.286190	-0.568250
H	4.967671	-0.077570	3.843406	C	-1.892646	-3.364819	-1.575443
H	5.162040	0.359199	1.398076	C	-3.232433	-3.730265	-1.835560
H	5.193736	-1.385705	1.051231	C	-4.180927	-3.817369	-0.813624
C	3.176212	1.651454	-0.134861	C	-3.789851	-3.573754	0.509357
C	2.583203	2.399746	-1.350242	C	-2.466000	-3.211768	0.833353
C	3.342271	3.717390	-1.599262	C	-0.896714	-3.445347	-2.730350
C	3.350273	4.616028	-0.351775	H	-3.524604	-3.968663	-2.870464
C	3.863087	3.864500	0.887689	H	-4.528737	-3.693340	1.315388
C	3.099960	2.545088	1.120912	C	-2.079128	-3.136239	2.315602
H	4.256412	1.476074	-0.342183	H	6.180526	0.437133	2.781502
H	2.596186	1.764616	-2.260119	H	-5.220703	-4.103218	-1.040223
H	1.508277	2.616166	-1.157292	H	1.190936	-4.207048	-0.723736
H	4.391605	3.482032	-1.895368	H	2.787960	-3.826406	1.066558
H	2.890238	4.255208	-2.460691	C	1.614760	1.085142	-0.177718
H	2.311518	4.962988	-0.157639	H	1.595486	1.285491	0.918567
H	3.960328	5.528127	-0.532927	C	2.746534	1.752497	-0.830780
H	3.785036	4.508214	1.790940	C	3.702147	2.407336	0.000573
H	4.947755	3.637864	0.761476	C	2.932674	1.813357	-2.241109
H	3.521831	2.031943	2.009027	C	4.802809	3.077845	-0.546880
H	2.036245	2.757431	1.361580	H	3.571347	2.368332	1.094158
C	3.253464	-1.031932	-1.394425	C	4.031424	2.495222	-2.783285
C	3.399511	-2.547283	-1.121328	H	2.195103	1.326416	-2.894565
C	3.801493	-3.311387	-2.396927	C	4.970785	3.124255	-1.944330
C	5.100728	-2.757355	-3.001897	H	5.533453	3.568831	0.115707
C	4.991312	-1.244004	-3.245311	H	4.156509	2.535816	-3.877126
C	4.576256	-0.476212	-1.972456	H	5.832966	3.655607	-2.379093
H	2.462516	-0.906840	-2.171767	P	-1.374015	1.672360	-0.028679
H	4.183505	-2.712535	-0.348527	C	-0.740360	3.400842	-0.571313
H	2.457514	-2.964350	-0.713986	C	-1.776080	4.437089	-1.067643
H	2.978792	-3.228774	-3.143118	C	0.248320	4.060008	0.420029
H	3.905699	-4.394248	-2.167854	H	-0.158031	3.101414	-1.468962
H	5.349502	-3.285795	-3.948074	C	-1.066476	5.646620	-1.710761
H	5.945793	-2.957250	-2.302475	H	-2.412400	4.795055	-0.227232
H	5.953480	-0.838909	-3.628705	H	-2.454879	3.980946	-1.816084

H	4.234415	-1.054702	-4.040838	C	0.955371	5.265445	-0.231299
H	5.388281	-0.557581	-1.214468	H	-0.284823	4.413694	1.329862
H	4.485480	0.599838	-2.223379	H	1.008346	3.330834	0.764346
C	-0.300681	-1.798851	0.477437	C	-0.056934	6.298428	-0.752670
C	-0.205774	-3.108676	-0.190356	H	-1.822955	6.389435	-2.046187
C	0.063741	-3.321207	-1.569819	H	-0.535289	5.303458	-2.627406
C	0.135646	-4.618477	-2.095055	H	1.649927	5.733430	0.499997
C	-0.040223	-5.741021	-1.262362	H	1.585671	4.903387	-1.074347
C	-0.295022	-5.555559	0.108114	H	0.469144	7.139214	-1.255105
C	-0.383312	-4.258280	0.633008	H	-0.604430	6.744729	0.110337
H	-0.557638	-1.932303	1.555856	C	-3.016814	1.441178	-0.956284
H	0.214075	-2.439563	-2.212388	C	-3.360644	-0.045937	-1.187646
H	0.337357	-4.758801	-3.169274	C	-4.274737	2.197788	-0.471794
H	0.024995	-6.758178	-1.681498	H	-2.721708	1.843929	-1.952357
H	-0.430294	-6.425941	0.770070	C	-4.507585	-0.191020	-2.205299
H	-0.591161	-4.113905	1.705222	H	-3.649974	-0.531484	-0.228564
C	-1.970991	0.669667	0.082779	H	-2.468167	-0.593442	-1.555302
N	-2.328105	1.999634	0.041318	C	-5.423839	2.061014	-1.492384
N	-3.127957	-0.037911	0.300348	H	-4.613018	1.773953	0.500574
C	-4.334279	0.820677	0.272249	H	-4.064934	3.270265	-0.295399
C	-3.739936	2.213076	0.438561	C	-5.760128	0.588620	-1.775122
H	-5.033527	0.542749	1.084590	H	-4.745856	-1.266036	-2.347052
H	-4.866462	0.695599	-0.697270	H	-4.156826	0.187040	-3.192667
H	-3.789857	2.562930	1.492470	H	-6.320427	2.605280	-1.122555
H	-4.218451	2.979580	-0.202078	H	-5.124319	2.560278	-2.442575
C	-3.344663	-1.459589	0.383265	H	-6.553530	0.512827	-2.550472
C	-3.653543	-2.188485	-0.802871	H	-6.182092	0.127200	-0.851740
C	-3.950805	-3.561282	-0.675666	C	-1.731959	1.892539	1.826005
C	-3.975557	-4.187440	0.576869	C	-2.548992	3.143815	2.240270
C	-3.717201	-3.443795	1.736347	C	-2.345729	0.633390	2.470825
C	-3.405811	-2.070231	1.672047	H	-0.704548	2.015472	2.242727
C	-3.775416	-1.518667	-2.174500	C	-2.617377	3.289379	3.772429
H	-4.211019	-5.261149	0.651172	H	-3.584141	3.057180	1.853315
C	-3.225171	-1.273657	2.967374	H	-2.126423	4.065294	1.796203
H	-4.178051	-4.149377	-1.578771	C	-2.477879	0.773393	4.001879
H	-3.765280	-3.939646	2.718748	H	-3.355625	0.460128	2.034517
C	-2.990413	-2.238976	-3.286231	H	-1.737675	-0.257729	2.208825
H	-3.342662	-0.500232	-2.089663	C	-3.239183	2.041882	4.416135
C	-5.265503	-1.390505	-2.575025	H	-3.200172	4.198661	4.036668
C	-4.597537	-0.980896	3.619742	H	-1.591530	3.447837	4.178725
C	-2.295390	-1.960352	3.986629	H	-2.973232	-0.125708	4.422007
H	-2.747544	-0.307801	2.702354	H	-1.460358	0.800842	4.451981
C	-1.535396	3.167644	-0.265361	H	-3.258973	2.135964	5.523732
C	-1.350049	3.532542	-1.636548	H	-4.302282	1.956624	4.091880
C	-0.683157	4.744157	-1.914323	H	1.498203	-3.563537	2.290537
C	-0.253167	5.594977	-0.887898	H	0.180799	-4.812964	0.637795
C	-0.480483	5.243198	0.447736	C	5.031742	-1.520882	-1.721646
C	-1.124448	4.035657	0.792796	C	5.149762	-3.568779	-0.241368
C	-1.947204	2.728073	-2.794542	H	3.340580	-2.562332	-0.936942
H	0.248548	6.545010	-1.132341	H	5.206749	-4.226563	-1.134258
C	-1.436558	3.770537	2.268875	H	6.191231	-3.328566	0.062435
H	-0.523007	5.040062	-2.961943	H	4.701686	-4.159726	0.585535
H	-0.159322	5.926593	1.249610	H	5.052359	-2.152412	-2.634244
C	-1.077735	2.736580	-4.065082	H	4.477466	-0.595044	-1.968006
H	-2.016480	1.670549	-2.469324	H	6.082656	-1.253646	-1.478416
C	-3.369856	3.238598	-3.126619	C	1.458796	1.132665	4.005923

C	-2.583223	4.691155	2.754022	H	0.711016	-0.349115	2.623194
H	-1.751325	2.710045	2.359171	C	1.414455	-1.360108	4.403085
C	-0.210778	3.936044	3.188125	H	0.459900	1.266277	4.466982
H	-5.368524	-0.822660	-3.523868	H	2.201232	1.255109	4.822218
H	-5.719709	-2.392174	-2.732120	H	1.613334	1.959875	3.282489
H	-5.871208	-0.876517	-1.799880	H	0.458490	-1.251551	4.957840
H	-3.110410	-1.695052	-4.246511	H	1.433807	-2.374096	3.956555
H	-1.910720	-2.272203	-3.052059	H	2.244369	-1.305822	5.139672
H	-3.353058	-3.276521	-3.446362	C	-1.312151	-2.594391	-3.946590
H	-4.473996	-0.342888	4.520374	H	0.071469	-3.034700	-2.383167
H	-5.292376	-0.460150	2.928190	C	-0.669622	-4.919265	-3.140568
H	-5.097588	-1.921058	3.937387	H	0.116612	-4.981078	-3.922315
H	-2.151099	-1.303663	4.869227	H	-0.346343	-5.546365	-2.282912
H	-2.711057	-2.922949	4.354439	H	-1.592410	-5.379106	-3.556202
H	-1.291844	-2.148551	3.555873	H	-0.533651	-2.660377	-4.734067
H	-1.504263	2.037891	-4.814097	H	-2.270773	-2.937455	-4.392376
H	-1.035975	3.738935	-4.542841	H	-1.406262	-1.522323	-3.679920
H	-0.046805	2.397024	-3.845706	C	-3.223527	-2.641474	3.222390
H	-3.821876	2.630580	-3.938683	C	-1.614877	-4.515331	2.847693
H	-4.053025	3.193431	-2.253976	H	-1.225904	-2.430301	2.407342
H	-3.343157	4.295470	-3.469241	H	-2.838934	-2.430623	4.241240
H	-2.869305	4.439797	3.797376	H	-3.702939	-1.723177	2.832892
H	-2.269065	5.756906	2.741088	H	-4.015309	-3.411657	3.336682
H	-3.492186	4.613601	2.122409	H	-1.339552	-4.444571	3.921338
H	-0.491081	3.698645	4.235602	H	-2.433469	-5.260468	2.756074
H	0.596672	3.237732	2.897018	H	-0.739447	-4.918680	2.304807
H	0.182828	4.974719	3.180311	Cl	-0.394643	1.173166	-3.005918

6-trans <sup>+</sup>				6-cis <sup>+</sup> c			
-3032.68874998				-3032.71131321			
Ru	0.107763	0.152826	0.077465	Ru	0.142761	-0.123898	-0.991859
C	1.862068	1.242497	-0.035913	C	0.415939	-1.392779	0.589473
N	3.164921	0.854182	-0.061640	N	1.357741	-1.503516	1.588985
N	1.813863	2.597524	-0.159235	N	-0.380007	-2.521117	0.654443
C	4.092402	2.001552	-0.247763	C	1.046334	-2.641289	2.492933
C	3.157340	3.222247	-0.211897	C	0.137156	-3.510668	1.631361
C	3.715259	-0.474965	0.067757	C	2.640550	-0.847873	1.749914
C	0.659363	3.440388	0.034913	C	-1.376561	-2.894209	-0.322971
C	4.053953	-1.209794	-1.105973	C	2.811368	0.140173	2.764883
C	4.602313	-2.498014	-0.935099	C	4.097362	0.686555	2.960721
C	4.838336	-3.030029	0.339032	C	5.194562	0.256010	2.205630
C	4.562146	-2.263862	1.479069	C	5.023892	-0.752359	1.249520
C	4.011745	-0.970115	1.374020	C	3.763339	-1.336517	1.009282
C	3.945071	-0.621353	-2.515265	C	1.685182	0.561311	3.706844
H	4.861673	-3.092793	-1.824135	H	4.245007	1.451738	3.737964
H	4.796000	-2.673635	2.473976	H	5.896975	-1.109558	0.683331
C	3.859358	-0.116609	2.637313	C	3.679993	-2.527976	0.053945
C	0.214504	3.693937	1.368631	C	-1.024296	-3.009417	-1.711610
C	-0.820933	4.629370	1.554499	C	-2.042431	-3.359856	-2.624414
C	-1.388261	5.304669	0.462236	C	-3.340635	-3.661387	-2.197407
C	-0.938631	5.042990	-0.837737	C	-3.649835	-3.613073	-0.834207
C	0.095830	4.114283	-1.085121	C	-2.695146	-3.220352	0.125873
C	0.819362	2.944440	2.557732	C	0.420871	-2.945388	-2.236995
H	-1.181551	4.848901	2.570753	H	-1.803951	-3.429880	-3.694219
H	-1.388830	5.583596	-1.684921	H	-4.666931	-3.873975	-0.504008
C	0.600744	3.900960	-2.511977	C	-3.117747	-3.217790	1.600038
H	5.265505	-4.039646	0.443767	H	6.191392	0.690906	2.379606
H	-2.184728	6.046279	0.630100	H	-4.108342	-3.952473	-2.931069
H	3.307235	3.863592	0.684385	H	0.690519	-4.317357	1.099278
H	4.855503	2.010485	0.556516	H	1.972754	-3.152862	2.814722
Cl	0.293481	-0.027025	-2.241449	C	1.723272	0.808499	-0.668953
C	0.739105	-1.434132	0.773748	H	1.857039	1.336566	0.299378
H	0.981230	-1.313376	1.863997	C	2.860994	1.013992	-1.562672
C	0.910136	-2.810815	0.322547	C	3.977997	1.742536	-1.052808
C	1.165134	-3.806149	1.311827	C	2.909163	0.578606	-2.919618
C	0.815951	-3.221710	-1.035796	C	5.090148	2.016922	-1.857239
C	1.292440	-5.156325	0.960534	H	3.957119	2.088641	-0.007130
H	1.257279	-3.503571	2.367390	C	4.020875	0.863256	-3.721873
C	0.958954	-4.570357	-1.383168	H	2.046321	0.047840	-3.345933
H	0.644594	-2.452877	-1.803700	C	5.114410	1.578543	-3.195427
C	1.188396	-5.542085	-0.388892	H	5.941127	2.581461	-1.445354
H	1.479312	-5.911835	1.739526	H	4.035130	0.531457	-4.771746
H	0.892335	-4.872047	-2.440269	H	5.985057	1.801470	-3.832312
H	1.292142	-6.602529	-0.668127	P	-1.206248	1.606743	-0.134812
P	-2.290615	-0.666567	0.001015	C	-0.453531	3.268040	-0.709595
C	-2.536362	-1.782791	-1.522649	C	-1.437327	4.358983	-1.200046
C	-3.416448	-3.046536	-1.375199	C	0.567539	3.887241	0.276491
C	-2.930553	-1.001263	-2.800825	H	0.107360	2.922269	-1.605755
H	-1.493170	-2.136640	-1.681037	C	-0.666569	5.521582	-1.859795
C	-3.292225	-3.939783	-2.626662	H	-2.029989	4.754348	-0.345405
H	-4.482969	-2.756709	-1.243348	H	-2.156789	3.943092	-1.933005
H	-3.129340	-3.634804	-0.479310	C	1.337713	5.049241	-0.384418

C	-2.810072	-1.897367	-4.049013	H	0.039807	4.275602	1.174822
H	-3.980287	-0.645528	-2.715410	H	1.287827	3.128284	0.643071
H	-2.287135	-0.107757	-2.922764	C	0.381795	6.128725	-0.915855
C	-3.645896	-3.180462	-3.914237	H	-1.388063	6.297302	-2.194158
H	-3.940848	-4.834205	-2.508456	H	-0.165274	5.144493	-2.780051
H	-2.247263	-4.320173	-2.694866	H	2.051952	5.484695	0.347031
H	-3.118088	-1.322657	-4.948690	H	1.951315	4.648071	-1.222877
H	-1.738429	-2.160707	-4.200100	H	0.951719	6.929549	-1.433076
H	-3.502253	-3.833874	-4.801117	H	-0.132665	6.618897	-0.057483
H	-4.727902	-2.914318	-3.897902	C	-2.870290	1.473566	-1.048948
C	-2.707452	-1.734480	1.520433	C	-3.360780	0.026382	-1.276008
C	-2.115767	-1.198971	2.845758	C	-4.044762	2.336275	-0.529171
C	-4.190789	-2.110512	1.758387	H	-2.559200	1.857208	-2.047509
H	-2.149063	-2.669604	1.272772	C	-4.533816	-0.001270	-2.275778
C	-2.249729	-2.235122	3.980791	H	-3.685875	-0.418288	-0.310722
H	-2.646565	-0.263760	3.133739	H	-2.542031	-0.614390	-1.663613
H	-1.048926	-0.930607	2.716287	C	-5.211583	2.325723	-1.538995
C	-4.318701	-3.178344	2.863233	H	-4.408138	1.920530	0.436419
H	-4.742781	-1.202351	2.086456	H	-3.735783	3.380127	-0.331476
H	-4.681570	-2.460685	0.831465	C	-5.697212	0.898131	-1.829561
C	-3.703010	-2.692679	4.184063	H	-4.877860	-1.048494	-2.409721
H	-1.838834	-1.812027	4.922933	H	-4.161515	0.333956	-3.270193
H	-1.617705	-3.119282	3.734240	H	-6.042057	2.951535	-1.147644
H	-5.389095	-3.439896	3.004537	H	-4.878116	2.807572	-2.486336
H	-3.811267	-4.113736	2.532930	H	-6.497512	0.909073	-2.599755
H	-3.752865	-3.489320	4.956465	H	-6.159165	0.474690	-0.907877
H	-4.305405	-1.841634	4.576650	C	-1.505338	1.717312	1.726567
C	-3.524274	0.753466	-0.182130	C	-2.242416	2.987695	2.227928
C	-5.018501	0.376224	-0.343374	C	-2.207245	0.448576	2.258890
C	-3.367504	1.845929	0.900871	H	-0.469424	1.738557	2.136053
H	-3.186590	1.202129	-1.146533	C	-2.360800	2.997286	3.765224
C	-5.859699	1.614836	-0.707828	H	-3.263543	3.019692	1.800262
H	-5.398969	-0.037948	0.612307	H	-1.730085	3.907438	1.883620
H	-5.155693	-0.418619	-1.103919	C	-2.349753	0.464081	3.792996
C	-4.236725	3.078026	0.577059	H	-3.222474	0.385806	1.808996
H	-3.667839	1.432082	1.890738	H	-1.661490	-0.457974	1.924376
H	-2.304896	2.157474	0.991721	C	-3.060065	1.733550	4.289088
C	-5.713607	2.715027	0.355099	H	-2.911181	3.908135	4.083572
H	-6.924839	1.321037	-0.823072	H	-1.346379	3.076225	4.217173
H	-5.534588	2.005333	-1.699478	H	-2.898309	-0.443974	4.124077
H	-4.137086	3.827851	1.390803	H	-1.339769	0.402258	4.258762
H	-3.834064	3.562791	-0.340863	H	-3.104906	1.744700	5.398843
H	-6.291849	3.617987	0.064723	H	-4.116966	1.725130	3.936422
H	-6.156441	2.358883	1.313657	H	0.523552	-2.268164	3.401654
H	4.623010	1.899592	-1.216189	H	-0.677842	-3.981533	2.207550
H	3.252363	3.868832	-1.107230	C	4.512617	-2.350504	-1.231128
C	3.189085	-0.856053	3.812678	C	4.108626	-3.829273	0.775037
C	5.237162	0.432287	3.082385	H	2.620007	-2.640460	-0.250462
H	3.216965	0.752894	2.380905	H	3.994485	-4.705622	0.103356
H	5.129833	1.111733	3.953868	H	5.175161	-3.775519	1.078718
H	5.913860	-0.395543	3.381258	H	3.517994	-4.026216	1.692980
H	5.747283	0.992358	2.271857	H	4.330547	-3.198091	-1.923981
H	3.040519	-0.166405	4.669453	H	4.263328	-1.412004	-1.763442
H	2.198207	-1.271912	3.535308	H	5.602312	-2.346037	-1.021650
H	3.811080	-1.697270	4.182882	C	1.614196	2.087341	3.912278
C	3.336466	-1.590874	-3.546941	H	0.728976	0.230851	3.246374

H	3.268341	0.257279	-2.462743	C	1.828306	-0.147203	5.075844
C	5.338789	-0.151203	-3.001876	H	0.730653	2.354471	4.527165
H	3.218280	-1.077848	-4.523522	H	2.504062	2.472811	4.451140
H	3.985217	-2.474783	-3.720968	H	1.541870	2.635863	2.951044
H	2.337832	-1.946402	-3.230391	H	0.969644	0.095809	5.736575
H	5.259153	0.355460	-3.986361	H	1.883077	-1.250019	4.976692
H	5.825975	0.550156	-2.293157	H	2.753824	0.181513	5.593604
H	6.025789	-1.015238	-3.122753	C	0.549261	-2.684297	-3.746407
C	0.044430	1.640426	2.826810	H	0.974142	-2.104205	-1.715303
H	1.853477	2.653398	2.275969	C	1.163326	-4.253678	-1.875576
C	0.918897	3.780878	3.847974	H	2.211662	-4.225662	-2.234416
H	1.464438	3.217047	4.632266	H	1.175143	-4.457535	-0.788054
H	1.460179	4.732362	3.671572	H	0.658009	-5.110947	-2.367807
H	-0.079281	4.029664	4.263906	H	1.617866	-2.543842	-4.007463
H	0.586447	0.953781	3.506823	H	0.189114	-3.549610	-4.339644
H	-0.967256	1.836107	3.236583	H	-0.003171	-1.776448	-4.058950
H	-0.153789	1.090469	1.852098	C	-4.452446	-2.483568	1.849261
C	-0.535118	3.518166	-3.483203	C	-3.216920	-4.663425	2.147493
C	1.361433	5.145813	-3.025178	H	-2.338494	-2.674411	2.175331
H	1.305921	3.043816	-2.487351	H	-4.652386	-2.414384	2.938464
H	-0.121536	3.318554	-4.493286	H	-4.444176	-1.455530	1.436203
H	-1.059336	2.601189	-3.148497	H	-5.312145	-3.020859	1.398479
H	-1.282554	4.332370	-3.589142	H	-3.442993	-4.657244	3.234158
H	1.794206	4.951040	-4.028397	H	-4.032576	-5.219305	1.639666
H	0.684803	6.021358	-3.118424	H	-2.286788	-5.247954	1.992512
H	2.188990	5.444356	-2.348178	Cl	-0.441593	0.678888	-3.160005

6-cis <sup>+</sup> t			
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Cl	1.231862	-0.716532	-2.841593
C	0.792504	-1.569510	0.051337
N	2.088594	-1.926414	0.388947
N	0.039373	-2.724988	0.086081
C	2.267731	-3.396974	0.355480
C	0.841780	-3.897277	0.520074
C	3.233455	-1.131691	0.778185
C	-1.367468	-2.992767	-0.140865
C	3.321979	-0.694198	2.138350
C	4.468603	0.021728	2.535436
C	5.518029	0.271058	1.639049
C	5.444564	-0.220272	0.332165
C	4.320180	-0.941894	-0.126273
C	2.257563	-1.045803	3.183012
H	4.554011	0.376922	3.573325
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C	4.365704	-1.552080	-1.526843
C	-1.798171	-3.405124	-1.439768
C	-3.131053	-3.845325	-1.591414
C	-4.003372	-3.929326	-0.500807
C	-3.553576	-3.567587	0.775430
C	-2.237594	-3.106938	0.990573
C	-0.859449	-3.511101	-2.641818
H	-3.478071	-4.164394	-2.586427
H	-4.234683	-3.669307	1.634552
C	-1.786021	-2.864300	2.434510
H	6.406632	0.830518	1.971370
H	-5.031226	-4.299674	-0.640580
H	0.608414	-4.774359	-0.113454
H	2.706844	-3.699829	-0.620182
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H	1.719429	0.944401	1.128115
C	2.270645	2.364812	-0.386462
C	2.799625	3.242916	0.605295
C	2.540376	2.655912	-1.753842
C	3.517194	4.390120	0.243940
H	2.639281	3.007922	1.669930
C	3.283944	3.788514	-2.108393
H	2.199292	1.951607	-2.528596
C	3.760996	4.666501	-1.114771
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H	3.503959	3.987387	-3.168955
H	4.340355	5.558693	-1.400060
P	-1.477204	1.428426	0.182254
C	-1.179366	2.280191	1.849994
C	-1.860277	3.657326	2.040510
C	-1.444032	1.343887	3.047964
H	-0.080063	2.462123	1.800051
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H	-0.878155	0.396099	2.921421
C	-1.796111	3.361473	4.569701
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H	0.011679	2.169487	4.443422
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H	-2.897302	3.202829	4.630374
C	-1.397673	2.843107	-1.083972
C	-0.869697	2.274128	-2.421377
C	-2.626323	3.747227	-1.335164
H	-0.583648	3.476877	-0.657881
C	-0.548551	3.381769	-3.443619
H	-1.603321	1.566094	-2.861231
H	0.083505	1.687108	-2.271151
C	-2.291932	4.863340	-2.345890
H	-3.460305	3.136306	-1.743042
H	-2.995354	4.192828	-0.390687
C	-1.768233	4.291275	-3.673140
H	-0.211837	2.923223	-4.397252
H	0.301285	3.991525	-3.063887
H	-3.194671	5.486642	-2.519344
H	-1.525939	5.542011	-1.905391
H	-1.503198	5.111006	-4.373769
H	-2.577338	3.707906	-4.168886
C	-3.199776	0.650937	0.146513
C	-4.339939	1.491040	0.774828
C	-3.558016	0.191112	-1.290974
H	-3.069615	-0.269527	0.761512
C	-5.695456	0.760860	0.693432
H	-4.426607	2.465637	0.250312
H	-4.111802	1.723066	1.834882
C	-4.934182	-0.499043	-1.354958
H	-3.574561	1.070875	-1.970879
H	-2.777046	-0.500795	-1.677912
C	-6.044630	0.371811	-0.750125
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H	-5.657812	-0.156905	1.323648
H	-5.163394	-0.756824	-2.410918
H	-4.879873	-1.462101	-0.803797
H	-7.016797	-0.164118	-0.783618
H	-6.177500	1.294117	-1.361593
H	2.949896	-3.730301	1.160628
H	0.598488	-4.155200	1.573014
C	4.790970	-0.542754	-2.611777
C	5.304501	-2.782685	-1.548193
H	3.339185	-1.883045	-1.783175
H	5.282901	-3.269077	-2.545832
H	6.355225	-2.488050	-1.341682
H	5.024306	-3.543658	-0.791118
H	4.692494	-1.002311	-3.616639
H	4.158303	0.365729	-2.592401
H	5.850154	-0.229472	-2.497801
C	2.046951	0.056400	4.237241

H	1.292883	-1.189092	2.649066
C	2.603808	-2.377871	3.891181
H	1.173045	-0.183354	4.876391
H	2.920083	0.154258	4.915036
H	1.870365	1.048377	3.772963
H	1.816518	-2.649859	4.625176
H	2.709410	-3.221266	3.180346
H	3.564082	-2.289256	4.441156
C	-1.419611	-2.817782	-3.900335
H	0.088181	-2.998383	-2.384140
C	-0.532183	-4.992635	-2.946011
H	0.207327	-5.063394	-3.770691
H	-0.108462	-5.519558	-2.065565
H	-1.438619	-5.553324	-3.258044
H	-0.670475	-2.848016	-4.717470
H	-2.338398	-3.315475	-4.275707
H	-1.658280	-1.751894	-3.710124
C	-2.777643	-1.996689	3.237002
C	-1.578769	-4.203455	3.185844
H	-0.813566	-2.326273	2.397510
H	-2.350002	-1.732231	4.226065
H	-3.029694	-1.056052	2.710731
H	-3.727360	-2.536715	3.431716
H	-1.171696	-4.022779	4.202651
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H	-0.888773	-4.892167	2.658897

7-trans				7-cis		
	-3026.41711147			-3026.40883466		
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Cl	0.037995	-0.335945	-2.418408	C	0.972634	-1.801817
P	-0.817911	2.052649	-0.010562	N	2.238578	-2.147427
N	0.062631	-3.209838	0.038878	N	0.171615	-2.904340
N	2.183187	-2.610438	0.024376	C	2.282920	-3.490720
C	0.901348	-2.131106	0.012503	C	0.968179	-4.102953
C	0.782078	-4.498720	0.161116	C	3.437912	-1.357458
H	0.429907	-5.215153	-0.609661	C	-1.264881	-3.028325
H	0.584260	-4.951838	1.157714	C	3.570644	-0.378010
C	2.249806	-4.087916	-0.021331	C	4.776759	0.342104
H	2.912793	-4.473798	0.780551	C	5.866239	0.094010
H	2.672318	-4.421339	-0.995298	C	5.725760	-0.924510
C	-1.379371	-3.248616	0.035084	C	4.539463	-1.669622
C	-2.083424	-3.272781	1.269532	C	2.455629	-0.140787
C	-1.370078	-3.177020	2.595959	H	4.870267	1.108045
H	-2.094158	-3.211433	3.433497	H	6.573164	-1.153592
H	-0.778107	-2.238714	2.680339	C	4.464482	-2.766112
H	-0.659548	-4.020291	2.739422	C	-2.010854	-3.392734
C	-3.485152	-3.431134	1.230772	C	-3.404270	-3.574346
H	-4.036644	-3.451643	2.185972	C	-4.068687	-3.448399
C	-4.191742	-3.593419	0.023961	C	-3.289294	-3.159885
C	-5.696164	-3.749076	0.010569	C	-1.896821	-2.969795
H	-6.021016	-4.508886	-0.730085	C	-1.365955	-3.683883
H	-6.193858	-2.794366	-0.269124	H	-3.984340	-3.847086
H	-6.086948	-4.046225	1.004422	H	-3.775829	-3.102963
C	-3.454472	-3.609513	-1.176970	C	-1.103379	-2.821149
H	-3.980791	-3.770799	-2.132943	C	7.143079	0.897920
C	-2.053607	-3.459258	-1.200342	C	-5.567533	-3.617045
C	-1.301143	-3.555673	-2.504359	H	1.102708	-4.736052
H	-1.993172	-3.763503	-3.343839	H	3.169955	-4.056031
H	-0.545741	-4.371015	-2.483675	C	2.107710	0.562019
H	-0.756809	-2.609279	-2.717211	H	2.333449	1.486344
C	3.423260	-1.882703	-0.018370	H	2.941711	0.182861
C	4.004897	-1.565568	-1.275478	P	-0.715584	1.553513
C	3.308731	-1.901742	-2.571732	C	-0.011111	3.178388
H	3.914050	-1.575759	-3.440235	C	-1.010365	4.278069
H	2.308025	-1.418749	-2.639696	C	1.145747	3.811984
H	3.141623	-2.995916	-2.676491	H	0.420646	2.775416
C	5.259841	-0.921924	-1.281683	C	-0.296329	5.370301
H	5.714447	-0.665319	-2.253462	H	-1.480440	4.745775
C	5.949832	-0.611670	-0.093833	H	-1.829583	3.846135
C	7.280862	0.106260	-0.126503	C	1.868679	4.894116
H	7.775912	0.009533	-1.113677	H	0.749670	4.283435
H	7.974006	-0.282907	0.647641	H	1.874994	3.047174
H	7.152642	1.193173	0.072838	C	0.890883	5.982017
C	5.359120	-0.978354	1.132767	H	-1.023841	6.160964
H	5.892419	-0.765253	2.074717	H	0.067250	4.920747
C	4.107559	-1.620596	1.200060	H	2.689146	5.342929
C	3.512007	-2.005661	2.531584	H	2.350679	4.416444
H	3.288405	-3.092984	2.586694	H	1.416927	6.728402
H	2.550950	-1.471486	2.706836	H	0.509471	6.539971

H	4.206755	-1.764470	3.359929	C	-2.539779	1.491157	-0.623011
C	1.986870	0.652637	-0.171396	C	-3.087606	0.047687	-0.664932
C	-2.669443	1.730022	-0.273008	C	-3.568028	2.419580	0.060455
C	-3.168877	1.713543	-1.735108	H	-2.431515	1.803538	-1.686009
C	-3.068037	0.410679	0.429047	C	-4.440694	-0.003462	-1.399009
H	-3.178883	2.577996	0.244447	H	-3.203734	-0.354062	0.366989
C	-4.693738	1.488331	-1.790507	H	-2.368662	-0.617647	-1.185594
H	-2.646596	0.902341	-2.289099	C	-4.918343	2.380450	-0.684594
H	-2.924598	2.666108	-2.249248	H	-3.737082	2.083111	1.108048
C	-4.590578	0.190463	0.386776	H	-3.203023	3.463812	0.116092
H	-2.564103	-0.435446	-0.096168	C	-5.473008	0.950003	-0.776097
H	-2.701452	0.383875	1.474415	H	-4.823913	-1.046198	-1.404382
C	-5.118765	0.205585	-1.056618	H	-4.275229	0.274676	-2.464770
H	-5.026326	1.457972	-2.851030	H	-5.646552	3.051743	-0.178543
H	-5.209278	2.362453	-1.328360	H	-4.778440	2.788287	-1.712041
H	-4.841693	-0.768756	0.886754	H	-6.420043	0.936776	-1.358808
H	-5.092612	0.993615	0.975742	H	-5.732630	0.594762	0.248703
H	-6.225990	0.101600	-1.070621	C	-0.677758	1.855766	1.795715
H	-4.710130	-0.678276	-1.597690	C	-1.294792	3.161093	2.361588
C	-0.446038	3.433312	-1.292177	C	-1.226146	0.647449	2.580809
C	0.633118	4.464154	-0.881825	H	0.419381	1.910328	1.988703
C	-0.125011	2.907174	-2.707180	C	-0.981111	3.305620	3.864350
H	-1.420996	3.978637	-1.326679	H	-2.395748	3.141413	2.235957
C	0.747560	5.606955	-1.912471	H	-0.935916	4.054716	1.813651
H	1.617501	3.949256	-0.794270	C	-0.962225	0.779363	4.093416
H	0.414227	4.908179	0.108874	H	-2.322236	0.564790	2.402765
C	-0.027663	4.046687	-3.737543	H	-0.781564	-0.287754	2.186972
H	0.839688	2.357067	-2.667101	C	-1.505377	2.100649	4.662261
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C	1.022697	5.090848	-3.332051	H	0.120804	3.395788	4.007203
H	1.541622	6.315251	-1.589530	H	-1.405024	-0.084882	4.634973
H	-0.204112	6.187768	-1.911807	H	0.135827	0.728550	4.274454
H	0.207625	3.621524	-4.737200	H	-1.242153	2.197617	5.738047
H	-1.021289	4.543609	-3.838207	H	-2.618884	2.090809	4.613756
H	1.045715	5.934822	-4.055637	H	2.345107	-3.403332	2.201380
H	2.034139	4.623756	-3.363488	H	0.457460	-4.707338	1.390617
C	-0.821716	3.083953	1.597610	Cl	-0.618986	0.680266	-3.123176
C	-1.804083	2.624755	2.701142	H	8.039383	0.262221	0.751933
C	0.593019	3.243968	2.206251	H	7.175323	1.692884	0.128054
H	-1.174139	4.084837	1.244260	H	7.238255	1.397031	1.890806
C	-1.809822	3.620248	3.879608	H	5.300743	-2.684162	-2.064539
H	-1.493667	1.619334	3.059036	H	4.540650	-3.773839	-0.875070
H	-2.836819	2.533578	2.306141	H	3.505038	-2.718335	-1.902166
C	0.591267	4.247484	3.374842	H	2.679084	0.722924	3.203723
H	0.917190	2.246403	2.569067	H	1.496372	0.044779	2.025270
H	1.332692	3.554152	1.442621	H	2.299584	-1.025220	3.203352
C	-0.405555	3.830240	4.468232	H	-5.859641	-4.097490	1.588457
H	-2.510999	3.260753	4.664282	H	-6.082892	-2.631884	0.594137
H	-2.211239	4.600645	3.530209	H	-5.970779	-4.228767	-0.199834
H	1.616867	4.332061	3.795959	H	-1.699782	-2.317225	3.649158
H	0.324176	5.264103	2.999887	H	-0.824921	-3.820388	3.268049
H	-0.434867	4.586390	5.283115	H	-0.164286	-2.253648	2.722582
H	-0.058254	2.878885	4.931132	H	-2.101303	-3.586659	-3.002993
H	2.421859	0.917372	-1.163987	H	-0.498089	-3.032520	-2.409719
H	2.593601	0.935416	0.720388	H	-0.993689	-4.733114	-2.200752

7-trans <sup>+</sup>				7-cis <sup>+</sup> c		
-2566.00524786				-2566.01599688		
Ru	0.362847	0.006341	-0.085751	Ru	0.024623	-0.485061
Cl	0.334094	0.216294	-2.406185	C	0.273241	-1.863892
P	-1.111892	1.918688	0.281609	N	1.421577	-2.441676
N	0.260474	-2.996979	-0.483113	N	-0.791962	-2.558946
N	2.364928	-2.332756	-0.446415	C	1.139864	-3.510550
C	1.074545	-1.922964	-0.321363	C	-0.364217	-3.753879
C	1.003997	-4.244227	-0.788249	C	2.789869	-2.195163
H	0.743393	-4.606511	-1.805135	C	-2.146470	-2.505500
H	0.731150	-5.041857	-0.066650	C	3.615694	-1.359802
C	2.474603	-3.797871	-0.670514	C	4.964919	-1.191706
H	3.006745	-4.272821	0.181790	C	5.524458	-1.856672
H	3.062369	-4.003595	-1.587846	C	4.693897	-2.735980
C	-1.165105	-3.020369	-0.275476	C	3.341321	-2.934381
C	-1.650657	-3.196636	1.048529	C	3.111274	-0.712369
C	-0.700756	-3.342454	2.216325	H	5.604186	-0.530939
H	-1.254588	-3.481556	3.164596	H	5.119251	-3.299562
H	-0.034526	-2.462443	2.332403	C	2.515796	-3.929441
H	-0.037464	-4.225619	2.093427	C	-2.423296	-2.886124
C	-3.042715	-3.296087	1.242382	C	-3.760927	-2.876140
H	-3.427705	-3.434465	2.266417	C	-4.829808	-2.545342
C	-3.949829	-3.268313	0.163332	C	-4.523840	-2.226016
C	-5.436678	-3.424779	0.384502	C	-3.201118	-2.203102
H	-5.789785	-4.410712	0.012307	C	-1.337172	-3.337182
H	-6.013921	-2.652014	-0.164150	H	-3.976509	-3.161672
H	-5.704342	-3.358658	1.457263	H	-5.345471	-1.988715
C	-3.426610	-3.132876	-1.139573	C	-2.952775	-1.899833
H	-4.117385	-3.134222	-1.999207	C	6.969442	-1.660432
C	-2.045359	-3.015422	-1.391892	C	-6.253396	-2.551863
C	-1.530975	-2.918227	-2.808292	H	-0.586416	-4.672320
H	-2.368412	-2.818832	-3.525487	H	1.757550	-4.407544
H	-0.962097	-3.828120	-3.099080	C	1.785999	-0.446775
H	-0.852943	-2.048993	-2.940119	H	2.551224	0.323810
C	3.563991	-1.550713	-0.311087	H	2.123744	-1.239363
C	4.241299	-1.104089	-1.479052	P	-0.086400	1.593839
C	3.689496	-1.366888	-2.859788	C	1.001337	2.767381
H	4.299198	-0.858993	-3.631515	C	0.438480	4.178777
H	2.641553	-1.010330	-2.952614	C	2.466264	2.872168
H	3.691342	-2.451151	-3.105950	H	1.004349	2.226471
C	5.444029	-0.391401	-1.310740	C	1.322102	4.895535
H	5.971407	-0.031856	-2.209965	H	0.402283	4.786870
C	5.995714	-0.129519	-0.038635	H	-0.597982	4.115226
C	7.309772	0.603455	0.098094	C	3.346177	3.583463
H	7.399938	1.423165	-0.643310	H	2.502887	3.454180
H	8.164268	-0.085962	-0.078846	H	2.893745	1.876563
H	7.438965	1.033787	1.110787	C	2.791822	4.974801
C	5.303342	-0.602869	1.094647	H	0.915167	5.911592
H	5.721840	-0.418517	2.098119	H	1.253426	4.347467
C	4.097078	-1.322431	0.986509	H	4.387344	3.660846
C	3.392898	-1.829306	2.224337	H	3.394576	2.959630
H	3.201902	-2.922015	2.177582	H	3.407679	5.449805
H	2.402807	-1.342299	2.362273	H	2.875031	5.634974
H	3.995192	-1.634309	3.132441	C	-1.882383	2.163746

C	1.954278	0.851069	0.134252	C	-2.916361	1.040299	-0.080414
C	-2.769860	1.986516	-0.623872	C	-2.337182	3.452319	0.398144
C	-2.820960	2.928822	-1.849609	H	-1.881058	2.351235	-1.427011
C	-3.235309	0.568052	-1.032400	C	-4.317161	1.469016	-0.558743
H	-3.472973	2.393310	0.141441	H	-2.951269	0.790676	1.002933
C	-4.238778	2.961639	-2.455328	H	-2.627217	0.111171	-0.615183
H	-2.102410	2.567906	-2.618332	C	-3.726407	3.892344	-0.108095
H	-2.517991	3.960394	-1.576064	H	-2.405913	3.254302	1.490584
C	-4.648683	0.597020	-1.645064	H	-1.610303	4.276826	0.268394
H	-2.511751	0.169906	-1.777961	C	-4.774310	2.786354	0.087975
H	-3.211690	-0.131537	-0.171077	H	-5.041386	0.654763	-0.345150
C	-4.729252	1.557663	-2.841671	H	-4.293183	1.584321	-1.665877
H	-4.245340	3.635536	-3.338289	H	-4.032636	4.821293	0.418644
H	-4.941571	3.410906	-1.716405	H	-3.655579	4.154756	-1.188230
H	-4.939446	-0.431298	-1.948123	H	-5.754795	3.101974	-0.327567
H	-5.381690	0.911113	-0.866570	H	-4.936331	2.626787	1.179040
H	-5.767521	1.604502	-3.233306	C	0.436022	1.819241	1.707013
H	-4.099110	1.164716	-3.671830	C	0.481189	3.285571	2.213185
C	-0.386267	3.663377	0.177637	C	-0.393762	0.947428	2.676973
C	0.513053	4.063453	1.368305	H	1.480646	1.432351	1.700869
C	0.369723	3.886930	-1.153977	C	1.038807	3.354934	3.649032
H	-1.287561	4.321273	0.197831	H	-0.541362	3.711767	2.214212
C	1.001612	5.521310	1.232579	H	1.086523	3.925243	1.541225
H	1.401798	3.391101	1.401761	C	0.108663	1.051767	4.132281
H	-0.019367	3.946713	2.335372	H	-1.457342	1.272991	2.639815
C	0.857029	5.342291	-1.290042	H	-0.380479	-0.111075	2.341974
H	1.244581	3.199605	-1.180943	C	0.197037	2.507732	4.615076
H	-0.254704	3.608689	-2.025129	H	1.066994	4.414648	3.980641
C	1.731269	5.761119	-0.098258	H	2.094335	2.998077	3.658193
H	1.659570	5.769815	2.092496	H	-0.557941	0.459768	4.795803
H	0.125468	6.205364	1.304931	H	1.115743	0.583742	4.208935
H	1.414070	5.456046	-2.244163	H	0.618820	2.548280	5.641583
H	-0.022983	6.021677	-1.363043	H	-0.827769	2.939183	4.682582
H	2.029680	6.827034	-0.187735	H	1.394641	-3.153127	2.840940
H	2.676639	5.171218	-0.110543	H	-0.911528	-3.825848	2.596352
C	-1.492215	1.619129	2.112295	Cl	-1.078486	0.322107	-3.045193
C	-2.788658	0.834590	2.410260	H	7.048905	-1.168464	-1.623369
C	-0.255567	0.864088	2.666087	H	7.515235	-1.034253	0.102032
H	-1.570257	2.605182	2.623920	H	7.498575	-2.632726	-0.713314
C	-2.928451	0.555846	3.918737	H	3.521104	0.310153	2.636652
H	-2.777158	-0.138111	1.868487	H	2.007995	-0.655405	2.538687
H	-3.674044	1.393737	2.043287	H	3.438592	-1.291822	3.403174
C	-0.404026	0.450939	4.143704	H	-6.981522	-2.376971	-0.237641
H	-0.108438	-0.085571	2.036336	H	-6.407722	-1.764454	-1.821992
H	0.662628	1.470589	2.545868	H	-6.504406	-3.520040	-1.535089
C	-1.734583	-0.254222	4.446862	H	-3.695192	-1.174734	3.124246
H	-3.879648	0.016226	4.111484	H	-3.053938	-2.816641	3.357652
H	-3.001274	1.520906	4.470161	H	-1.941427	-1.486544	2.909179
H	0.461374	-0.173704	4.452602	H	3.134832	-4.444804	-2.180929
H	-0.337498	1.383604	4.749742	H	2.077428	-4.711465	-0.765758
H	-1.829179	-0.426469	5.539661	H	1.668050	-3.448788	-1.953498
H	-1.738584	-1.260007	3.971305	H	-1.770499	-3.863640	-2.794659
H	2.565080	1.195107	-0.728104	H	-0.766558	-2.476602	-2.354953
H	2.379486	1.061374	1.145212	H	-0.606132	-4.015003	-1.438776

7-cis <sup>+</sup> t			
-2566.00618726			
Ru	-0.547350	0.048925	-1.055633
Cl	-0.849758	1.271010	-3.010643
C	-1.285512	1.502425	0.100187
N	-2.607035	1.704998	0.421024
N	-0.602270	2.642515	0.454468
C	-2.873562	3.094266	0.863711
C	-1.470449	3.635136	1.133136
C	-3.759365	0.843993	0.315348
C	0.805705	2.968753	0.431962
C	-4.101064	0.040468	1.437646
C	-5.247931	-0.770615	1.357506
C	-6.074231	-0.785741	0.213069
C	-5.727071	0.055910	-0.860717
C	-4.590940	0.893154	-0.833873
C	-3.249186	0.041331	2.685206
H	-5.508375	-1.406129	2.220301
H	-6.366673	0.071101	-1.758956
C	-4.317774	1.821127	-1.993717
C	1.317342	3.781427	-0.623643
C	2.641719	4.249871	-0.519073
C	3.452269	3.992767	0.605372
C	2.897876	3.234579	1.653375
C	1.580282	2.734299	1.601693
C	0.474891	4.212582	-1.798496
H	3.038609	4.877440	-1.334335
H	3.496947	3.053175	2.561687
C	1.004726	2.067728	2.830540
C	-7.316024	-1.645417	0.163495
C	4.848947	4.562460	0.695219
H	-1.299640	4.645419	0.710696
H	-3.399435	3.648198	0.055358
C	-1.815773	-1.242207	-0.789364
H	-2.771960	-1.099987	-0.249424
H	-1.703109	-2.234937	-1.290703
P	1.010367	-1.392087	0.064682
C	0.400788	-2.373488	1.566546
C	1.013853	-3.777571	1.788524
C	0.427539	-1.536617	2.862744
H	-0.669440	-2.522615	1.288893
C	0.321433	-4.499265	2.963714
H	2.100126	-3.694218	2.006163
H	0.915908	-4.394737	0.872772
C	-0.240814	-2.278535	4.036759
H	1.481141	-1.303281	3.134756
H	-0.074328	-0.562420	2.690864
C	0.372582	-3.669844	4.255541
H	0.795860	-5.492079	3.114348
H	-0.740913	-4.700364	2.694658
H	-0.161313	-1.662866	4.957951
H	-1.329329	-2.386413	3.826504
H	-0.154057	-4.199453	5.077235
H	1.431452	-3.561722	4.585193

C	1.141459	-2.671888	-1.331073
C	0.887697	-2.008295	-2.708293
C	2.377863	-3.598438	-1.421124
H	0.256333	-3.315954	-1.107364
C	0.680088	-3.061487	-3.813520
H	1.740119	-1.349347	-2.976548
H	-0.013097	-1.336987	-2.707650
C	2.175888	-4.660692	-2.522340
H	3.276916	-2.991424	-1.664089
H	2.584444	-4.095695	-0.452819
C	1.878203	-4.024019	-3.890128
H	0.519236	-2.553416	-4.787300
H	-0.248916	-3.638017	-3.600409
H	3.077655	-5.306314	-2.581457
H	1.334341	-5.330713	-2.231907
H	1.688849	-4.810486	-4.650764
H	2.775904	-3.464599	-4.239181
C	2.695280	-0.626331	0.408874
C	3.715086	-1.543326	1.128991
C	3.294018	-0.021743	-0.887653
H	2.448703	0.220213	1.090113
C	5.046001	-0.806415	1.381111
H	3.913705	-2.445719	0.512929
H	3.302411	-1.901797	2.093951
C	4.641831	0.676783	-0.625447
H	3.452957	-0.831617	-1.633045
H	2.578334	0.695772	-1.346205
C	5.643688	-0.249114	0.080639
H	5.758034	-1.498176	1.879439
H	4.871826	0.030060	2.096148
H	5.055039	1.045701	-1.588233
H	4.461063	1.574420	0.003900
H	6.588640	0.294933	0.291591
H	5.917733	-1.093299	-0.593390
H	-3.528012	3.095524	1.758273
H	-1.222247	3.675085	2.216934
H	-4.719086	1.402570	-2.937553
H	-4.823753	2.800380	-1.840889
H	-3.238014	2.010447	-2.142281
H	-3.688469	-0.607564	3.467134
H	-2.220184	-0.320852	2.479082
H	-3.146772	1.059936	3.116523
H	1.748640	1.408169	3.321261
H	0.718256	2.829402	3.588813
H	0.104913	1.466139	2.604818
H	0.947406	5.063576	-2.325434
H	0.328572	3.389331	-2.527062
H	-0.543131	4.524602	-1.487633
H	5.398534	4.174102	1.574899
H	5.441727	4.330880	-0.214115
H	4.818562	5.670037	0.781155
H	-7.610566	-1.881861	-0.878134
H	-7.177629	-2.599109	0.711549
H	-8.175652	-1.121690	0.636443

8-trans				8-cis			
-2671.58885702				-2671.59607223			
Ru	0.287050	0.628866	0.273878	Ru	-0.251931	0.905909	-0.253219
Cl	0.511200	0.203816	2.669979	Cl	-0.862672	3.196872	-0.734585
C	0.509752	-1.390831	-0.092162	Cl	0.314841	0.765416	-2.606890
N	-0.441488	-2.368552	-0.117182	C	-0.433580	-1.109339	-0.343668
N	1.722190	-1.995193	-0.292881	N	-1.642360	-1.702747	-0.658204
C	0.110728	-3.705627	-0.434406	C	-1.485513	-3.072720	-1.187092
C	1.627662	-3.470379	-0.364192	H	-1.601182	-3.070599	-2.294498
C	-1.868094	-2.225791	-0.019841	H	-2.252811	-3.752225	-0.764339
C	3.016959	-1.361275	-0.348366	C	-0.059528	-3.425847	-0.753339
C	-2.622000	-1.924812	-1.185522	H	-0.033048	-4.081353	0.148033
C	-4.024657	-1.880743	-1.073172	H	0.522607	-3.928809	-1.551550
C	-4.687833	-2.130685	0.145787	N	0.518076	-2.101165	-0.440213
C	-3.906695	-2.433469	1.277732	C	-2.968725	-1.173649	-0.469242
C	-2.498560	-2.491618	1.222299	C	-3.627294	-0.442014	-1.498398
C	-1.944293	-1.643842	-2.504859	C	-4.935546	0.022181	-1.248809
H	-4.617337	-1.641962	-1.972331	H	-5.436050	0.610860	-2.035817
H	-4.405871	-2.636039	2.240521	C	-5.628947	-0.260139	-0.055944
C	-1.688336	-2.802131	2.458291	C	-4.983915	-1.065040	0.902631
C	3.791842	-1.223039	0.836715	H	-5.520579	-1.339862	1.826714
C	5.058385	-0.610492	0.732331	C	-3.670037	-1.539971	0.714607
C	5.587697	-0.178966	-0.499036	C	-3.014902	-0.234985	-2.861283
C	4.829803	-0.415829	-1.662685	H	-3.049980	-1.182454	-3.444555
C	3.557047	-1.018493	-1.619249	H	-1.952600	0.084595	-2.825318
C	3.322863	-1.758426	2.168013	H	-3.582458	0.523336	-3.435096
H	5.657883	-0.488462	1.650309	C	-7.019357	0.284710	0.181481
H	5.245228	-0.136257	-2.645558	H	-7.636574	0.241812	-0.739481
C	2.813562	-1.312915	-2.898780	H	-6.980416	1.351797	0.492561
C	-6.196297	-2.056341	0.228874	H	-7.549541	-0.273377	0.979209
C	6.931008	0.512382	-0.572466	C	-3.076521	-2.488953	1.733133
H	2.088378	-3.929006	0.538841	H	-3.481033	-2.297188	2.747205
H	-0.247030	-4.461551	0.294778	H	-1.972298	-2.429873	1.776646
Cl	0.565680	1.152193	-2.079616	H	-3.334294	-3.543576	1.486206
C	-1.538469	0.816970	0.521718	C	1.914516	-2.068058	-0.088914
H	-1.902471	0.331523	1.458910	C	2.290754	-2.255216	1.267872
C	-2.628070	1.545242	-0.147507	C	3.661545	-2.299066	1.592235
C	-3.878272	1.593204	0.535599	H	3.952009	-2.432288	2.648371
C	-2.530940	2.207668	-1.402201	C	4.662777	-2.196481	0.608130
C	-4.975852	2.282155	0.000197	C	4.255632	-2.068651	-0.734347
H	-3.970698	1.075714	1.504328	H	5.021230	-2.011507	-1.526240
C	-3.634670	2.883872	-1.940200	C	2.899809	-2.016216	-1.113569
H	-1.574913	2.160211	-1.946755	C	1.255702	-2.452648	2.351172
C	-4.858141	2.929925	-1.243256	H	1.691070	-2.287348	3.356775
H	-5.928295	2.313753	0.553564	H	0.853180	-3.490376	2.341478
H	-3.541124	3.384857	-2.917412	H	0.393428	-1.770453	2.227118
H	-5.718919	3.470104	-1.669654	C	6.129843	-2.211733	0.973195
P	0.800817	2.921284	0.761861	H	6.716193	-2.849466	0.279500
C	0.459937	4.217557	-0.508218	H	6.294441	-2.582716	2.004768
C	0.103947	3.644464	2.311008	H	6.562778	-1.189208	0.912519
C	2.630320	3.035953	1.013383	C	2.523378	-1.938329	-2.571172
H	-2.691688	-1.462323	-3.301636	H	2.011097	-2.867037	-2.908229
H	-1.279878	-0.754101	-2.440945	H	3.422966	-1.811411	-3.204637
H	-1.305240	-2.492235	-2.831904	H	1.826637	-1.093221	-2.761199

H	-2.348143	-2.972865	3.331561	C	1.421856	0.897565	0.567459
H	-1.064509	-3.713360	2.329461	H	1.590514	0.359728	1.531345
H	-0.991870	-1.967895	2.699420	C	2.624537	1.627258	0.155995
H	-6.572914	-2.422894	1.204641	P	-1.173734	1.438762	1.831931
H	-6.549708	-1.009911	0.102092	C	-1.146834	0.270537	3.275093
H	-6.678238	-2.656108	-0.571843	C	-2.941200	1.973643	1.771973
H	3.439409	-1.073502	-3.780773	C	-0.344270	2.906014	2.603299
H	2.524038	-2.383248	-2.970256	C	3.801659	1.464085	0.944548
H	1.883269	-0.708394	-2.955506	C	4.983763	2.148635	0.635124
H	4.063789	-1.535482	2.960856	C	5.018659	3.020262	-0.470353
H	2.348752	-1.317324	2.471475	C	3.864859	3.200196	-1.257150
H	3.197386	-2.862953	2.137794	C	2.679416	2.516901	-0.954567
H	7.460146	0.281093	-1.519570	H	3.770269	0.779091	1.807844
H	6.812734	1.617881	-0.529525	H	5.881237	2.009182	1.259249
H	7.588920	0.222316	0.271733	H	5.945177	3.565135	-0.714207
H	-0.227849	-4.027504	-1.444941	H	3.888115	3.887949	-2.117493
H	2.170589	-3.856190	-1.251787	H	1.775946	2.662482	-1.564143
H	2.943200	4.075569	1.244045	H	-1.622421	0.746105	4.158378
H	2.915438	2.366390	1.849251	H	-1.682591	-0.666240	3.036967
H	3.145054	2.690142	0.094586	H	-0.097013	0.024769	3.530379
H	0.550955	4.634686	2.536626	H	-0.860030	3.209672	3.537752
H	-0.993120	3.752957	2.192706	H	0.711355	2.653639	2.829151
H	0.296206	2.933160	3.138776	H	-0.359612	3.731483	1.865716
H	0.906955	5.189555	-0.213710	H	-3.285094	2.299906	2.775738
H	0.871515	3.876683	-1.478601	H	-3.003201	2.814715	1.053939
H	-0.636344	4.335527	-0.622784	H	-3.578568	1.143807	1.409303

8-trans <sup>+</sup>				8-cis <sup>+</sup> c			
-2211.17519546				-2211.19670842			
Ru	0.615056	0.405455	0.249928	Ru	0.048554	0.725362	0.556874
Cl	0.637590	-0.284365	2.531321	Cl	-0.200040	0.698271	2.852620
C	0.118961	-1.508207	-0.312486	C	0.490755	-1.146915	0.130501
N	-0.985148	-2.262745	-0.462067	N	1.768803	-1.667463	0.153218
N	1.208734	-2.225810	-0.701465	C	1.764396	-3.137361	0.330908
C	-0.649460	-3.636419	-0.933256	H	2.008583	-3.387834	1.387864
C	0.845655	-3.528594	-1.307398	H	2.526430	-3.614754	-0.315755
C	-2.346543	-1.914357	-0.140475	C	0.328613	-3.507050	-0.045357
C	2.478044	-1.571227	-0.756732	H	0.241965	-3.900666	-1.082823
C	-3.157291	-1.337390	-1.151106	H	-0.125862	-4.251597	0.638058
C	-4.506470	-1.070262	-0.846942	N	-0.378209	-2.208649	0.063734
C	-5.061655	-1.369055	0.413759	C	3.037699	-0.987964	0.126742
C	-4.221023	-1.942008	1.391099	C	3.620310	-0.473217	1.316040
C	-2.865660	-2.234917	1.142086	C	4.893803	0.133926	1.225039
C	-2.597595	-0.997313	-2.513432	H	5.342827	0.546163	2.144142
H	-5.146054	-0.623601	-1.626084	C	5.621206	0.192424	0.023439
H	-4.635376	-2.182310	2.384321	C	5.046510	-0.401098	-1.123165
C	-2.005257	-2.860866	2.214076	H	5.614916	-0.406760	-2.068545
C	3.633232	-2.181296	-0.194084	C	3.777767	-1.006534	-1.095150
C	4.859681	-1.500936	-0.291269	C	2.988055	-0.623465	2.680184
C	4.985436	-0.231612	-0.901270	H	3.684851	-1.159863	3.357926
C	3.822885	0.367442	-1.411540	H	2.032379	-1.176556	2.656914
C	2.556249	-0.270867	-1.358307	H	2.779161	0.360162	3.148163
C	3.555803	-3.508122	0.523633	C	6.989955	0.828540	-0.043165
H	5.755352	-1.975759	0.142517	H	7.281419	1.281094	0.924343
H	3.897985	1.345792	-1.914329	H	7.029837	1.621775	-0.819119
C	1.372648	0.382348	-2.029450	H	7.763981	0.079317	-0.314390
C	-6.525380	-1.124207	0.699477	C	3.274354	-1.727271	-2.327277
C	6.335095	0.439515	-1.006177	H	3.630817	-1.239182	-3.256294
H	1.447293	-4.359650	-0.893266	H	2.169806	-1.796317	-2.362850
H	-0.832496	-4.365717	-0.115721	H	3.663448	-2.769423	-2.356801
C	-1.111279	1.107321	0.458582	C	-1.810503	-2.232252	-0.102452
H	-1.611887	0.759482	1.391458	C	-2.356234	-2.228966	-1.413139
C	-1.940873	2.050699	-0.288225	C	-3.757215	-2.314061	-1.553194
C	-3.239679	2.330694	0.230765	H	-4.189471	-2.302897	-2.567763
C	-1.542122	2.728826	-1.475777	C	-4.614503	-2.428285	-0.440893
C	-4.095812	3.239316	-0.405883	C	-4.030671	-2.465041	0.842815
H	-3.564769	1.816809	1.149397	H	-4.681142	-2.573948	1.726523
C	-2.396911	3.635981	-2.110748	C	-2.639159	-2.381439	1.042143
H	-0.540895	2.549903	-1.895905	C	-1.478658	-2.151984	-2.643759
C	-3.677390	3.893797	-1.578325	H	-2.040533	-1.750227	-3.510062
H	-5.093352	3.441414	0.014030	H	-1.112551	-3.158613	-2.944596
H	-2.069009	4.153489	-3.025823	H	-0.585811	-1.514716	-2.482644
H	-4.346417	4.610963	-2.079402	C	-6.112680	-2.533231	-0.607620
P	1.702604	2.418768	1.089763	H	-6.485352	-3.514668	-0.244137
C	2.155905	3.762883	-0.099014	H	-6.419500	-2.428352	-1.666671
C	0.709902	3.296605	2.370639	H	-6.639904	-1.754565	-0.017355
C	3.286316	2.035539	1.952445	C	-2.060649	-2.457071	2.434283
H	-3.408597	-0.760010	-3.228346	H	-1.244220	-3.206555	2.502502
H	-1.931987	-0.108082	-2.461872	H	-2.838197	-2.738238	3.170030
H	-1.999491	-1.827046	-2.944296	H	-1.625777	-1.485093	2.748317
H	-2.579687	-2.994429	3.150739	C	-1.650024	0.876339	-0.190840

H	-1.633700	-3.865035	1.915083	H	-2.078993	0.051179	-0.794415
H	-1.116573	-2.232715	2.440950	C	-2.541710	2.016948	-0.011178
H	-6.694712	-0.831325	1.755376	P	0.999927	1.877712	-1.260343
H	-6.947456	-0.335460	0.045470	C	1.106658	1.166796	-2.956169
H	-7.119134	-2.047841	0.522469	C	2.702203	2.466090	-0.864683
H	1.713630	1.225631	-2.664316	C	0.107487	3.468925	-1.559715
H	0.784161	-0.314978	-2.657624	C	-3.689216	2.115953	-0.852231
H	0.518367	0.985351	-1.421114	C	-4.564288	3.203984	-0.744536
H	4.439136	-3.652179	1.174912	C	-4.328162	4.203487	0.219221
H	2.648438	-3.570204	1.158617	C	-3.215003	4.109661	1.078926
H	3.535264	-4.366321	-0.183460	C	-2.328857	3.032171	0.967267
H	6.259159	1.461187	-1.427045	H	-3.881038	1.321893	-1.591852
H	6.828950	0.510862	-0.014423	H	-5.443624	3.270189	-1.403943
H	7.018088	-0.143766	-1.659881	H	-5.023823	5.052206	0.312627
H	-1.293843	-3.918032	-1.789846	H	-3.049203	4.878156	1.849868
H	1.013485	-3.495421	-2.406506	H	-1.486511	2.939360	1.672473
H	3.732133	2.954573	2.384717	H	1.569376	1.896204	-3.652480
H	3.067447	1.306193	2.757477	H	1.709314	0.240934	-2.943031
H	3.999619	1.573525	1.241345	H	0.085224	0.923653	-3.309589
H	1.293569	4.117562	2.833996	H	0.670310	4.073200	-2.300270
H	-0.207478	3.711369	1.907407	H	-0.912845	3.273386	-1.942098
H	0.418531	2.556371	3.142039	H	0.019647	4.045756	-0.617742
H	2.648161	4.605287	0.429256	H	3.057837	3.140738	-1.670950
H	2.851238	3.372970	-0.868816	H	2.678755	3.028624	0.089946
H	1.244796	4.143840	-0.602493	H	3.401292	1.615149	-0.761934

8-cis <sup>+</sup> t			
-2211.183666631			
Ru	-0.627457	0.627443	0.302147
Cl	-1.822761	2.627355	0.792636
C	-0.230566	-1.214215	-0.478068
N	-1.354205	-1.794110	-1.005603
C	-1.059052	-2.956250	-1.871632
H	-1.227466	-2.691171	-2.939281
H	-1.709165	-3.820662	-1.631127
C	0.425184	-3.218777	-1.545874
H	0.569534	-4.125096	-0.919777
H	1.057595	-3.331789	-2.449526
N	0.832966	-2.004479	-0.785811
C	-2.581949	-1.052196	-1.037876
C	-2.602152	0.238324	-1.651820
C	-3.819394	0.953506	-1.664418
H	-3.838749	1.951518	-2.129808
C	-5.004175	0.423770	-1.124514
C	-4.953572	-0.868784	-0.555816
H	-5.875840	-1.305057	-0.136937
C	-3.767924	-1.621654	-0.495089
C	-1.393450	0.820694	-2.359735
H	-1.699836	1.656012	-3.019281
H	-0.847809	0.070075	-2.963818
H	-0.608641	1.308898	-1.698803
C	-6.289879	1.215335	-1.135413
H	-6.285816	1.992991	-1.924099
H	-6.437872	1.734563	-0.163286
H	-7.171539	0.562151	-1.293138
C	-3.769242	-3.002647	0.120144
H	-4.602839	-3.118625	0.840271
H	-2.818093	-3.221780	0.646796
H	-3.905763	-3.793200	-0.650590
C	2.233821	-1.782610	-0.531009
C	2.891162	-2.517259	0.490296
C	4.275375	-2.314412	0.674148
H	4.788002	-2.873227	1.474990
C	5.023378	-1.448374	-0.144822
C	4.346602	-0.777908	-1.186279
H	4.916665	-0.119270	-1.862218
C	2.966629	-0.934658	-1.409001
C	2.186108	-3.560141	1.329399
H	2.533376	-3.535311	2.382237
H	2.413889	-4.581039	0.951130
H	1.087125	-3.441297	1.325479
C	6.512658	-1.276599	0.044941
H	7.075535	-1.801789	-0.757027
H	6.855437	-1.687273	1.014715
H	6.810127	-0.208859	-0.004427
C	2.305362	-0.230271	-2.570095
H	1.615834	-0.900363	-3.123966
H	3.062072	0.142037	-3.286691
H	1.712749	0.645417	-2.231207
C	1.155706	1.080762	0.664101

H	1.755044	0.499829	1.403601
C	1.920297	2.188237	0.098439
P	-0.930920	0.039562	2.473709
C	-0.198218	-1.538451	3.071901
C	-2.720668	-0.106659	2.887485
C	-0.301120	1.290355	3.670248
C	3.321549	2.244752	0.364536
C	4.110627	3.282941	-0.144294
C	3.519752	4.299946	-0.919105
C	2.133838	4.278755	-1.172278
C	1.340558	3.239229	-0.672523
H	3.780955	1.451689	0.975982
H	5.190370	3.309823	0.070220
H	4.138462	5.121797	-1.312740
H	1.668610	5.091312	-1.751807
H	0.250331	3.257872	-0.822970
H	-0.399406	-1.666773	4.155469
H	-0.636772	-2.390852	2.517888
H	0.895549	-1.528374	2.903761
H	-0.556011	0.993629	4.708082
H	0.798552	1.386065	3.575436
H	-0.763251	2.266648	3.426715
H	-2.844433	-0.396861	3.951244
H	-3.199625	0.874247	2.700670
H	-3.202859	-0.862188	2.236982

9-trans				9-cis			
-2897.25819551				-2897.272178			
Ru	-0.249205	0.421527	0.089037	Ru	-0.234228	0.692880	-0.504199
Cl	-0.808622	0.191127	2.446761	Cl	-1.012526	2.788251	-1.411231
P	-0.551967	2.745007	0.278543	Cl	0.244989	0.086892	-2.796725
O	-0.357183	3.619905	-1.096569	C	-0.299759	-1.321954	-0.143212
O	-2.063904	3.196170	0.816831	N	-1.466921	-2.021374	-0.326811
O	0.342429	3.696326	1.286598	C	-1.256450	-3.481436	-0.414693
N	-1.619545	-2.247598	-0.467886	H	-1.376423	-3.819719	-1.467808
N	0.548528	-2.593483	-0.347366	H	-2.000714	-4.022665	0.204483
C	-0.419365	-1.645451	-0.209047	C	0.182298	-3.637017	0.090634
C	-2.941134	-1.682998	-0.336195	H	0.233912	-4.041723	1.126812
C	-4.930842	-0.681979	-1.305940	H	0.802405	-4.289371	-0.556633
C	-3.602127	-1.790780	0.920578	N	0.691892	-2.246333	0.061937
C	2.412769	-2.694847	1.256738	C	-2.810332	-1.506385	-0.447042
C	1.571822	0.532857	0.444843	C	-3.408112	-1.326517	-1.724999
C	-5.584266	-0.696247	-0.059264	C	-4.741016	-0.866704	-1.772983
C	3.909853	1.292497	0.633382	H	-5.200059	-0.703916	-2.762525
C	0.009253	-3.936658	-0.668677	C	-5.503717	-0.636611	-0.613161
C	-3.626076	-1.190136	-1.481012	C	-4.906989	-0.912296	0.633273
C	2.586313	2.181042	-1.220034	H	-5.498395	-0.787868	1.556210
C	-3.199823	2.370609	0.516710	C	-3.576497	-1.357681	0.742253
C	-3.033461	-1.268753	-2.867068	C	-2.699652	-1.688195	-3.007016
C	2.669508	1.350149	-0.067737	H	-2.698945	-2.791613	-3.156170
C	-2.950300	-2.462916	2.103565	H	-1.646964	-1.337856	-3.020478
C	2.859440	-2.281726	-1.144482	H	-3.217657	-1.244769	-3.879923
C	4.912168	2.861355	-0.928384	C	-6.918594	-0.109905	-0.702190
C	5.013572	2.047209	0.215768	H	-7.419560	-0.436938	-1.635909
C	4.237509	-2.270135	-0.855711	H	-6.929701	1.002676	-0.701661
C	3.699953	2.918189	-1.643352	H	-7.535713	-0.442813	0.157178
C	-1.480188	-3.652322	-0.915365	C	-3.012294	-1.736361	2.091567
C	4.732113	-2.464598	0.450201	H	-3.710740	-1.449977	2.901815
C	2.359598	-2.070834	-2.553052	H	-2.037275	-1.251841	2.291862
C	1.443004	-2.888732	2.398680	H	-2.855863	-2.835826	2.165970
C	-6.973531	-0.120232	0.103314	C	2.094589	-2.069315	0.341521
C	0.276205	3.579074	2.717175	C	2.522554	-1.964347	1.691925
C	3.803720	-2.674421	1.488813	C	3.906922	-1.902853	1.953999
C	-0.532990	5.044883	-1.116193	H	4.242378	-1.816526	3.001568
C	6.219957	-2.432326	0.721669	C	4.866352	-1.969243	0.925636
C	-4.907852	-1.274727	1.033601	C	4.406748	-2.121181	-0.397508
C	1.955165	-2.486664	-0.069853	H	5.139489	-2.200436	-1.218038
H	-5.459495	-0.283405	-2.188287	C	3.036674	-2.191594	-0.716944
H	4.947052	-2.101414	-1.683163	C	1.533056	-1.948882	2.832837
H	4.169929	-2.831135	2.517569	H	2.054517	-1.821451	3.802124
H	-5.418311	-1.346856	2.008800	H	0.964041	-2.902733	2.891258
H	0.184322	-4.631965	0.182573	H	0.786649	-1.134722	2.727508
H	0.524336	-4.358689	-1.555956	C	6.346638	-1.884393	1.223626
H	-1.758647	-3.740099	-1.988225	H	6.909440	-2.701223	0.724744
H	-2.155733	-4.314534	-0.334934	H	6.551397	-1.941827	2.311325
H	1.639369	2.223578	-1.777855	H	6.774919	-0.928590	0.850511
H	5.779842	3.452593	-1.263526	C	2.598643	-2.432268	-2.139539
H	5.958595	2.000510	0.780443	H	2.161636	-3.449157	-2.258839
H	3.622274	3.550566	-2.542338	H	3.458497	-2.362260	-2.833975
H	1.900513	-0.136557	1.271547	H	1.823719	-1.702254	-2.458369

H	-3.587223	-0.615016	-3.569424	C	1.500915	0.936762	0.161301
H	-3.103961	-2.305651	-3.266188	H	1.758819	0.659806	1.208830
H	-1.967989	-0.960455	-2.880576	C	2.634958	1.559232	-0.524695
H	-3.689037	-2.642744	2.909113	P	-1.029675	1.438976	1.471539
H	-2.136027	-1.824159	2.510221	O	-0.584813	0.563086	2.810927
H	-2.499671	-3.439602	1.828099	C	-0.998933	0.957682	4.131715
H	1.637771	-1.226184	-2.602640	O	-2.649957	1.489837	1.764029
H	1.828187	-2.968483	-2.939042	C	-3.512042	2.448061	1.123604
H	3.199471	-1.860867	-3.243666	O	-0.689901	2.989115	1.957491
H	0.803173	-1.989116	2.546460	C	0.492122	3.713336	1.590225
H	1.981747	-3.088367	3.345584	C	3.898858	1.535622	0.136463
H	0.752036	-3.740311	2.220314	C	5.028171	2.131801	-0.438090
H	-7.519791	-0.088763	-0.860902	C	4.920823	2.781382	-1.683007
H	-6.932389	0.921472	0.491541	C	3.678038	2.831312	-2.342694
H	-7.577733	-0.707983	0.824613	C	2.545245	2.229707	-1.778027
H	6.632422	-1.413082	0.558270	H	3.978217	1.027444	1.111319
H	6.772465	-3.113443	0.040467	H	5.996015	2.098760	0.087542
H	6.454188	-2.727625	1.763804	H	5.805945	3.258329	-2.134422
H	3.988279	0.642888	1.520298	H	3.589086	3.351105	-3.309903
Cl	-0.195425	0.588017	-2.308878	H	1.571808	2.279846	-2.286555
H	-0.651342	5.335203	-2.178625	H	0.363185	4.739516	1.987321
H	-1.438956	5.346079	-0.549391	H	1.402885	3.266885	2.044263
H	0.353135	5.556416	-0.687415	H	0.600216	3.760144	0.487278
H	1.130188	4.157287	3.121504	H	-0.348875	0.414911	4.845892
H	-0.674673	4.009061	3.096906	H	-0.878022	2.050692	4.275391
H	0.347171	2.520083	3.043260	H	-2.058649	0.680437	4.307734
H	-4.070995	2.833659	1.020079	H	-4.545951	2.074649	1.254812
H	-3.398095	2.323825	-0.575689	H	-3.404041	3.441103	1.607530
H	-3.066495	1.341630	0.916490	H	-3.279116	2.542051	0.042703

9-cis <sup>+</sup> c				9-cis <sup>+</sup> t			
-2436.859991626				-2436.85135843			
C	-1.449281	2.868075	0.161719	Ru	-0.208819	0.471150	-0.625621
Ru	-0.437476	0.745778	0.096084	Cl	-0.374523	0.244144	-2.913145
P	-1.033066	0.215970	2.149661	C	-0.401514	-1.332696	0.173094
O	-2.654510	0.127506	2.370935	N	0.518019	-2.259297	0.569492
O	-0.568858	1.213688	3.362926	N	-1.648984	-1.881482	0.300663
O	-0.586238	-1.267016	2.662208	C	-0.124856	-3.497185	1.080270
N	-1.308744	-1.761080	-1.075959	C	-1.606906	-3.299461	0.717631
N	0.852847	-2.028061	-0.698916	C	1.955933	-2.219575	0.500950
C	0.421253	-3.337182	-1.259677	C	-2.877498	-1.303365	-0.192490
C	-0.193852	-1.172669	-0.555143	C	2.706775	-1.952867	1.674969
C	4.298828	-2.186873	0.770105	C	4.114239	-1.964566	1.579557
C	-6.334854	0.858920	-2.214486	C	4.782943	-2.252442	0.372704
C	-1.348214	0.479884	-2.985944	C	3.999848	-2.535871	-0.766648
C	-3.822278	0.627763	-2.504041	C	2.592393	-2.539300	-0.729792
C	-3.709074	-2.690633	0.283007	C	2.036525	-1.670570	3.000517
C	-4.947985	-0.902289	-1.010800	H	4.706073	-1.750134	2.485196
C	-5.019881	0.181599	-1.909532	H	4.501088	-2.775087	-1.719206
C	2.284419	1.901621	-0.139585	C	1.795688	-2.865759	-1.970752
C	-0.938240	-1.739315	3.932259	C	-3.233505	-1.473229	-1.561672
C	2.901651	-2.336566	0.657501	C	-4.445181	-0.907784	-2.004893
C	4.404197	-1.073293	-1.370996	C	-5.327056	-0.236579	-1.135660
C	3.652712	1.900117	0.263607	C	-4.986832	-0.174427	0.231033
C	5.072199	-1.565967	-0.230729	C	-3.786261	-0.712361	0.729356
C	2.134936	-3.094172	1.714792	C	-2.432450	-2.325869	-2.518564
C	-3.456920	1.216526	2.731727	H	-4.717263	-1.019402	-3.067606
C	2.347526	-0.658871	-2.780216	H	-5.690152	0.293920	0.939754
C	-2.544678	-1.061054	-1.306704	C	-3.538488	-0.740565	2.219461
C	3.010465	-1.183599	-1.529145	C	6.292060	-2.303664	0.305736
C	0.216134	2.372587	3.335693	C	-6.601393	0.388180	-1.652983
C	2.260143	-1.800916	-0.490429	H	-1.937136	-3.950257	-0.121147
C	-1.021012	-3.061984	-1.721672	H	0.329263	-4.387456	0.600138
C	6.575773	-1.474707	-0.111128	C	1.629449	0.767439	-0.422418
C	2.816043	3.674708	-1.753319	H	2.265703	0.035414	0.115695
C	1.360073	1.002546	0.545810	C	2.362596	1.876366	-1.011929
C	1.884471	2.817109	-1.157391	C	3.782535	1.902389	-0.865072
C	-2.581518	0.017147	-2.240103	C	1.736100	2.928814	-1.743248
C	-3.732559	-1.532936	-0.686280	C	4.539752	2.939947	-1.420768
C	4.579892	2.761738	-0.334915	H	4.276456	1.086761	-0.312321
C	4.165321	3.648322	-1.347159	C	2.496867	3.966394	-2.289892
H	4.800765	-2.591451	1.664985	H	0.644023	2.917769	-1.889286
H	4.989099	-0.593832	-2.173053	C	3.898240	3.974008	-2.130630
H	-5.873973	-1.269655	-0.538227	H	5.634848	2.945898	-1.307120
H	-3.856385	1.462755	-3.222778	H	2.002828	4.772201	-2.854234
H	3.975797	1.205747	1.055399	H	4.494317	4.789709	-2.569453
H	2.488616	4.384589	-2.528743	P	-0.673964	1.575751	1.328461
H	0.822049	2.884474	-1.439703	O	-0.515767	0.766365	2.759186
H	5.631432	2.750154	-0.008336	O	0.088907	3.012776	1.615600
H	4.892888	4.331830	-1.812585	O	-2.205580	2.120370	1.218314
H	-6.471952	1.758788	-1.575496	H	0.039135	-3.581446	2.175973
H	-7.196221	0.187876	-2.027352	H	-2.290694	-3.474073	1.572824
H	-6.382732	1.201648	-3.267696	H	2.457902	-3.223279	-2.782304
H	-0.661294	1.100443	-2.355758	H	1.041751	-3.658404	-1.779380

H	-1.625410	1.128794	-3.838958	H	1.244168	-1.979567	-2.351122
H	-0.745249	-0.365574	-3.372412	H	2.720125	-1.123490	3.679493
H	-2.767303	-2.712522	0.865401	H	1.109343	-1.075467	2.880191
H	-3.806269	-3.666775	-0.242374	H	1.764630	-2.615286	3.521775
H	-4.555537	-2.626732	0.994151	H	-4.042414	0.108240	2.722443
H	1.128449	-2.665970	1.884279	H	-3.963577	-1.668240	2.663934
H	2.685493	-3.092382	2.676214	H	-2.461653	-0.715805	2.470361
H	2.009849	-4.161720	1.426001	H	-2.401035	-1.870545	-3.527238
H	1.749701	0.253437	-2.569254	H	-1.387073	-2.480445	-2.196551
H	1.658733	-1.402509	-3.232730	H	-2.913403	-3.323597	-2.624147
H	3.101336	-0.389251	-3.544304	H	-7.369303	0.475299	-0.858745
H	6.973734	-0.568454	-0.610245	H	-6.408135	1.413100	-2.039422
H	7.061124	-2.349948	-0.596396	H	-7.032133	-0.195821	-2.490994
H	6.905657	-1.466207	0.946868	H	6.675237	-1.888701	-0.648637
H	1.815964	0.501315	1.427769	H	6.762135	-1.749140	1.141919
H	0.471782	-4.117542	-0.470413	H	6.650701	-3.354523	0.365331
H	1.096167	-3.642811	-2.084079	C	1.417684	3.125967	2.157956
H	-1.115772	-2.965058	-2.826416	C	-0.934784	1.325172	4.025838
H	-1.735075	-3.839881	-1.387101	C	-2.758062	3.351425	1.738339
H	-4.493310	0.892363	2.813795	H	-3.661610	3.562928	1.136869
H	-3.123173	1.611591	3.690090	H	-3.048238	3.225986	2.801764
H	-3.378438	1.992728	1.971942	H	-2.035870	4.184285	1.640715
H	0.311286	2.770371	4.344967	H	1.586808	4.203381	2.344463
H	1.204096	2.132728	2.945411	H	1.514470	2.568594	3.112792
H	-0.256369	3.116117	2.695518	H	2.175381	2.760707	1.436768
H	-0.541316	-2.744176	4.068729	H	-0.320019	0.845434	4.811259
H	-0.524018	-1.079019	4.692752	H	-0.781179	2.423070	4.060378
H	-2.023196	-1.762130	4.023214	H	-2.003891	1.091719	4.206899

9-trans <sup>+</sup>			
-2436.83974887			
Cl	-0.519175	-0.495826	2.423250
Ru	-0.499216	0.042923	0.107543
P	-1.920999	1.883598	0.552271
O	-2.391860	2.655298	-0.826146
O	-1.410246	3.201655	1.404202
O	-3.277625	1.392233	1.327096
N	-0.534511	-2.710820	-0.627950
N	1.619708	-2.322897	-0.357508
C	1.557512	-3.763218	-0.738794
C	0.390931	-1.781989	-0.272145
C	4.665868	-1.262166	1.539599
C	-6.029567	-0.958273	-1.056914
C	-1.134598	-0.294339	-2.175191
C	-3.546226	-0.654967	-1.509779
C	-2.643786	-4.304629	0.667644
C	-4.258957	-2.598443	-0.269375
C	-4.590228	-1.403186	-0.949039
C	1.709656	2.127552	-0.424083
C	-4.210196	2.230640	2.036612
C	3.395772	-1.815324	1.284397
C	4.891802	-0.563987	-0.765876
C	3.026919	2.524614	-0.044521
C	5.435291	-0.641544	0.532473
C	2.608407	-2.481784	2.387152
C	-3.093506	3.917056	-0.865390
C	3.064345	-0.968213	-2.476335
C	-1.900159	-2.299965	-0.739834
C	3.622884	-1.091485	-1.076952
C	-0.685039	3.094622	2.645940
C	2.884106	-1.710275	-0.037042
C	0.076287	-3.962208	-1.133548
C	6.818050	-0.111296	0.834547
C	1.717504	3.909039	-2.112410
C	1.107397	1.014290	0.295972
C	1.066431	2.850928	-1.470926
C	-2.192782	-1.078023	-1.434328
C	-2.938413	-3.058781	-0.134266
C	3.676694	3.583404	-0.691643
C	3.024625	4.275767	-1.728560
H	5.072735	-1.332507	2.562106
H	5.475747	-0.082630	-1.567617
H	-5.065584	-3.186565	0.199134
H	-3.771715	0.279452	-2.047366
H	3.532931	1.976316	0.766152
H	1.206141	4.464491	-2.914067
H	0.031859	2.598941	-1.749157
H	4.693817	3.874532	-0.386850
H	3.531616	5.111270	-2.236763
H	-6.471425	-0.791441	-0.051719
H	-6.651720	-1.731398	-1.555003
H	-6.128610	-0.018812	-1.634771
H	-0.419503	0.501806	-1.618369
H	-1.608755	0.420184	-2.876872
H	-0.419623	-0.932807	-2.729193

H	-1.743053	-4.172401	1.301153
H	-2.476942	-5.191862	0.018091
H	-3.493646	-4.550837	1.332747
H	1.621558	-1.990756	2.537282
H	3.162158	-2.443669	3.344797
H	2.410647	-3.552908	2.165720
H	2.251964	-0.209973	-2.516425
H	2.635885	-1.922436	-2.847094
H	3.847538	-0.650519	-3.191146
H	7.148532	0.633170	0.083407
H	7.564506	-0.935575	0.829941
H	6.867003	0.358414	1.838018
H	1.742303	0.661093	1.140098
H	1.856865	-4.390889	0.127619
H	2.262543	-3.972401	-1.568043
H	-0.070492	-4.038786	-2.233493
H	-0.371438	-4.858871	-0.664611
H	-0.421003	4.127887	2.940240
H	-1.304111	2.624232	3.437054
H	0.240482	2.496845	2.514664
H	-3.099518	4.242272	-1.923034
H	-4.141800	3.798056	-0.520845
H	-2.578374	4.676628	-0.244806
H	-4.468368	1.715630	2.982544
H	-3.773689	3.223891	2.265976
H	-5.131664	2.359015	1.431949

10-trans				10-cis			
-2851.53978176				-2851.55147530			
Ru	-0.288414	0.597107	-0.211052	Ru	-0.340754	0.897357	-0.083933
Cl	-0.599492	0.161974	-2.556137	Cl	-1.102986	3.164321	-0.199768
C	-0.483751	-1.477113	0.115787	Cl	0.100583	1.059118	-2.433773
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N	-1.720776	-2.029310	0.265765	N	-1.609580	-1.726720	-0.714907
C	-0.186481	-3.803710	0.453275	C	-1.483048	-3.164631	-1.031817
C	-1.688764	-3.508962	0.323928	H	-1.945263	-3.388787	-2.015363
C	1.861598	-2.396151	0.094283	H	-2.011774	-3.771414	-0.264258
C	-2.987615	-1.335113	0.272126	C	0.040038	-3.379220	-1.018942
C	2.611554	-2.129083	1.270218	H	0.360742	-4.211687	-0.358530
C	4.015288	-2.101653	1.163038	H	0.452224	-3.574190	-2.032244
C	4.681004	-2.339249	-0.057729	N	0.557330	-2.086158	-0.507029
C	3.900830	-2.607772	-1.199534	C	-2.923526	-1.142761	-0.573362
C	2.491545	-2.646012	-1.151386	C	-3.559226	-0.547650	-1.699557
C	1.931538	-1.855414	2.590782	C	-4.842567	0.003689	-1.516571
H	4.607454	-1.886431	2.068421	H	-5.331569	0.486041	-2.379277
H	4.401642	-2.794563	-2.164393	C	-5.520752	-0.052501	-0.283022
C	1.681084	-2.897873	-2.401550	C	-4.898581	-0.730890	0.781125
C	-3.712209	-1.165966	-0.939028	H	-5.426536	-0.823761	1.745005
C	-4.935185	-0.465293	-0.885187	C	-3.615066	-1.296787	0.658890
C	-5.474822	0.015521	0.321766	C	-2.920078	-0.534088	-3.065482
C	-4.782650	-0.272460	1.515610	H	-2.612987	-1.553929	-3.382577
C	-3.554775	-0.960094	1.523691	H	-2.003480	0.094312	-3.085162
C	-3.281806	-1.801834	-2.239926	H	-3.627694	-0.144535	-3.822834
H	-5.488688	-0.305526	-1.825699	C	-6.870739	0.604148	-0.107596
H	-5.216386	0.038851	2.480630	H	-7.468222	0.570112	-1.041297
C	-2.902069	-1.332152	2.833157	H	-6.751453	1.676300	0.163470
C	6.191641	-2.307770	-0.126810	H	-7.459417	0.125217	0.700663
C	-6.758180	0.814064	0.340743	C	-3.049419	-2.099646	1.809568
H	-2.131066	-3.931881	-0.604647	H	-3.348279	-1.666141	2.783963
H	0.175716	-4.563622	-0.268647	H	-1.945519	-2.157706	1.791464
Cl	-0.518114	0.982218	2.145091	H	-3.441993	-3.140845	1.787210
C	1.569844	0.732934	-0.295834	C	1.963203	-2.007478	-0.201466
H	2.045532	-0.134516	-0.800758	C	2.387895	-2.324909	1.116647
C	2.527692	1.757875	0.094076	C	3.771045	-2.346636	1.389332
C	3.817647	1.726634	-0.513432	H	4.104047	-2.589433	2.412477
C	2.261325	2.762866	1.066160	C	4.732254	-2.088892	0.393145
C	4.783717	2.689233	-0.197189	C	4.274889	-1.814335	-0.911101
H	4.040019	0.938264	-1.250512	H	5.009278	-1.625086	-1.711904
C	3.243216	3.705393	1.397897	C	2.906137	-1.780967	-1.241010
H	1.289205	2.761151	1.581827	C	1.395558	-2.652345	2.208111
C	4.498949	3.681968	0.760712	H	1.915924	-2.992059	3.124795
H	5.767115	2.665566	-0.693260	H	0.695755	-3.459412	1.902240
H	3.027463	4.469452	2.161479	H	0.767637	-1.780052	2.480571
H	5.261103	4.435635	1.016111	C	6.212564	-2.112052	0.701072
P	-0.647674	2.787993	-0.622285	H	6.755348	-2.806779	0.025610
F	-0.690290	3.921403	0.529332	H	6.411489	-2.426319	1.744838
F	0.202769	3.628881	-1.707019	H	6.666598	-1.108059	0.556533
F	-2.117658	3.083151	-1.223958	C	2.475896	-1.538295	-2.666260
H	2.678299	-1.701860	3.393885	H	2.112651	-2.475606	-3.144250
H	1.285325	-0.951510	2.540750	H	3.325427	-1.173394	-3.275792
H	1.276115	-2.697598	2.900862	H	1.657218	-0.790104	-2.723575

H	2.342185	-3.063610	-3.274428	C	1.422422	0.928752	0.592178
H	1.030065	-3.793489	-2.302949	H	1.697171	0.352765	1.503477
H	1.010940	-2.038616	-2.628244	C	2.535108	1.742949	0.121865
H	6.559436	-2.476135	-1.158356	P	-1.051550	0.972958	1.983121
H	6.590275	-1.331851	0.223096	F	-0.798403	-0.250961	3.035075
H	6.640676	-3.088345	0.524297	F	-2.608657	1.194271	2.329130
H	-3.511273	-0.978308	3.687612	F	-0.461176	2.119460	2.949653
H	-2.794128	-2.434317	2.934747	C	3.807525	1.527807	0.733975
H	-1.892592	-0.880209	2.919968	C	4.924613	2.283546	0.362045
H	-3.647228	-1.216734	-3.106512	C	4.796167	3.286751	-0.618711
H	-2.183058	-1.872578	-2.334871	C	3.545245	3.529732	-1.217279
H	-3.719599	-2.822314	-2.326653	C	2.423443	2.772281	-0.857448
H	-7.342122	0.630889	1.265783	H	3.901129	0.748189	1.507281
H	-6.542439	1.904658	0.302862	H	5.898547	2.100709	0.843311
H	-7.402147	0.578148	-0.530402	H	5.672191	3.890245	-0.906697
H	0.101633	-4.142028	1.473232	H	3.440877	4.327838	-1.969104
H	-2.283166	-3.879357	1.183767	H	1.441594	2.976246	-1.307206

10-trans <sup>+</sup>				10-cis <sup>+</sup> c			
-2391.11595389				-2391.13422931			
Ru	0.615056	0.405455	0.249928	Ru	-0.632186	0.600109	0.458356
Cl	0.637590	-0.284365	2.531321	Cl	-1.822112	2.426445	1.312802
C	0.118961	-1.508207	-0.312486	C	-0.250661	-1.040086	-0.727034
N	-0.985148	-2.262745	-0.462067	N	-1.376191	-1.503026	-1.327291
N	1.208734	-2.225810	-0.701465	C	-1.095277	-2.552086	-2.334461
C	-0.649460	-3.636419	-0.933256	H	-1.251285	-2.146876	-3.358406
C	0.845655	-3.528594	-1.307398	H	-1.763287	-3.425389	-2.205789
C	-2.346543	-1.914357	-0.140475	C	0.384262	-2.880898	-2.034878
C	2.478044	-1.571227	-0.756732	H	0.508466	-3.850942	-1.507936
C	-3.157291	-1.337390	-1.151106	H	1.020965	-2.902435	-2.941559
C	-4.506470	-1.070262	-0.846942	N	0.807801	-1.770582	-1.133615
C	-5.061655	-1.369055	0.413759	C	-2.616919	-0.801068	-1.150758
C	-4.221023	-1.942008	1.391099	C	-2.683024	0.579746	-1.513065
C	-2.865660	-2.234917	1.142086	C	-3.900116	1.266006	-1.320479
C	-2.597595	-0.997313	-2.513432	H	-3.954252	2.332044	-1.591546
H	-5.146054	-0.623601	-1.626084	C	-5.041835	0.626167	-0.806756
H	-4.635376	-2.182310	2.384321	C	-4.944059	-0.745762	-0.480350
C	-2.005257	-2.860866	2.214076	H	-5.830421	-1.262710	-0.076830
C	3.633232	-2.181296	-0.194084	C	-3.756614	-1.481240	-0.635094
C	4.859681	-1.500936	-0.291269	C	-1.510247	1.300918	-2.146103
C	4.985436	-0.231612	-0.901270	H	-1.837318	2.259310	-2.593968
C	3.822885	0.367442	-1.411540	H	-0.995335	0.695644	-2.917970
C	2.556249	-0.270867	-1.358307	H	-0.687346	1.629382	-1.435909
C	3.555803	-3.508122	0.523633	C	-6.328175	1.382262	-0.582739
H	5.755352	-1.975759	0.142517	H	-6.377716	2.302092	-1.197544
H	3.897985	1.345792	-1.914328	H	-6.414547	1.691397	0.481906
C	1.372648	0.382348	-2.029450	H	-7.214650	0.757812	-0.812916
C	-6.525380	-1.124207	0.699478	C	-3.708324	-2.945517	-0.266774
C	6.335095	0.439515	-1.006177	H	-4.516274	-3.199395	0.446203
H	1.447293	-4.359650	-0.893266	H	-2.741670	-3.221823	0.198965
H	-0.832496	-4.365717	-0.115721	H	-3.852774	-3.595727	-1.157867
C	-1.111279	1.107321	0.458582	C	2.192487	-1.628970	-0.760203
H	-1.611887	0.759482	1.391458	C	2.721603	-2.415389	0.296463
C	-1.940873	2.050699	-0.288225	C	4.093824	-2.284138	0.591118
C	-3.239679	2.330694	0.230765	H	4.513104	-2.879021	1.419616
C	-1.542122	2.728826	-1.475777	C	4.945493	-1.438606	-0.147893
C	-4.095812	3.239316	-0.405883	C	4.385052	-0.695764	-1.209096
H	-3.564769	1.816809	1.149397	H	5.035272	-0.036563	-1.807494
C	-2.396911	3.635981	-2.110748	C	3.018628	-0.773742	-1.537744
H	-0.540895	2.549903	-1.895905	C	1.884570	-3.412834	1.064998
C	-3.677390	3.893797	-1.578325	H	2.203607	-3.468775	2.124267
H	-5.093352	3.441414	0.014030	H	2.007551	-4.434696	0.642979
H	-2.069009	4.153489	-3.025823	H	0.804290	-3.176239	1.047651
H	-4.346417	4.610963	-2.079402	C	6.422740	-1.365838	0.160663
P	1.702604	2.418768	1.089763	H	6.969687	-2.187788	-0.351209
F	2.069994	3.508142	0.126286	H	6.621244	-1.473638	1.245909
F	0.894659	3.133226	2.132248	H	6.870838	-0.413024	-0.184339
F	2.991083	2.106980	1.791625	C	2.457711	0.037798	-2.682601
H	-3.408597	-0.760010	-3.228346	H	1.858979	-0.581784	-3.382901
H	-1.931987	-0.108082	-2.461872	H	3.269178	0.511774	-3.267015
H	-1.999491	-1.827046	-2.944296	H	1.794185	0.850496	-2.316321
H	-2.579687	-2.994429	3.150739	C	1.174341	1.079199	0.769238

H	-1.633700	-3.865035	1.915083	H	1.830474	0.450681	1.404599
H	-1.116573	-2.232715	2.440950	C	1.838413	2.269476	0.270382
H	-6.694712	-0.831325	1.755376	P	-0.677956	-0.588383	2.232656
H	-6.947456	-0.335460	0.045470	F	-1.271191	-2.084103	2.139380
H	-7.119134	-2.047841	0.522470	F	-1.510437	-0.098159	3.498279
H	1.713630	1.225631	-2.664316	F	0.700602	-0.937647	2.978736
H	0.784161	-0.314978	-2.657624	C	3.261162	2.328904	0.405600
H	0.518367	0.985351	-1.421114	C	3.977790	3.443515	-0.041059
H	4.439136	-3.652179	1.174912	C	3.295272	4.535739	-0.612330
H	2.648438	-3.570204	1.158617	C	1.890713	4.512013	-0.727045
H	3.535264	-4.366321	-0.183460	C	1.166491	3.395985	-0.294913
H	6.259159	1.461187	-1.427044	H	3.790056	1.479681	0.865697
H	6.828950	0.510862	-0.014422	H	5.072839	3.473311	0.068935
H	7.018088	-0.143766	-1.659880	H	3.858933	5.419052	-0.951724
H	-1.293843	-3.918032	-1.789846	H	1.358295	5.382541	-1.140320
H	1.013485	-3.495421	-2.406506	H	0.066514	3.412669	-0.326023

10-cis <sup>+</sup> t			
-2391.12777209			
Ru	-0.286357	0.687668	-0.403682
Cl	-0.279155	0.933199	-2.679364
C	-0.461727	-1.260228	-0.009676
N	0.457966	-2.252340	0.095930
N	-1.710451	-1.796613	0.044432
C	-0.192261	-3.576893	0.299699
C	-1.689922	-3.275104	0.091035
C	1.897895	-2.180663	0.058811
C	-2.927592	-1.040642	-0.128982
C	2.626977	-2.170721	1.276708
C	4.035576	-2.132352	1.202931
C	4.723993	-2.131580	-0.026829
C	3.961127	-2.172130	-1.213366
C	2.553695	-2.208790	-1.202316
C	1.945865	-2.220556	2.626150
H	4.611810	-2.114321	2.142993
H	4.479743	-2.188342	-2.186267
C	1.780216	-2.271817	-2.498326
C	-3.394383	-0.747893	-1.443290
C	-4.574778	0.013606	-1.567127
C	-5.323940	0.429752	-0.450076
C	-4.884463	0.028932	0.830315
C	-3.707209	-0.714471	1.019743
C	-2.760638	-1.325058	-2.688192
H	-4.934278	0.262580	-2.579235
H	-5.483873	0.301628	1.714626
C	-3.342724	-1.203040	2.404113
C	6.234007	-2.134367	-0.079245
C	-6.566462	1.272172	-0.610053
H	-2.086702	-3.687883	-0.861685
H	0.212355	-4.311646	-0.424920
C	1.541021	0.989355	-0.001906
H	2.163243	0.145382	0.361881
C	2.244742	2.235760	-0.167785
C	3.619119	2.293191	0.223496
C	1.637041	3.410120	-0.711221
C	4.347292	3.478634	0.088356
H	4.095500	1.389027	0.635065
C	2.370907	4.589687	-0.843739
H	0.587220	3.379158	-1.045936
C	3.724273	4.625793	-0.442867
H	5.404273	3.515972	0.393313
H	1.898362	5.489224	-1.266654
H	4.299652	5.558810	-0.551620
P	-0.739408	1.300000	1.683640
F	-0.461184	0.384930	2.980123
F	0.033573	2.613301	2.186572
F	-2.229003	1.775612	2.036565
H	0.032857	-3.947572	1.322050
H	-2.328852	-3.646911	0.917196

H	2.455913	-2.478447	-3.350151
H	1.007609	-3.068951	-2.481838
H	1.254762	-1.316713	-2.710269
H	2.577428	-1.753228	3.407065
H	0.964890	-1.707661	2.630125
H	1.774060	-3.271509	2.948202
H	-3.633568	-0.469035	3.180673
H	-3.889097	-2.143904	2.635918
H	-2.263088	-1.416260	2.518270
H	-2.711623	-0.573322	-3.499757
H	-1.734831	-1.702820	-2.525602
H	-3.381372	-2.168684	-3.062156
H	-7.368839	0.951794	0.085151
H	-6.348293	2.338165	-0.380448
H	-6.962689	1.230903	-1.643426
H	6.616840	-1.487558	-0.894647
H	6.681890	-1.796145	0.875848
H	6.616191	-3.159608	-0.277174

11-trans				11-cis			
-2694.46916665				-2694.47345179			
Ru	0.002247	0.857194	-0.227170	Ru	-0.066101	-1.137536	-0.326019
Cl	-0.453046	0.563761	-2.569000	Cl	0.832474	-1.988093	1.720100
C	-0.572043	-1.042338	0.131002	C	-0.266258	0.582893	0.714840
N	0.128758	-2.221027	0.217210	N	0.654789	1.491333	1.181968
N	-1.899447	-1.358313	0.353815	N	-1.440892	0.822183	1.400838
C	-0.757888	-3.399686	0.345483	C	0.094565	2.391878	2.217382
C	-2.074895	-2.762426	0.783507	C	-1.261766	1.750199	2.533207
C	1.545906	-2.453458	0.120397	C	1.977582	1.795732	0.691912
C	-3.035782	-0.461748	0.301324	C	-2.755164	0.321590	1.080582
C	2.355742	-2.298676	1.284434	C	2.123079	2.607616	-0.476754
C	3.723137	-2.629117	1.184628	C	3.422453	2.994279	-0.863466
C	4.273172	-3.109123	-0.012084	C	4.548243	2.611572	-0.121015
C	3.461014	-3.257157	-1.144262	C	4.387958	1.829694	1.027696
C	2.088845	-2.930960	-1.107820	C	3.112843	1.409814	1.463460
C	1.776078	-1.835266	2.621633	C	0.924949	3.113122	-1.286471
H	4.369936	-2.510224	2.067230	H	3.555406	3.618004	-1.761073
H	3.901359	-3.628607	-2.083461	H	5.275141	1.532830	1.608679
C	1.246526	-3.092660	-2.375765	C	3.006095	0.603360	2.758215
C	-3.716824	-0.277656	-0.944370	C	-3.256103	-0.860874	1.702279
C	-4.796795	0.629055	-0.981878	C	-4.557685	-1.288464	1.356669
C	-5.232380	1.295444	0.169794	C	-5.358812	-0.556936	0.470772
C	-4.618931	1.029549	1.399651	C	-4.875628	0.638469	-0.079909
C	-3.529272	0.138966	1.502452	C	-3.578933	1.105554	0.214422
C	-3.409264	-1.113955	-2.189800	C	-2.482721	-1.619294	2.779538
H	-5.316114	0.803503	-1.936043	H	-4.953401	-2.210080	1.810942
H	-5.000644	1.516638	2.309887	H	-5.521818	1.226333	-0.751418
C	-3.017460	-0.238542	2.895469	C	-3.134411	2.461475	-0.339575
H	5.343169	-3.367767	-0.062304	H	5.554195	2.928213	-0.439991
H	-6.074424	2.004193	0.113481	H	-6.373152	-0.909527	0.223485
H	-2.963066	-3.217136	0.303523	H	-1.248523	1.185108	3.492002
H	-0.845831	-3.923945	-0.633104	H	0.762762	2.434658	3.099787
Cl	-0.057373	1.385005	2.103566	C	1.517357	-0.670113	-1.163835
C	1.812477	0.556933	-0.445872	H	1.568939	0.286808	-1.739009
H	2.097903	-0.308027	-1.082689	C	2.766640	-1.422672	-1.268951
C	2.975432	1.351716	-0.044373	C	3.860828	-0.806381	-1.945321
C	4.238853	1.004213	-0.607895	C	2.945621	-2.742055	-0.763520
C	2.930827	2.438349	0.874641	C	5.084033	-1.469684	-2.099872
C	5.399046	1.720185	-0.285283	H	3.735113	0.215843	-2.338743
H	4.290929	0.153296	-1.306611	C	4.171278	-3.401816	-0.926864
C	4.096998	3.141179	1.205322	H	2.102577	-3.233618	-0.258092
H	1.968581	2.690395	1.343790	C	5.242779	-2.772504	-1.588929
C	5.332002	2.792537	0.624468	H	5.918402	-0.973128	-2.620787
H	6.363110	1.438334	-0.738293	H	4.291695	-4.424690	-0.535765
H	4.045078	3.972412	1.926876	H	6.202565	-3.300035	-1.712593
H	6.244032	3.353562	0.885125	N	-1.234103	-0.690423	-2.032587
N	0.140255	2.991247	-0.667257	H	-0.000979	3.426250	1.817783
H	-0.351487	-4.118686	1.083905	H	-2.091609	2.484082	2.580163
H	-2.213171	-2.815027	1.886167	C	3.921670	-0.637402	2.750427
C	1.817417	-2.286485	-3.561099	C	3.309532	1.489363	3.989142
C	1.081434	-4.581932	-2.754185	H	1.966224	0.223007	2.830580
H	0.242647	-2.669483	-2.164994	H	3.158978	0.915054	4.927649
H	0.411779	-4.690876	-3.633353	H	4.362215	1.845888	3.980617

H	2.058252	-5.039947	-3.019882	H	2.662758	2.391265	4.035529
H	0.654869	-5.180305	-1.922068	H	3.748800	-1.239316	3.666645
H	1.159940	-2.395308	-4.448781	H	3.704483	-1.285410	1.879434
H	1.867033	-1.205380	-3.322666	H	4.997824	-0.361002	2.732628
H	2.831113	-2.637193	-3.850358	C	1.164925	3.085455	-2.810401
C	2.705282	-0.875010	3.387586	H	0.070662	2.436418	-1.072623
H	0.849059	-1.266277	2.404929	C	0.525440	4.544493	-0.856444
C	1.405727	-3.048596	3.506210	H	0.218579	3.288111	-3.353365
H	2.177272	-0.471628	4.275849	H	1.893741	3.860145	-3.129648
H	3.625768	-1.379535	3.752723	H	1.553989	2.104381	-3.152160
H	3.004385	-0.014036	2.757557	H	-0.371443	4.889365	-1.413384
H	0.939003	-2.712272	4.456204	H	0.299383	4.610541	0.226857
H	0.691289	-3.732800	3.003115	H	1.350001	5.259226	-1.064247
H	2.307528	-3.645113	3.763500	C	-2.455247	-3.142993	2.549281
C	-3.587455	-0.349292	-3.515080	H	-1.427458	-1.278169	2.743228
H	-2.345414	-1.420385	-2.130639	C	-3.054880	-1.280988	4.176528
C	-4.295151	-2.384368	-2.204433	H	-2.449155	-1.769034	4.968950
H	-4.041654	-3.025975	-3.075007	H	-3.059652	-0.188256	4.374684
H	-4.180761	-2.997264	-1.286987	H	-4.101648	-1.639644	4.283713
H	-5.370130	-2.114583	-2.284189	H	-1.816456	-3.625053	3.317255
H	-3.219387	-0.969755	-4.358550	H	-3.466529	-3.597829	2.626949
H	-4.654563	-0.120176	-3.725040	H	-2.023733	-3.396257	1.559376
H	-3.007206	0.593346	-3.513709	C	-3.284913	2.572460	-1.869579
C	-2.935068	0.948034	3.875240	C	-3.892910	3.611336	0.363981
C	-3.919520	-1.342341	3.504015	H	-2.055704	2.577700	-0.107946
H	-1.986840	-0.634257	2.778529	H	-2.901201	3.552287	-2.224412
H	-2.442352	0.625545	4.816202	H	-2.724802	1.774244	-2.395165
H	-2.338163	1.777064	3.449820	H	-4.347155	2.505074	-2.186844
H	-3.941057	1.329104	4.152636	H	-3.523182	4.598901	0.015464
H	-3.515967	-1.682287	4.481581	H	-4.981368	3.564133	0.147573
H	-4.946062	-0.955081	3.679531	H	-3.776564	3.572743	1.467044
H	-4.016750	-2.229764	2.846074	Cl	-0.509538	-3.411899	-0.979776
C	0.800889	3.448685	-1.762274	C	-2.513486	-1.159079	-2.022800
C	0.778360	4.795182	-2.148032	C	-3.341225	-1.131827	-3.151786
C	0.036068	5.713615	-1.387941	C	-2.849741	-0.609919	-4.357814
C	-0.652274	5.241197	-0.258659	C	-1.532228	-0.123470	-4.372222
C	-0.571162	3.881324	0.070575	C	-0.766123	-0.182300	-3.202184
H	1.344817	2.691141	-2.344321	H	-2.872847	-1.577337	-1.071666
H	1.338715	5.110094	-3.041194	H	-4.362288	-1.532206	-3.070071
H	-0.004985	6.777424	-1.670558	H	-3.474094	-0.586443	-5.264330
H	-1.248915	5.915230	0.374372	H	-1.081971	0.292456	-5.286076
H	-1.065724	3.466670	0.963301	H	0.274442	0.168260	-3.195549

11-trans <sup>+</sup>				11-cis <sup>+</sup> c			
-2234.06058224				-2234.05648817			
Ru	0.489320	0.653754	0.253331	Ru	-0.299980	-0.53248	-1.060933
C	0.016854	-1.303687	0.052712	C	-0.293248	0.171787	0.845320
N	-1.107812	-2.060070	0.014434	N	0.628463	0.736673	1.681125
N	1.098183	-2.131519	-0.060439	N	-1.447966	-0.024665	1.550876
C	-0.800535	-3.494934	-0.229054	C	0.027156	1.060067	3.003972
C	0.728630	-3.563650	-0.048501	C	-1.276148	0.248488	2.995850
C	-2.482649	-1.624305	0.070873	C	2.046346	0.923326	1.471214
C	2.439849	-1.631360	0.087566	C	-2.585461	-0.715755	0.986329
C	-3.154545	-1.256951	-1.130725	C	2.547870	2.221215	1.163660
C	-4.514001	-0.891201	-1.032214	C	3.942403	2.375958	1.015920
C	-5.187726	-0.901573	0.196133	C	4.815163	1.294571	1.188508
C	-4.513084	-1.287258	1.363273	C	4.308389	0.036473	1.541298
C	-3.154073	-1.661330	1.328438	C	2.925501	-0.177823	1.707301
C	-2.484449	-1.305406	-2.504682	C	1.651525	3.457801	1.077847
H	-5.058554	-0.599922	-1.943561	H	4.354000	3.368966	0.776547
H	-5.057328	-1.309440	2.320707	H	5.006522	-0.797877	1.707210
C	-2.469865	-2.123688	2.617420	C	2.434297	-1.529985	2.229506
C	2.834123	-1.084198	1.348993	C	-2.506503	-2.124816	0.742885
C	4.129021	-0.533108	1.456702	C	-3.608434	-2.738726	0.107129
C	5.018957	-0.564311	0.374184	C	-4.758312	-2.011712	-0.221410
C	4.629690	-1.149104	-0.839449	C	-4.848417	-0.650154	0.105354
C	3.338335	-1.685713	-1.018636	C	-3.775527	0.026848	0.716894
C	1.918414	-1.130879	2.580803	C	-1.375640	-3.003107	1.293759
H	4.459123	-0.100872	2.413426	H	-3.569890	-3.815144	-0.115059
H	5.344405	-1.180279	-1.676211	H	-5.776226	-0.102100	-0.119695
C	2.953149	-2.317436	-2.355488	C	-3.938665	1.486075	1.146779
H	-6.251270	-0.618760	0.243074	H	5.900648	1.437471	1.069967
H	6.031507	-0.145048	0.483485	H	-5.604164	-2.516175	-0.714254
H	1.029579	-4.026148	0.918741	H	-1.190983	-0.708468	3.556959
H	-1.353622	-4.136948	0.484819	H	0.714660	0.776731	3.823525
Cl	0.681812	0.821001	-2.069994	C	1.314368	0.185420	-1.632755
C	-1.240162	1.329398	0.466210	H	1.345727	1.271944	-1.888675
H	-1.888081	0.813812	1.213886	C	2.557899	-0.507800	-1.938398
C	-1.916165	2.467890	-0.136169	C	3.715213	0.274913	-2.226206
C	-3.241063	2.755528	0.317253	C	2.661385	-1.926494	-2.031382
C	-1.345001	3.316730	-1.130391	C	4.926233	-0.335152	-2.572188
C	-3.958389	3.842003	-0.194664	H	3.646367	1.373025	-2.174231
H	-3.699654	2.100067	1.075220	C	3.871909	-2.529538	-2.392499
C	-2.071244	4.397886	-1.642028	H	1.764701	-2.546029	-1.875991
H	-0.336918	3.093284	-1.506831	C	5.007474	-1.738566	-2.656978
C	-3.373911	4.666592	-1.175733	H	5.810223	0.283350	-2.792177
H	-4.977997	4.048792	0.165829	H	3.930796	-3.625160	-2.484565
H	-1.622038	5.040690	-2.415095	H	5.955994	-2.217978	-2.946181
H	-3.937190	5.522250	-1.580782	N	-1.301133	1.064394	-1.776772
N	1.527702	2.552104	0.458398	H	-0.159068	2.154399	3.075998
H	-1.120810	-3.772486	-1.256094	H	-2.137960	0.810208	3.403498
H	1.234214	-4.120467	-0.861216	C	3.127438	-2.738802	1.572113
C	-2.583289	-1.082851	3.751929	C	2.592106	-1.602591	3.767782
C	-3.017775	-3.493020	3.080911	H	1.350588	-1.605329	1.996931
H	-1.389410	-2.252796	2.392160	H	2.184761	-2.557632	4.160243
H	-2.472509	-3.852977	3.978332	H	3.663173	-1.549368	4.055374
H	-4.093303	-3.424361	3.347274	H	2.073600	-0.771636	4.288581

H	-2.925560	-4.266416	2.290652	H	2.646231	-3.681906	1.903751
H	-2.008924	-1.411762	4.643175	H	3.076971	-2.692465	0.466519
H	-2.199811	-0.087634	3.443105	H	4.197436	-2.808872	1.858333
H	-3.635002	-0.943773	4.078059	C	1.898433	4.295817	-0.193679
C	-2.718035	-0.023039	-3.327670	H	0.596968	3.103854	1.056676
H	-1.388862	-1.386827	-2.346290	C	1.813541	4.337679	2.340558
C	-2.954830	-2.549676	-3.295593	H	1.174171	5.134928	-0.254765
H	-2.139671	-0.069016	-4.273069	H	2.911215	4.748918	-0.194438
H	-3.785929	0.105293	-3.603091	H	1.807803	3.691104	-1.119882
H	-2.387706	0.878509	-2.775759	H	1.109946	5.196031	2.317265
H	-2.419776	-2.618687	-4.265570	H	1.628278	3.765570	3.272405
H	-2.780470	-3.495460	-2.740975	H	2.842722	4.748134	2.407632
H	-4.042142	-2.496285	-3.515072	C	-0.988674	-4.187154	0.385927
C	1.102815	0.167178	2.745340	H	-0.469884	-2.367086	1.415008
H	1.189517	-1.953310	2.419116	C	-1.768514	-3.523811	2.699221
C	2.677056	-1.449013	3.886255	H	-0.938403	-4.109466	3.146244
H	1.960629	-1.634758	4.712592	H	-2.029983	-2.704562	3.399733
H	3.309100	-2.352526	3.772844	H	-2.653579	-4.190533	2.629952
H	3.333759	-0.613597	4.205396	H	-0.093797	-4.698604	0.795978
H	0.525626	0.161377	3.696464	H	-1.794692	-4.948442	0.339044
H	1.730202	1.077513	2.744749	H	-0.766880	-3.864752	-0.651382
H	0.192249	0.228982	2.031304	C	-4.609860	2.373478	0.081103
C	3.311466	-1.425688	-3.561623	C	-4.731198	1.568716	2.474728
C	3.591911	-3.719092	-2.502557	H	-2.919526	1.893272	1.325444
H	1.848455	-2.430943	-2.354962	H	-4.601324	3.434615	0.405244
H	2.929935	-1.883102	-4.497720	H	-4.094065	2.308572	-0.896590
H	2.859172	-0.419095	-3.462935	H	-5.672558	2.096079	-0.078826
H	4.409351	-1.311157	-3.681698	H	-4.783755	2.616650	2.836981
H	3.249272	-4.206864	-3.438647	H	-5.771910	1.209017	2.332916
H	4.699132	-3.648147	-2.547894	H	-4.282419	0.948709	3.277899
H	3.343337	-4.390396	-1.654089	Cl	-0.790931	-2.093882	-2.751812
C	1.141419	3.539260	1.309970	C	-2.259382	0.854343	-2.732253
C	1.887690	4.708379	1.498502	C	-2.870151	1.911601	-3.414121
C	3.086693	4.875432	0.784133	C	-2.511136	3.236123	-3.115919
C	3.487067	3.859410	-0.097776	C	-1.556129	3.449120	-2.110232
C	2.683245	2.719586	-0.237050	C	-0.977668	2.350728	-1.463720
H	0.193661	3.375576	1.845489	H	-2.499551	-0.194011	-2.954314
H	1.523968	5.477328	2.196204	H	-3.621168	1.677127	-4.182847
H	3.695348	5.784060	0.911288	H	-2.972157	4.082026	-3.648015
H	4.413114	3.941899	-0.685820	H	-1.245435	4.462479	-1.816710
H	2.946946	1.908219	-0.933019	H	-0.228192	2.479418	-0.673270

11-cis <sup>+</sup> t			
-2234.06320829			
Ru	0.048715	0.677165	-0.845434
Cl	0.412255	-0.263068	-2.912858
C	-0.240651	-0.991154	0.127098
N	0.647563	-1.912554	0.614273
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C	-0.047157	-3.121152	1.124624
C	-1.448988	-2.983350	0.524287
C	2.071520	-1.818664	0.839452
C	-2.762754	-0.870886	-0.021187
C	2.540542	-1.294913	2.081505
C	3.932122	-1.282605	2.310177
C	4.829542	-1.777767	1.353637
C	4.346674	-2.308515	0.150606
C	2.964879	-2.354658	-0.133422
C	1.600511	-0.775236	3.171786
H	4.320449	-0.885571	3.261173
H	5.059228	-2.708174	-0.587180
C	2.488184	-3.012029	-1.428873
C	-3.392989	-0.908893	-1.302419
C	-4.634933	-0.249003	-1.443300
C	-5.254613	0.382170	-0.357283
C	-4.649991	0.352747	0.907893
C	-3.405507	-0.277540	1.110422
C	-2.843329	-1.721137	-2.475805
H	-5.136711	-0.256329	-2.422803
H	-5.163735	0.819274	1.762542
C	-2.838617	-0.383403	2.528544
H	5.912568	-1.761449	1.553487
H	-6.229244	0.878003	-0.490969
H	-1.575750	-3.595431	-0.395694
H	0.481925	-4.034205	0.790103
C	1.761210	1.141512	-0.320898
H	2.356265	0.456612	0.317322
C	2.451270	2.339006	-0.776673
C	3.769374	2.597185	-0.299414
C	1.870789	3.263948	-1.694410
C	4.469324	3.738279	-0.712327
H	4.235668	1.881980	0.397149
C	2.575725	4.397963	-2.108676
H	0.863173	3.075430	-2.104443
C	3.875303	4.639550	-1.615627
H	5.487102	3.924946	-0.336036
H	2.120442	5.098027	-2.826096
H	4.428824	5.532608	-1.945694
N	-0.961159	2.115107	0.278977
H	-0.049490	-3.113299	2.237511
H	-2.257806	-3.250420	1.231315
C	3.230286	-2.481012	-2.672013
C	2.614609	-4.551438	-1.337504
H	1.415454	-2.759259	-1.558961
H	2.212835	-5.029684	-2.254935
H	3.676064	-4.861236	-1.234952

H	2.066795	-4.970806	-0.467627
H	2.791781	-2.919064	-3.591989
H	3.148483	-1.379016	-2.753741
H	4.306422	-2.753782	-2.661051
C	1.973251	0.647453	3.640388
H	0.579570	-0.720396	2.736674
C	1.553350	-1.743353	4.376623
H	1.206758	1.041996	4.339303
H	2.943555	0.663994	4.178838
H	2.060762	1.351131	2.786404
H	0.825035	-1.392106	5.137191
H	1.265124	-2.771169	4.074636
H	2.545273	-1.814107	4.870258
C	-2.928535	-0.982287	-3.825940
H	-1.769190	-1.919093	-2.278078
C	-3.579835	-3.080640	-2.563583
H	-3.138412	-3.709090	-3.364768
H	-3.529570	-3.651298	-1.613646
H	-4.654630	-2.935565	-2.802219
H	-2.425128	-1.577487	-4.614600
H	-3.978688	-0.832868	-4.153666
H	-2.427881	0.005685	-3.788126
C	-2.918840	0.931689	3.328595
C	-3.551389	-1.515354	3.308486
H	-1.764588	-0.653212	2.439557
H	-2.414950	0.812871	4.310050
H	-2.434011	1.773998	2.796933
H	-3.967959	1.224576	3.541983
H	-3.099726	-1.644469	4.314117
H	-4.627088	-1.279645	3.449620
H	-3.498405	-2.490591	2.783102
C	-2.163820	2.501939	-0.237510
C	-2.824600	3.660499	0.184008
C	-2.244743	4.457511	1.185128
C	-1.023191	4.043002	1.740856
C	-0.415211	2.872650	1.273280
H	-2.594228	1.855322	-1.020392
H	-3.786734	3.924290	-0.278403
H	-2.738706	5.378741	1.529886
H	-0.529640	4.619704	2.537013
H	0.539401	2.519269	1.684698

12-trans				12-cis		
				-2289.09428194		
-2289.08844906						
Ru	0.393947	0.981342	-0.468894	Ru	-0.243119	-1.186516
C	0.635354	-0.972359	0.252971	Cl	0.092399	-2.055632
Cl	0.287400	1.503210	1.910118	Cl	-1.823495	-2.973483
Cl	0.705191	-0.033077	-2.683499	C	0.173683	0.618373
C	-1.417393	0.970789	-0.857505	C	1.452604	-1.762136
H	-1.675790	0.338766	-1.737683	C	2.589866	-2.506554
C	0.726680	3.217349	-0.458399	H	1.953305	-1.646977
C	1.060077	2.721817	-1.719534	C	-0.034748	-0.007104
H	2.106692	2.479759	-1.974228	C	-1.078903	-0.935940
H	0.381004	2.807881	-2.581513	H	-2.132851	-0.631835
N	1.869056	-1.453991	0.576040	H	-0.931401	-1.879616
N	-0.282939	-1.934502	0.527501	N	-0.856067	1.403860
C	1.810882	-2.791580	1.209160	N	1.346530	1.222371
C	0.339510	-3.191871	1.011280	C	-0.396124	2.571530
H	2.522762	-3.485792	0.717488	C	1.132046	2.522478
H	2.093682	-2.714793	2.281647	H	-0.855551	3.504142
H	-0.151390	-3.528254	1.947044	H	-0.696680	2.464447
H	0.208109	-3.993868	0.252086	H	1.688982	2.553166
H	-0.242150	3.710310	-0.275915	H	1.514784	3.349592
C	3.143509	-0.793388	0.404737	H	-0.249452	1.060207
C	-1.713381	-1.910829	0.346935	C	-2.258927	1.162871
C	3.871437	-1.012737	-0.800410	C	2.693584	0.825646
C	5.106564	-0.354605	-0.958972	C	-2.864033	1.733495
C	5.655515	0.468044	0.044818	C	-4.222175	1.454367
C	4.961074	0.569628	1.264472	C	-4.997601	0.667746
C	3.723817	-0.071451	1.484321	C	-4.391451	0.202819
C	-2.538627	-1.551435	1.446710	C	-3.038573	0.445797
C	-3.934450	-1.596253	1.269856	C	3.463181	0.123166
C	-4.524810	-2.004273	0.056923	C	4.784846	-0.229235
C	-3.674735	-2.399113	-0.993322	C	5.371382	0.112228
C	-2.269265	-2.376049	-0.873783	C	4.604444	0.866186
C	3.379865	-1.962698	-1.863543	C	3.275666	1.249728
H	5.664832	-0.507058	-1.897923	C	-2.138309	2.686368
C	6.955562	1.206648	-0.180049	H	-4.689980	1.880041
H	5.402128	1.152735	2.090384	C	-6.434564	0.327711
C	3.119086	-0.058692	2.868155	H	-4.992478	-0.372531
C	-1.948614	-1.149690	2.776501	C	-2.470401	-0.023849
H	-4.580628	-1.305705	2.115102	C	2.899692	-0.217447
C	-6.028299	-2.010766	-0.104213	H	5.379205	-0.787272
H	-4.115010	-2.750373	-1.941801	C	6.778615	-0.325334
C	-1.400696	-2.844383	-2.016360	H	5.054737	1.182272
H	4.147161	-2.101405	-2.650120	C	2.558159	2.146943
H	3.146555	-2.963263	-1.440151	H	3.622182	-0.817444
H	2.452092	-1.578193	-2.339685	H	2.676946	0.699596
H	3.472449	0.818412	3.445366	H	1.951975	-0.792570
H	2.013741	-0.017222	2.842962	H	2.579293	1.723024
H	3.433575	-0.965659	3.432685	H	1.500016	2.315109
H	7.473627	1.427855	0.774931	H	3.058922	3.137700
H	7.648459	0.629124	-0.825595	H	7.227848	0.308417
H	6.775086	2.179729	-0.688125	H	7.441563	-0.292654
H	-2.747218	-0.908823	3.505024	H	6.788840	-1.373628

H	-1.334191	-1.966643	3.215096	H	-2.200122	2.354689	-2.640756
H	-1.281919	-0.265996	2.675908	H	-2.604374	3.694308	-1.538687
H	-2.021741	-3.166078	-2.875204	H	-1.068890	2.801469	-1.326093
H	-0.709593	-2.043792	-2.362937	H	-3.266661	-0.461843	3.396636
H	-0.769092	-3.711514	-1.723671	H	-1.678655	-0.792758	2.615443
H	-6.342638	-2.562241	-1.012751	H	-2.010604	0.811427	3.334997
H	-6.530155	-2.473909	0.770940	H	-7.057959	0.276793	0.556046
H	-6.421208	-0.973933	-0.187986	H	-6.889292	1.066088	-1.050547
H	1.498232	3.400501	0.306467	H	-6.498702	-0.668077	-0.850997
C	-2.584760	1.708537	-0.364931	H	0.947409	-0.211135	-2.889624
C	-3.790674	1.552409	-1.111715	C	3.741563	-2.642557	-1.191970
C	-2.607311	2.580279	0.759400	C	4.839610	-3.361305	-0.704430
C	-4.957797	2.244346	-0.762160	C	4.785960	-3.944050	0.567392
H	-3.790100	0.875869	-1.981492	C	3.634263	-3.808047	1.351673
C	-3.779543	3.263114	1.109971	C	2.536216	-3.089299	0.864134
H	-1.693029	2.682823	1.363205	H	3.783295	-2.189264	-2.181265
C	-4.955766	3.104314	0.352000	H	5.735465	-3.467096	-1.314489
H	-5.873376	2.116040	-1.361531	H	5.640083	-4.503133	0.946628
H	-3.777130	3.930842	1.986500	H	3.592531	-4.261339	2.340969
H	-5.871221	3.651453	0.629602	H	1.640361	-2.983508	1.474193

12-trans <sup>+</sup>				12-cis <sup>+</sup> c			
-1828.67204010				-1828.69043640			
Ru	0.551962	0.935643	-0.314525	Ru	0.590532	0.731798	-0.667798
C	0.595355	-1.068635	0.119597	Cl	1.431147	2.876286	-0.538663
Cl	0.598490	1.179375	2.013553	C	0.463314	-1.070468	0.284102
C	-1.195295	1.145040	-0.796557	C	-1.192672	1.008311	-1.140749
H	-1.262899	0.686891	-1.830839	C	-2.167182	1.870866	-0.494857
C	1.224660	3.130087	-0.224245	H	-1.573807	0.541794	-2.077406
C	1.523565	2.580095	-1.470719	C	0.731570	-0.650069	-2.327454
H	2.546533	2.217791	-1.684006	C	1.494784	0.534427	-2.557858
H	0.886246	2.779420	-2.350898	H	2.591440	0.530847	-2.415073
N	1.817401	-1.614136	0.312557	H	1.123977	1.326766	-3.230458
N	-0.358316	-2.015956	0.233462	N	1.635540	-1.569344	0.750758
C	1.752413	-3.075496	0.558152	N	-0.551372	-1.888335	0.644277
C	0.228998	-3.342704	0.573938	C	1.442550	-2.768317	1.599075
H	2.282753	-3.619328	-0.252537	C	-0.051242	-3.087539	1.374019
H	2.244279	-3.332165	1.518007	H	2.116773	-3.588488	1.280519
H	-0.139942	-3.666358	1.569106	H	1.680989	-2.524504	2.657580
H	-0.089405	-4.103320	-0.167854	H	-0.616794	-3.225500	2.317169
H	0.314372	3.729041	-0.059478	H	-0.210008	-3.992741	0.749562
C	3.048766	-0.898889	0.085586	H	1.254319	-1.592598	-2.103088
C	-1.782948	-1.872116	0.070094	C	2.892418	-0.876929	0.607732
C	3.432604	-0.595909	-1.251355	C	-1.963005	-1.732583	0.405237
C	4.646988	0.089435	-1.456014	C	3.856660	-1.367740	-0.317693
C	5.488747	0.456125	-0.385919	C	5.064553	-0.658124	-0.451631
C	5.085723	0.113759	0.922559	C	5.353508	0.490277	0.315381
C	3.883592	-0.567805	1.189275	C	4.400057	0.910318	1.263910
C	-2.597427	-1.626952	1.207285	C	3.172605	0.244081	1.442543
C	-3.988862	-1.548062	1.010736	C	-2.733007	-1.015972	1.362879
C	-4.584573	-1.720440	-0.256678	C	-4.121441	-0.932001	1.168028
C	-3.741820	-1.980163	-1.356012	C	-4.763255	-1.541694	0.066791
C	-2.342065	-2.069460	-1.219577	C	-3.969107	-2.253351	-0.851292
C	2.580066	-0.998588	-2.434297	C	-2.571546	-2.380638	-0.699099
H	4.955365	0.324397	-2.488234	C	3.650758	-2.638889	-1.111949
C	6.798510	1.169146	-0.625132	H	5.814162	-1.023318	-1.173333
H	5.734080	0.384573	1.772329	C	6.642588	1.252342	0.124093
C	3.511815	-0.943378	2.603203	H	4.621846	1.783374	1.899327
C	-2.005662	-1.474018	2.588683	C	2.216582	0.726293	2.512633
H	-4.631714	-1.352298	1.884934	C	-2.082357	-0.370175	2.563844
C	-6.085321	-1.652481	-0.415389	H	-4.725726	-0.376387	1.903874
H	-4.187454	-2.133314	-2.352925	C	-6.263034	-1.455643	-0.092306
C	-1.476111	-2.383375	-2.419670	H	-4.452560	-2.746322	-1.711259
H	3.128577	-0.864002	-3.386289	C	-1.794263	-3.235994	-1.674690
H	2.247183	-2.055096	-2.375589	H	-2.835220	0.132479	3.200158
H	1.651710	-0.380253	-2.506060	H	-1.551338	-1.111361	3.199045
H	4.098043	-0.355898	3.335726	H	-1.334163	0.395013	2.266620
H	2.435656	-0.765083	2.799692	H	-2.126226	-3.057509	-2.717675
H	3.725673	-2.016150	2.806252	H	-0.703887	-3.057034	-1.627480
H	7.657866	0.508818	-0.379447	H	-1.966310	-4.315855	-1.472848
H	6.910199	1.487298	-1.679832	H	-6.592083	-1.782342	-1.098052
H	6.892580	2.067521	0.019631	H	-6.775425	-2.102691	0.652395
H	-2.772008	-1.128900	3.309027	H	-6.630841	-0.422698	0.076739
H	-1.614856	-2.441836	2.973357	H	3.998346	-2.521643	-2.158308
H	-1.165908	-0.748975	2.602884	H	4.242757	-3.472537	-0.674987

H	-2.089302	-2.483151	-3.335824	H	2.593304	-2.965617	-1.135873
H	-0.713388	-1.597793	-2.610039	H	2.775041	1.043419	3.415891
H	-0.919739	-3.337092	-2.293257	H	1.645235	1.615095	2.165922
H	-6.391430	-1.692503	-1.479006	H	1.486744	-0.047385	2.819743
H	-6.578187	-2.499759	0.108002	H	7.031094	1.644879	1.085257
H	-6.495745	-0.721735	0.028591	H	7.428156	0.624585	-0.340345
H	1.988941	3.190418	0.566058	H	6.481826	2.128714	-0.541333
C	-2.398715	1.806523	-0.343073	H	-0.235836	-0.784545	-2.841308
C	-3.520138	1.849148	-1.224250	C	-3.483789	1.909570	-1.047406
C	-2.495526	2.446670	0.926718	C	-4.465124	2.746647	-0.505799
C	-4.690108	2.522038	-0.853443	C	-4.159277	3.562552	0.600874
H	-3.456053	1.352746	-2.205593	C	-2.865826	3.541793	1.161260
C	-3.672388	3.108819	1.290128	C	-1.878578	2.711164	0.621609
H	-1.633520	2.405296	1.609778	H	-3.717866	1.276707	-1.918139
C	-4.768073	3.152582	0.403257	H	-5.470960	2.775661	-0.952554
H	-5.545758	2.559122	-1.545201	H	-4.928412	4.229776	1.020933
H	-3.739945	3.603657	2.271426	H	-2.625459	4.196340	2.013253
H	-5.687639	3.685002	0.693426	H	-0.858632	2.738328	1.033322

12-cis <sup>+</sup> t			
-1828.68703231			
Ru	0.271877	0.826443	0.155150
Cl	0.187626	1.058784	2.441946
C	0.538299	-1.134200	-0.005830
C	-1.507642	1.102903	-0.321221
C	-2.159202	2.395749	-0.284699
H	-2.132619	0.258117	-0.680133
C	0.659922	0.776700	-2.109595
C	1.245740	1.865272	-1.432014
H	2.322915	1.836220	-1.177168
H	0.795890	2.875111	-1.482936
N	1.801645	-1.652203	-0.053919
N	-0.355952	-2.152640	0.068083
C	1.806891	-3.119169	0.144514
C	0.317963	-3.476279	-0.013424
H	2.458815	-3.614462	-0.602648
H	2.201748	-3.358427	1.156160
H	-0.059525	-4.148225	0.782679
H	0.090740	-3.948062	-0.993844
H	1.266886	-0.093084	-2.389086
C	3.019004	-0.876078	-0.072564
C	-1.797616	-2.100464	0.037955
C	3.722244	-0.724511	-1.302613
C	4.869066	0.091278	-1.315742
C	5.356992	0.724671	-0.152316
C	4.693616	0.468679	1.062869
C	3.546987	-0.350012	1.141268
C	-2.511856	-2.085089	1.265841
C	-3.919218	-2.068357	1.207984
C	-4.625000	-2.086281	-0.012982
C	-3.878763	-2.130998	-1.207984
C	-2.468514	-2.155175	-1.212018
C	3.334212	-1.464079	-2.566208
H	5.411452	0.224458	-2.266838
C	6.562994	1.632055	-0.210225
H	5.096978	0.894714	1.996465
C	3.018899	-0.735650	2.504073
C	-1.803406	-2.085875	2.599734
H	-4.483351	-2.050001	2.155141
C	-6.135732	-2.102133	-0.032214
H	-4.410144	-2.162531	-2.173903
C	-1.722985	-2.265120	-2.524175
H	-2.513367	-2.299638	3.421455
H	-0.998078	-2.848539	2.642880
H	-1.326605	-1.104916	2.809653
H	-2.334680	-1.878717	-3.363049
H	-0.763025	-1.712106	-2.516672
H	-1.490863	-3.325891	-2.766454
H	-6.539519	-1.820317	-1.024551
H	-6.520019	-3.118459	0.203775
H	-6.561732	-1.414666	0.726621
H	3.372142	-0.802720	-3.455532
H	4.052812	-2.290186	-2.759061

H	2.325146	-1.915651	-2.512511
H	2.979525	0.136899	3.184661
H	2.005088	-1.173158	2.476422
H	3.704876	-1.479788	2.965001
H	7.076660	1.694826	0.769286
H	7.296333	1.290104	-0.967880
H	6.264973	2.666079	-0.491178
H	-0.269912	0.911831	-2.683756
C	-3.445659	2.524028	-0.891946
C	-4.101944	3.759436	-0.917380
C	-3.499617	4.886892	-0.325436
C	-2.238505	4.778429	0.297514
C	-1.572802	3.549834	0.320651
H	-3.914525	1.635810	-1.344753
H	-5.091135	3.847895	-1.392386
H	-4.021024	5.856945	-0.338496
H	-1.784138	5.659198	0.776637
H	-0.607033	3.463684	0.846221

13-trans			13-cis		
-2403.64111756			-2403.63053379		
C	0.284921	-1.431561	0.098432	Ru	0.349236
N	-0.670440	-2.415428	0.223732	Cl	0.079715
C	-0.100285	-3.776730	0.277288	O	0.371116
C	1.394793	-3.507020	0.488134	N	1.173680
C	-2.853108	-2.210489	1.333789	N	-1.036024
C	-4.257821	-2.161184	1.230661	C	-3.531538
H	-4.853032	-2.076111	2.155498	C	1.608487
C	-4.918605	-2.212329	-0.013767	C	-2.423299
C	-4.133531	-2.304992	-1.181617	C	3.432980
H	-4.630867	-2.333621	-2.165981	C	0.066868
C	-2.725948	-2.355327	-1.135200	C	-4.589669
C	-2.098199	-2.304818	0.136679	C	-0.679432
C	-2.166176	-2.117200	2.675816	C	-2.167576
H	-2.906065	-2.056533	3.497772	C	2.521331
H	-1.506578	-1.223463	2.728569	C	2.935884
H	-1.518229	-2.999064	2.870172	C	1.611625
C	-6.429510	-2.199214	-0.093541	C	3.041565
H	-6.786112	-1.738291	-1.037054	C	-1.390850
H	-6.880606	-1.645046	0.754421	C	-6.669478
H	-6.838939	-3.233298	-0.061729	C	-4.381357
C	-1.910212	-2.395128	-2.406449	C	-1.833490
H	-2.566473	-2.442800	-3.297243	C	-5.193778
H	-1.233545	-3.275539	-2.441106	C	0.838373
H	-1.264947	-1.494324	-2.497812	C	1.909037
C	2.821341	-1.497346	0.008276	C	-1.262847
C	3.576414	-1.117250	1.151627	C	-2.584819
C	4.864631	-0.578158	0.949744	C	1.989245
H	5.445372	-0.263850	1.833598	C	-2.610606
C	5.437679	-0.457309	-0.329648	C	6.563318
C	4.700488	-0.938036	-1.430496	C	4.740306
H	5.150792	-0.908187	-2.437036	C	-3.213354
C	3.407364	-1.476067	-1.289646	C	4.252142
C	3.088694	-1.365290	2.559682	C	-0.887786
H	3.585883	-0.682334	3.276688	C	5.166947
H	3.336932	-2.403446	2.877252	C	-3.003721
H	1.997166	-1.214291	2.658457	C	-3.155325
C	6.804661	0.161320	-0.519607	H	-5.208777
H	7.360568	-0.320410	-1.350038	H	-1.233534
H	7.420718	0.085944	0.399237	H	-0.950313
H	6.720498	1.241819	-0.770819	H	-1.348447
C	2.691091	-2.050675	-2.487732	H	-1.690958
H	3.369947	-2.104499	-3.361489	H	-2.783956
H	1.819673	-1.418853	-2.762025	H	2.364016
H	2.311509	-3.075281	-2.287881	H	2.091916
C	-1.682461	0.771725	-0.134421	H	2.900027
H	-2.427960	-0.044690	-0.143381	H	3.830365
C	-2.226370	2.111346	-0.263978	H	-6.834197
C	-3.611172	2.357828	-0.445446	H	-7.163219
H	-4.295305	1.494455	-0.476287	H	-7.195870
C	-4.098528	3.664062	-0.586580	H	-4.833797
H	-5.175353	3.843440	-0.728392	H	1.400404
C	-3.199814	4.746498	-0.545248	H	1.097916

H	-3.573868	5.776847	-0.655840	H	1.306285	4.317230	1.925162
C	-1.818714	4.540250	-0.361060	H	2.975330	3.741089	1.671465
C	1.009738	3.888992	0.173853	H	1.756537	2.633386	2.368857
C	-1.336910	3.227279	-0.223396	H	2.478457	0.682740	3.589055
N	1.509244	-2.074016	0.159873	H	1.644418	-0.896278	3.498535
Cl	0.457869	0.773681	2.328466	H	1.077892	0.451020	2.482788
Cl	0.714506	0.720581	-2.285379	H	-1.714868	-3.130931	-1.586617
Ru	0.142217	0.522638	-0.004098	H	-3.345329	-3.885014	-1.761985
H	-1.140475	5.403699	-0.329599	H	-2.287637	-4.343462	-0.397446
O	-0.026289	2.870983	-0.057275	H	6.618228	0.971662	-0.084626
H	0.810312	4.705437	-0.555551	H	7.308721	-0.599835	0.401324
C	2.354225	3.253238	-0.158762	H	6.878395	0.618283	1.649925
H	2.595255	2.437624	0.553469	H	5.449231	-1.763351	-0.906802
H	2.354822	2.839011	-1.185565	H	4.577812	0.771297	2.496590
H	3.147967	4.024312	-0.080604	H	-4.560027	4.003105	-0.326651
C	0.918830	4.406669	1.609704	H	-2.103024	0.111263	-1.903198
H	1.080623	3.570089	2.318882	H	-0.545581	4.487594	1.255083
H	1.693399	5.183415	1.777629	H	-2.871172	5.317888	0.991791
H	-0.070409	4.857196	1.826180	H	-3.880591	1.814849	-1.376277
H	1.713257	-3.690353	1.539359	H	1.413526	3.606194	-1.850212
H	2.045722	-4.115925	-0.173070	H	2.618361	4.506644	-0.877910
H	-0.558644	-4.360378	1.102318	H	0.875221	4.851086	-0.645953
H	-0.307260	-4.321495	-0.672762	Cl	1.919946	1.051364	-2.531076

13-trans <sup>+</sup>				13-cis <sup>+</sup>			
-1943.21796377				-1943.21617094			
C	0.195498	-1.570172	-0.150573	Ru	0.346199	0.112485	-1.025607
N	1.374683	-2.232179	-0.226609	Cl	0.487207	-1.328175	-2.788054
C	1.173562	-3.703481	-0.305661	O	0.438891	2.053541	0.086667
C	-0.337507	-3.843956	-0.580519	N	1.286916	-1.732609	0.938811
C	3.403018	-1.389017	-1.329103	N	-0.931893	-1.798886	0.961506
C	4.726498	-0.915866	-1.230144	C	-3.399479	3.747713	-0.273770
H	5.269534	-0.663358	-2.156096	C	1.714186	3.287769	-1.648760
C	5.375448	-0.767161	0.013068	C	-2.322694	-1.554634	0.690529
C	4.659884	-1.107722	1.179638	C	3.464526	-1.857834	-0.250990
H	5.150601	-1.004201	2.161614	C	0.152100	-1.187371	0.412323
C	3.335609	-1.587885	1.141039	C	-4.352356	-2.112112	-0.515661
C	2.714480	-1.706282	-0.129667	C	-0.530165	-2.775310	2.006781
C	2.735086	-1.522704	-2.679574	C	-2.358338	0.158229	2.593307
H	3.446164	-1.299385	-3.497937	C	2.615390	-1.228603	0.700959
H	1.877410	-0.822584	-2.782424	C	3.086315	-0.166521	1.524884
H	2.337635	-2.544998	-2.854056	C	1.738551	2.762025	-0.219356
C	6.808069	-0.293470	0.095502	C	3.039922	-3.090303	-1.012546
H	6.964315	0.387981	0.956342	C	-1.432329	0.619295	-1.132273
H	7.122543	0.232634	-0.827384	C	-6.578230	-1.017108	0.033527
H	7.498834	-1.153311	0.236891	C	-4.411572	-0.448977	1.240650
C	2.613860	-1.953637	2.416447	C	-1.807067	1.930089	-0.644703
H	3.259008	-1.775985	3.297988	C	-5.092050	-1.183467	0.247624
H	2.324223	-3.026658	2.434289	C	0.992449	-2.901093	1.797502
H	1.683800	-1.360525	2.545739	C	2.129393	3.796128	0.832682
C	-2.173309	-2.030208	-0.344140	C	-1.073068	3.984748	0.489959
C	-2.477430	-0.934269	-1.212842	C	-2.380110	4.494875	0.349192
C	-3.814160	-0.474479	-1.286500	C	2.221761	0.402687	2.627652
H	-4.052527	0.349186	-1.979264	C	-2.224532	-3.337040	-1.142235
C	-4.847144	-1.066824	-0.540509	C	6.641266	0.288555	0.119968
C	-4.504934	-2.132084	0.322018	C	4.763739	-1.334935	-0.419253
H	-5.294522	-2.591097	0.940082	C	-2.976034	-2.326326	-0.310569
C	-3.192576	-2.621951	0.452168	C	4.394807	0.308472	1.317270
C	-1.441974	-0.347103	-2.149907	C	-0.792375	2.709765	-0.016613
H	-1.940226	0.265131	-2.929423	C	5.247724	-0.251642	0.340991
H	-0.820337	-1.118034	-2.644981	C	-3.035700	-0.621545	1.489944
H	-0.668711	0.470904	-1.800875	C	-3.117850	2.466633	-0.759592
C	-6.277745	-0.596225	-0.654251	H	-4.866662	-2.703379	-1.291327
H	-6.918460	-1.382091	-1.108281	H	-1.067021	-3.733818	1.862484
H	-6.366083	0.312328	-1.281255	H	-0.794211	-2.384982	3.014292
H	-6.708735	-0.370328	0.343390	H	-1.366261	0.545774	2.284795
C	-2.885730	-3.712661	1.450600	H	-2.195963	-0.471548	3.495504
H	-3.694796	-3.794542	2.201503	H	-2.979535	1.017879	2.911167
H	-1.937721	-3.507825	1.988954	H	2.434985	1.902190	-0.135371
H	-2.793952	-4.710633	0.968311	H	1.983070	-3.039892	-1.339178
C	1.171907	1.175429	-0.309558	H	3.164228	-4.000261	-0.384477
H	2.125498	0.654442	-0.533677	H	3.666222	-3.233427	-1.914048
C	1.237416	2.611528	-0.237871	H	-6.940978	-0.034454	0.394768
C	2.457711	3.321981	-0.415946	H	-7.142543	-1.798321	0.588687
H	3.371026	2.747604	-0.638193	H	-6.853738	-1.121235	-1.035383
C	2.497833	4.713158	-0.297011	H	-4.971883	0.276908	1.852990
H	3.443963	5.258349	-0.430258	H	1.568475	-2.845187	2.743023
C	1.311134	5.413564	-0.001211	H	1.273329	-3.843301	1.277931

H	1.333388	6.510530	0.094420	H	1.649138	4.781441	0.675763
C	0.084011	4.745955	0.174932	H	3.224709	3.957040	0.759713
C	-2.370011	3.202002	0.554626	H	1.914033	3.438281	1.858139
C	0.045205	3.346363	0.058249	H	2.758399	1.195615	3.183998
N	-0.823777	-2.486016	-0.254059	H	1.937711	-0.378407	3.364813
Cl	-0.416295	0.194600	2.331511	H	1.276160	0.832429	2.236036
Ru	-0.435195	0.280140	0.018208	H	-1.489456	-2.845304	-1.816410
H	-0.816204	5.333064	0.397866	H	-2.919251	-3.928126	-1.768865
O	-1.074200	2.563856	0.206727	H	-1.650355	-4.049185	-0.512842
H	-2.117499	4.034312	1.244417	H	6.664001	0.983891	-0.747781
C	-3.209690	2.183886	1.308838	H	7.362296	-0.523698	-0.102234
H	-3.462680	1.314511	0.668326	H	7.010596	0.848300	1.001911
H	-2.680443	1.816323	2.207883	H	5.426691	-1.810222	-1.161029
H	-4.157983	2.665428	1.622766	H	4.772370	1.123313	1.957427
C	-3.028735	3.736931	-0.714730	H	-4.410884	4.169823	-0.371730
H	-3.299455	2.906096	-1.398069	H	-2.218461	0.004240	-1.617581
H	-3.960908	4.277469	-0.452252	H	-0.311771	4.580451	1.005780
H	-2.372855	4.441227	-1.264150	H	-2.602289	5.497135	0.747848
H	-0.560757	-4.083612	-1.644072	H	-3.898606	1.857821	-1.241226
H	-0.812113	-4.618293	0.051396	H	1.497372	2.482178	-2.383404
H	1.804002	-4.138965	-1.106235	H	2.710118	3.703155	-1.904403
H	1.476168	-4.170763	0.656259	H	0.965299	4.095700	-1.778229

14-trans				14-cis			
-2608.12442252				-2608.11724990			
C	-1.143056	1.423367	0.076648	C	0.920444	-1.280007	-0.259717
C	-1.486154	3.776186	0.194224	C	0.721510	-3.334972	-1.427348
H	-1.403794	4.341929	-0.762116	H	0.419450	-3.274097	-2.498450
H	-1.262739	4.482817	1.019845	H	0.427559	-4.335865	-1.052363
C	-2.840744	3.073215	0.351926	C	2.209846	-3.029767	-1.209794
H	-3.250213	3.168794	1.383028	H	2.676365	-3.714870	-0.467308
H	-3.611904	3.446150	-0.353438	H	2.808100	-3.077380	-2.142752
C	1.569985	3.140605	1.380708	C	-2.036667	-3.104508	0.365992
C	2.930574	3.503365	1.316477	C	-3.445825	-3.166782	0.334287
H	3.489887	3.626397	2.259166	H	-3.960897	-3.791074	1.083537
C	3.594965	3.705496	0.089641	C	-4.210816	-2.467443	-0.619379
C	2.861283	3.524594	-1.101935	C	-3.523788	-1.689755	-1.575625
H	3.365625	3.664319	-2.072974	H	-4.099870	-1.144981	-2.342592
C	1.500255	3.160780	-1.094814	C	-2.120994	-1.586624	-1.585298
C	0.867181	2.968703	0.161283	C	-1.383234	-2.285054	-0.591532
C	0.891380	2.894065	2.707515	C	-1.254169	-3.892482	1.388018
H	1.592553	3.058734	3.548712	H	-1.927532	-4.331181	2.150245
H	0.501432	1.855073	2.771949	H	-0.501202	-3.254076	1.899189
H	0.021618	3.569414	2.858766	H	-0.702289	-4.735989	0.916169
C	5.045897	4.130496	0.049398	C	-5.721417	-2.518706	-0.609822
H	5.575034	3.699750	-0.824679	H	-6.130324	-2.657194	-1.632431
H	5.588691	3.823417	0.965691	H	-6.142176	-1.567301	-0.217029
H	5.133047	5.236868	-0.029431	H	-6.100298	-3.341851	0.027931
C	0.757520	2.915567	-2.388035	C	-1.422632	-0.740628	-2.624064
H	1.397772	3.143174	-3.262334	H	-2.146566	-0.329799	-3.354387
H	-0.157525	3.540055	-2.470534	H	-0.662049	-1.318405	-3.191089
H	0.427668	1.856762	-2.466740	H	-0.887520	0.112263	-2.154954
C	-3.568788	0.713671	-0.125981	C	3.366576	-0.842511	-0.692448
C	-4.220954	0.128854	0.992864	C	4.351916	-0.975294	0.323238
C	-5.257822	-0.797637	0.749541	C	5.516755	-0.186559	0.216979
H	-5.752214	-1.270491	1.615130	H	6.276036	-0.268482	1.012588
C	-5.694854	-1.113049	-0.549607	C	5.748668	0.681496	-0.866282
C	-5.095656	-0.434022	-1.630456	C	4.782347	0.732450	-1.891713
H	-5.460406	-0.620130	-2.654686	H	4.959790	1.373951	-2.771564
C	-4.050830	0.490173	-1.448126	C	3.596716	-0.022629	-1.831473
C	-3.919227	0.540229	2.415039	C	4.210501	-1.963902	1.453205
H	-4.080343	-0.302690	3.116080	H	4.954594	-1.761528	2.248060
H	-4.606087	1.358575	2.728723	H	4.390298	-3.001955	1.093721
H	-2.876310	0.881607	2.544785	H	3.198952	-1.936002	1.910071
C	-6.778875	-2.140815	-0.785178	C	6.992300	1.539470	-0.923416
H	-7.458345	-1.837947	-1.608435	H	7.267656	1.796096	-1.966432
H	-7.390436	-2.309227	0.123940	H	7.859345	1.035951	-0.449653
H	-6.340279	-3.121317	-1.074459	H	6.837154	2.497148	-0.379195
C	-3.491904	1.243774	-2.631024	C	2.612808	0.005008	-2.980478
H	-4.125976	1.092500	-3.526622	H	2.918306	0.743590	-3.747475
H	-2.466127	0.892888	-2.869777	H	1.585341	0.255615	-2.645860
H	-3.433650	2.335039	-2.434732	H	2.547121	-0.984135	-3.484498
C	1.394248	-0.091579	-0.034240	C	-1.150916	0.125085	1.204971
H	1.861769	0.909275	-0.073213	H	-1.613406	-0.592435	1.915893
C	2.318016	-1.212898	-0.103440	C	-2.040875	1.063654	0.538211
C	3.709023	-1.035870	-0.268831	C	-3.446670	0.985148	0.631377
H	4.143294	-0.028298	-0.337700	H	-3.924937	0.199440	1.232302

C	4.545715	-2.156244	-0.348694	C	-4.238081	1.916277	-0.051991
C	4.038133	-3.464588	-0.265229	C	-3.668396	2.943284	-0.824385
H	4.736802	-4.309715	-0.334980	H	-4.330546	3.652583	-1.339671
C	2.660641	-3.663774	-0.093359	C	-2.273006	3.044061	-0.918019
C	-0.241358	-3.868610	0.415910	C	0.616327	3.353586	-0.666089
C	1.804457	-2.546716	-0.014445	C	-1.460699	2.107761	-0.244438
N	-0.531384	2.648042	0.203923	N	0.052980	-2.268942	-0.647683
N	-2.504021	1.666641	0.064718	N	2.175011	-1.651291	-0.679378
Cl	-0.751186	-0.644112	2.391682	Cl	0.990196	-1.355262	2.707135
Cl	-0.853278	-0.885193	-2.194710	Cl	1.656346	1.843735	2.473556
Ru	-0.420717	-0.403451	0.067387	Ru	0.670942	0.257732	1.022920
H	2.269647	-4.687706	-0.026256	H	-1.836854	3.852691	-1.518956
O	0.454972	-2.596324	0.136502	O	-0.088424	2.095698	-0.272480
H	0.199456	-4.618412	-0.277324	H	0.162530	3.648739	-1.637697
C	-1.708487	-3.666804	0.059189	C	2.078051	3.013112	-0.888969
H	-2.181750	-2.921130	0.730704	H	2.546525	2.666068	0.053242
H	-1.821818	-3.323810	-0.987356	H	2.198586	2.235621	-1.663867
H	-2.243420	-4.630797	0.181455	H	2.606817	3.925307	-1.233358
C	-0.014281	-4.263574	1.874308	C	0.400190	4.433644	0.391254
H	-0.411536	-3.470133	2.538814	H	0.864271	4.116416	1.346388
H	-0.539581	-5.217008	2.088636	H	0.876358	5.375317	0.047979
H	1.060121	-4.406598	2.106406	H	-0.673406	4.642339	0.568261
N	6.002294	-1.959449	-0.523799	N	-5.711920	1.818089	0.036403
O	6.417281	-0.797664	-0.592695	O	-6.379210	2.679279	-0.545154
O	6.711689	-2.969325	-0.589955	O	-6.185752	0.877737	0.686244

14-trans <sup>+</sup>			14-cis <sup>+t</sup>				
-2147.69690969			-2147.69596950				
C	-1.035345	-1.653379	-0.168420	C	-0.922681	-1.194733	0.352090
C	-1.229591	-3.984046	-0.392327	C	-0.661664	-3.038962	1.791794
H	-1.227102	-4.564358	0.555414	H	-0.287850	-2.838557	2.819575
H	-0.869689	-4.652376	-1.199489	H	-0.401836	-4.085279	1.535355
C	-2.604361	-3.353434	-0.694560	C	-2.164831	-2.737098	1.634606
H	-2.882085	-3.421531	-1.769951	H	-2.701710	-3.533241	1.075267
H	-3.418795	-3.809339	-0.100675	H	-2.683483	-2.587479	2.603126
C	1.884645	-3.041607	-1.295222	C	1.877085	-3.013407	-0.449063
C	3.267300	-3.269903	-1.157161	C	3.273604	-3.134758	-0.600505
H	3.893135	-3.292681	-2.064728	H	3.662300	-3.773488	-1.410439
C	3.869048	-3.476212	0.102822	C	4.183501	-2.487817	0.260709
C	3.041553	-3.449549	1.243744	C	3.658665	-1.689466	1.302898
H	3.491146	-3.613184	2.236974	H	4.354309	-1.185207	1.994140
C	1.650989	-3.228663	1.166440	C	2.276011	-1.523077	1.495327
C	1.090943	-3.007665	-0.117984	C	1.389168	-2.176397	0.594295
C	1.281301	-2.801384	-2.661524	C	0.935972	-3.754503	-1.366237
H	2.017263	-3.007967	-3.462026	H	1.495529	-4.381478	-2.086229
H	0.950843	-1.746028	-2.781792	H	0.284083	-3.062734	-1.943451
H	0.393200	-3.439940	-2.850900	H	0.255798	-4.425342	-0.798916
C	5.349115	-3.756001	0.218242	C	5.675867	-2.635797	0.089962
H	5.740411	-3.491141	1.220226	H	6.136305	-3.085305	0.995420
H	5.932944	-3.199541	-0.542229	H	6.157145	-1.645682	-0.056490
H	5.556515	-4.837073	0.059598	H	5.931516	-3.276151	-0.776130
C	0.805612	-3.222354	2.418416	C	1.760765	-0.676899	2.636587
H	1.430036	-3.403235	3.314096	H	2.569602	-0.054627	3.065922
H	0.028516	-4.016670	2.396430	H	1.365528	-1.303714	3.465766
H	0.280601	-2.253579	2.556895	H	0.936607	-0.003794	2.321314
C	-3.311719	-0.873961	-0.412992	C	-3.327705	-0.651948	0.702340
C	-3.003858	0.250244	-1.244477	C	-4.353731	-1.021782	-0.213274
C	-3.931284	1.317410	-1.318771	C	-5.503426	-0.209661	-0.274975
H	-3.709069	2.166997	-1.985024	H	-6.297210	-0.480417	-0.990886
C	-5.144276	1.298482	-0.610030	C	-5.684271	0.910822	0.561535
C	-5.405136	0.180055	0.213192	C	-4.669842	1.213135	1.493977
H	-6.338564	0.158130	0.799909	H	-4.810363	2.061652	2.183964
C	-4.516289	-0.902712	0.342615	C	-3.491865	0.447449	1.592324
C	-1.785751	0.263697	-2.145023	C	-4.267616	-2.273937	-1.051585
H	-1.892760	1.052957	-2.917589	H	-4.949675	-2.214332	-1.921646
H	-1.605387	-0.705938	-2.647061	H	-4.577074	-3.164718	-0.460990
H	-0.725615	0.602645	-1.754316	H	-3.243511	-2.450737	-1.433809
C	-6.146888	2.422315	-0.721808	C	-6.941493	1.743609	0.470374
H	-7.089036	2.067576	-1.191265	H	-6.963712	2.543789	1.235459
H	-5.762195	3.261741	-1.333045	H	-7.847569	1.116400	0.605411
H	-6.419222	2.819936	0.278228	H	-7.033251	2.222443	-0.527927
C	-4.831596	-2.031574	1.294817	C	-2.452140	0.769066	2.641958
H	-5.597281	-1.720117	2.030958	H	-2.805907	1.572309	3.316911
H	-3.928848	-2.351131	1.854220	H	-1.494459	1.103229	2.189305
H	-5.238215	-2.922185	0.767335	H	-2.217340	-0.114951	3.271493
C	1.173355	0.235446	-0.205020	C	1.063078	0.101372	-1.172001
H	1.747283	-0.690375	-0.414417	H	1.552270	-0.676454	-1.793551
C	1.950471	1.447776	-0.103284	C	1.916563	1.109577	-0.563548
C	3.359687	1.443939	-0.248689	C	3.331951	1.076387	-0.589974
H	3.905491	0.512770	-0.459459	H	3.877610	0.263471	-1.088967

C	4.064449	2.639530	-0.113032	C	4.037899	2.106674	0.036051
C	3.410674	3.852775	0.163083	C	3.394141	3.175415	0.685760
H	4.013228	4.767580	0.259386	H	4.007664	3.951324	1.166039
C	2.014962	3.881103	0.307651	C	1.990049	3.222229	0.715689
C	-0.895485	3.772835	0.612256	C	-0.812124	3.333348	-0.527883
C	1.281784	2.684441	0.178815	C	1.270146	2.191029	0.095147
N	-0.331817	-2.805667	-0.253960	N	-0.027189	-2.102746	0.827981
N	-2.369005	-1.941437	-0.321055	N	-2.157386	-1.479796	0.853003
Cl	-0.827679	0.145679	2.354535	Cl	-1.382590	-1.110486	-2.728031
Ru	-0.672580	0.264837	0.053491	Ru	-0.773139	0.234113	-0.975389
H	1.525061	4.840743	0.516529	H	1.475109	4.043167	1.236331
O	-0.074320	2.568450	0.298989	O	-0.121378	2.136241	0.085449
H	-0.270676	4.391175	1.289133	H	-0.133667	4.190248	-0.342020
C	-2.130221	3.317947	1.372884	C	-2.131797	3.542582	0.187420
H	-2.774968	2.664588	0.750578	H	-2.815089	2.678722	0.055213
H	-1.857123	2.767561	2.292707	H	-1.977993	3.711616	1.270916
H	-2.721223	4.212688	1.655782	H	-2.630547	4.439887	-0.231953
C	-1.194135	4.521191	-0.683347	C	-0.922247	3.074223	-2.027158
H	-1.822975	3.902979	-1.356070	H	-1.561063	2.179612	-2.245690
H	-1.752575	5.451989	-0.456270	H	-1.427115	3.923418	-2.531654
H	-0.271448	4.804970	-1.227846	H	0.069743	2.938538	-2.502016
N	5.545918	2.628789	-0.268267	N	5.530918	2.064664	0.026093
O	6.074452	1.542278	-0.510414	O	6.121144	3.011624	0.542333
O	6.129603	3.705487	-0.144299	O	6.058342	1.080411	-0.496268

15-trans				15-cis		
-2552.88019889				-2552.88363035		
Ru	-0.508949	0.588053	0.182310	Ru	0.590652	0.263408
Cl	-0.727794	0.580850	2.538273	Cl	0.590145	-1.309113
Cl	-1.137401	1.115059	-2.024211	Cl	1.503546	1.888032
O	-0.334206	2.742484	0.406496	O	0.656588	1.781393
O	0.570151	4.793850	0.404176	O	0.091245	3.780040
O	5.997822	1.774281	-0.634058	O	-5.673402	2.445273
N	-2.311016	-1.752355	0.129093	N	2.121166	-1.697678
N	-0.240238	-2.494200	0.256884	N	-0.002801	-2.298537
C	-0.989647	-1.345360	0.124715	C	0.848523	-1.332356
C	-2.478343	-3.184655	0.438930	C	2.183794	-3.049228
H	-2.854039	-3.314232	1.479042	H	2.608810	-3.773215
H	-3.212916	-3.653480	-0.248083	H	2.827729	-3.057057
C	-1.056075	-3.727457	0.265375	C	0.704075	-3.336743
H	-0.920944	-4.284116	-0.690943	H	0.461560	-3.229473
H	-0.742112	-4.400170	1.090019	H	0.387227	-4.351519
C	-3.489958	-0.955330	-0.102364	C	3.295426	-0.885493
C	-4.246545	-0.450820	0.989324	C	4.148739	-1.097277
C	-5.403789	0.304381	0.702774	C	5.289505	-0.277382
H	-5.981230	0.718549	1.546658	H	5.946793	-0.422851
C	-5.852421	0.524481	-0.611902	C	5.613789	0.710480
C	-5.131067	-0.073931	-1.664587	C	4.771982	0.855464
H	-5.491342	0.041657	-2.700796	H	5.026812	1.598804
C	-3.962927	-0.824453	-1.438980	C	3.617899	0.069070
C	-3.903874	-0.769295	2.425542	C	3.870859	-2.168622
H	-4.319152	-1.761645	2.713421	H	3.967058	-3.186818
H	-2.811142	-0.779883	2.604707	H	2.843244	-2.076057
H	-4.350291	-0.022861	3.112139	H	4.591216	-2.102217
C	-7.071330	1.374574	-0.892545	C	6.819969	1.602363
H	-7.666412	0.970801	-1.737592	H	7.213453	1.972404
H	-7.733991	1.448864	-0.006729	H	7.640263	1.076611
H	-6.776137	2.410304	-1.171319	H	6.557893	2.493938
C	-3.251616	-1.484377	-2.595835	C	2.753271	0.229625
H	-2.303056	-0.949659	-2.817113	H	1.762852	0.655512
H	-2.997557	-2.543299	-2.378499	H	2.565602	-0.741519
H	-3.881198	-1.463778	-3.507232	H	3.235526	0.903130
C	1.179207	-2.674109	0.150964	C	-1.438976	-2.305426
C	1.940905	-2.846663	1.335451	C	-2.117070	-3.151903
C	3.317626	-3.121061	1.205665	C	-3.524669	-3.205749
H	3.918635	-3.250271	2.121708	H	-4.058475	-3.857122
C	3.941622	-3.241890	-0.052749	C	-4.262935	-2.461582
C	3.154211	-3.053564	-1.207784	C	-3.554912	-1.632422
H	3.624474	-3.133082	-2.202742	H	-4.111200	-1.038580
C	1.774924	-2.772796	-1.134379	C	-2.149575	-1.545144
C	1.298023	-2.712377	2.695190	C	-1.358880	-3.956323
H	2.055636	-2.777767	3.500558	H	-2.053605	-4.489477
H	0.755303	-1.747333	2.793323	H	-0.699513	-3.294033
H	0.550913	-3.516075	2.876057	H	-0.706314	-4.721714
C	5.406169	-3.607828	-0.160701	C	-5.769644	-2.579199
H	5.858723	-3.228986	-1.099698	H	-6.239083	-1.634480
H	5.993468	-3.213956	0.693920	H	-6.211239	-2.851641
H	5.540148	-4.712367	-0.161245	H	-6.071823	-3.369718
C	0.967131	-2.528724	-2.387530	C	-1.420424	-0.654492

H	0.074983	-3.187686	-2.444053	H	-0.673582	-1.218765	3.317258
H	0.586238	-1.484757	-2.423455	H	-0.861613	0.144089	2.187930
H	1.576415	-2.707147	-3.295030	H	-2.125978	-0.174565	3.424544
C	1.320832	0.478817	-0.015758	C	-1.242280	0.356903	-0.930411
H	1.803607	-0.512053	-0.117860	H	-1.785585	-0.384976	-1.558170
C	2.302395	1.565102	-0.085472	C	-2.084634	1.445777	-0.431311
C	3.649587	1.160927	-0.308006	C	-3.461382	1.398585	-0.779055
H	3.846565	0.082523	-0.396604	H	-3.803755	0.539105	-1.372131
C	4.696211	2.095789	-0.415109	C	-4.353772	2.419890	-0.403424
C	4.414141	3.479457	-0.291742	C	-3.876796	3.524280	0.349478
H	5.242497	4.198301	-0.376253	H	-4.585417	4.317585	0.629853
C	3.104631	3.895331	-0.067063	C	-2.533079	3.587828	0.703762
H	2.881195	4.966754	0.033086	H	-2.161098	4.443738	1.284211
C	2.037971	2.968945	0.038217	C	-1.617673	2.568165	0.333585
C	0.674472	3.455790	0.289647	C	-0.221594	2.659707	0.764522
C	-0.751138	5.310111	0.650285	C	1.476041	3.965262	1.788137
C	6.351651	0.403775	-0.773146	C	-6.210926	1.392343	-1.513165
H	5.834487	-0.068736	-1.637859	H	-6.110857	0.405398	-1.009563
H	7.443814	0.382899	-0.947463	H	-7.283998	1.624523	-1.647271
H	6.117389	-0.177324	0.146356	H	-5.721308	1.340437	-2.510898
H	-1.439514	5.027741	-0.171482	H	2.119477	3.832717	0.895550
H	-0.636633	6.407810	0.702920	H	1.548517	4.996717	2.177828
H	-1.153972	4.913919	1.604129	H	1.787028	3.240993	2.567832

15-trans <sup>+</sup>				15-cis <sup>+</sup> t			
-2092.46032948				-2092.46711267			
Ru	-0.799851	0.303073	-0.219076	Ru	-0.454147	0.274834	-0.752298
Cl	-0.772914	0.584934	2.083922	Cl	-0.742074	-0.477388	-2.891204
N	0.132625	-2.695810	-0.093449	N	-0.167491	-2.345343	0.759148
N	-2.027013	-2.223902	-0.127461	N	-2.232018	-1.562598	0.548496
O	-1.181724	2.426348	-0.327063	O	-0.692827	1.725963	0.697842
O	-0.753821	4.537485	0.295677	O	-0.285471	3.806691	1.437326
O	5.297501	2.888692	-0.025186	O	5.464566	3.013365	-0.965818
C	-0.764135	-1.682635	-0.113501	C	-0.916513	-1.313750	0.283014
C	-0.532937	-4.023489	-0.006216	C	-1.004128	-3.335274	1.484662
C	-2.019814	-3.696277	-0.263170	C	-2.438782	-2.914725	1.111701
C	-3.148890	-1.347590	-0.237752	C	-3.320849	-0.679954	0.210114
C	-4.251365	-1.449471	0.652569	C	-3.744062	0.270425	1.182963
C	-5.281895	-0.497681	0.541225	C	-4.821054	1.115497	0.861810
C	-5.248983	0.572647	-0.380507	C	-5.496554	1.031918	-0.375512
C	-4.138269	0.665353	-1.234117	C	-5.087177	0.040479	-1.287607
C	-3.089119	-0.285339	-1.199891	C	-4.021419	-0.842849	-1.016415
C	-4.306852	-2.500326	1.736196	C	-3.093504	0.334183	2.546193
C	-6.378408	1.573976	-0.436038	C	-6.626554	1.977173	-0.709972
C	-2.013593	-0.237888	-2.266787	C	-3.724644	-1.969494	-1.977938
C	1.568871	-2.610930	-0.007452	C	1.261367	-2.499373	0.725481
C	2.192347	-2.515936	1.263693	C	2.044810	-1.991914	1.794409
C	3.601828	-2.507626	1.302509	C	3.438852	-2.193177	1.747066
C	4.390607	-2.606490	0.138186	C	4.060387	-2.889198	0.689980
C	3.731016	-2.696465	-1.105874	C	3.245448	-3.382285	-0.351225
C	2.325817	-2.708971	-1.204290	C	1.847217	-3.208350	-0.356284
C	1.389115	-2.429689	2.539979	C	1.416905	-1.258572	2.958507
C	5.898610	-2.669831	0.224902	C	5.551024	-3.138796	0.691795
C	1.651881	-2.814874	-2.554601	C	1.006186	-3.747486	-1.489939
C	1.000237	0.628892	-0.577389	C	1.378736	0.337280	-0.546888
C	1.721636	1.864877	-0.304076	C	2.080537	1.594411	-0.338042
C	1.112231	3.115292	0.053370	C	1.469903	2.750835	0.267764
C	1.943009	4.217440	0.369903	C	2.248053	3.928112	0.434914
C	3.331895	4.114523	0.347143	C	3.569013	3.988467	0.009546
C	3.950320	2.891402	-0.020192	C	4.186453	2.851165	-0.584380
C	3.140144	1.784717	-0.354138	C	3.444437	1.660620	-0.729616
C	5.997707	1.703842	-0.405637	C	6.163624	1.929556	-1.585127
C	-0.347526	3.300113	0.004043	C	0.107282	2.708261	0.795021
C	-2.173686	4.797014	0.287193	C	-1.626060	3.860210	1.972386
H	-0.106992	-4.723450	-0.752674	H	-0.753695	-4.364476	1.159276
H	-0.361945	-4.459049	1.002015	H	-0.808148	-3.266076	2.577305
H	-2.353793	-3.986126	-1.284044	H	-2.893509	-3.582154	0.346932
H	-2.691902	-4.185983	0.466726	H	-3.123050	-2.876637	1.982958
H	-5.059296	-2.232222	2.502173	H	-3.577578	1.104355	3.177762
H	-4.592044	-3.499397	1.340021	H	-3.182894	-0.632995	3.085817
H	-3.326083	-2.603870	2.244665	H	-2.012264	0.569954	2.477960
H	-0.906905	0.104155	-2.044767	H	-2.675691	-2.314362	-1.924230
H	-1.835274	-1.233830	-2.720763	H	-4.387761	-2.837709	-1.766585
H	-2.282915	0.488319	-3.058177	H	-3.920212	-1.661779	-3.023654
H	2.399212	-2.905084	-3.366144	H	1.630533	-4.300108	-2.217857
H	0.983487	-3.699593	-2.620816	H	0.221594	-4.445552	-1.127756
H	1.023965	-1.924400	-2.774034	H	0.484822	-2.932693	-2.036031
H	0.750400	-1.520447	2.565089	H	0.672175	-0.506874	2.624961

H	0.713830	-3.303499	2.663680	H	0.890455	-1.956153	3.646352
H	2.056333	-2.404305	3.422780	H	2.186942	-0.736795	3.559169
H	6.286544	-2.105507	1.096748	H	6.098508	-2.366133	1.267764
H	6.238603	-3.721807	0.346467	H	5.782991	-4.119393	1.162557
H	6.383617	-2.280102	-0.692630	H	5.964877	-3.170964	-0.336232
H	-6.181715	2.377728	-1.171973	H	-6.246574	2.867785	-1.257417
H	-7.333764	1.082956	-0.718523	H	-7.382920	1.496470	-1.362040
H	-6.543465	2.047755	0.554519	H	-7.137509	2.346331	0.201614
H	-4.087345	1.480790	-1.973350	H	-5.628570	-0.069141	-2.241856
H	-6.135313	-0.574571	1.235513	H	-5.161144	1.849630	1.611416
H	4.327364	-2.777621	-2.030044	H	3.711001	-3.931415	-1.186506
H	4.098039	-2.436358	2.284662	H	4.057419	-1.798665	2.570463
H	1.648419	-0.168989	-1.001256	H	2.015591	-0.559144	-0.695292
H	3.592321	0.822026	-0.633106	H	3.898401	0.763411	-1.172911
H	7.073041	1.946826	-0.328229	H	7.175816	2.310664	-1.810985
H	5.762348	0.857473	0.275572	H	6.244107	1.057938	-0.900291
H	5.762409	1.413552	-1.452908	H	5.668571	1.619328	-2.530614
H	3.973615	4.971267	0.601027	H	4.166186	4.905108	0.125239
H	1.474502	5.175994	0.632489	H	1.789601	4.804844	0.913213
H	-2.697066	4.097793	0.968376	H	-1.729064	3.152895	2.818599
H	-2.580110	4.687870	-0.738017	H	-1.759073	4.898064	2.324264
H	-2.284875	5.838915	0.634850	H	-2.369379	3.612403	1.189651

16-trans			16-cis				
-2380.17242034			-2380.17908706				
C	0.518034	-1.390054	0.131766	C	0.163991	-1.192363	-0.449460
C	0.408071	-3.760214	0.382614	C	-0.499483	-2.864179	-1.986977
H	0.273548	-4.364245	-0.544054	H	-0.828174	-2.522105	-2.994820
H	0.009959	-4.356268	1.229438	H	-0.975407	-3.846730	-1.794052
C	1.859215	-3.308379	0.592438	C	1.031237	-2.903114	-1.841809
H	2.192836	-3.432166	1.647118	H	1.382136	-3.818611	-1.315476
H	2.582839	-3.845170	-0.055421	H	1.564471	-2.843220	-2.813007
C	-2.570892	-2.563188	1.236644	C	-3.063508	-2.484871	0.067407
C	-3.961830	-2.683811	1.043256	C	-4.450398	-2.246952	0.175726
H	-4.618048	-2.696998	1.929964	H	-5.045713	-2.905303	0.830420
C	-4.534474	-2.784294	-0.240982	C	-5.093762	-1.207255	-0.521560
C	-3.673788	-2.749290	-1.357143	C	-4.310510	-0.387342	-1.360794
H	-4.101385	-2.815358	-2.372003	H	-4.792764	0.426792	-1.928019
C	-2.276315	-2.627296	-1.220166	C	-2.924593	-0.580666	-1.506601
C	-1.737228	-2.532321	0.089533	C	-2.305187	-1.623389	-0.766516
C	-1.987950	-2.438111	2.624234	C	-2.417818	-3.619542	0.823451
H	-2.788166	-2.415717	3.389760	H	-3.148495	-4.114729	1.492513
H	-1.376480	-1.514981	2.722946	H	-1.564012	-3.250959	1.434891
H	-1.318528	-3.291812	2.868070	H	-2.019966	-4.398933	0.136322
C	-6.027735	-2.955490	-0.414109	C	-6.582925	-0.975275	-0.389598
H	-6.595122	-2.428577	0.379982	H	-7.051009	-1.702442	0.303000
H	-6.315068	-4.029080	-0.359925	H	-7.094831	-1.064436	-1.371889
H	-6.373640	-2.575495	-1.396699	H	-6.802013	0.044991	-0.007866
C	-1.387152	-2.536127	-2.438819	C	-2.120538	0.297328	-2.436955
H	-1.965744	-2.711058	-3.366850	H	-2.758522	1.073814	-2.901626
H	-0.560822	-3.277263	-2.410141	H	-1.654193	-0.289069	-3.258136
H	-0.909195	-1.534979	-2.512129	H	-1.294927	0.806316	-1.898557
C	3.042662	-1.165942	0.043132	C	2.626284	-1.172828	-0.867214
C	3.763237	-0.653808	1.154958	C	3.523438	-1.724506	0.086799
C	4.986679	0.005156	0.906537	C	4.816307	-1.166799	0.170507
H	5.540508	0.422866	1.764503	H	5.511690	-1.574850	0.922769
C	5.529654	0.122560	-0.385766	C	5.245155	-0.118807	-0.665719
C	4.829451	-0.475258	-1.453164	C	4.346652	0.362045	-1.640804
H	5.255954	-0.434708	-2.469672	H	4.673651	1.155434	-2.334404
C	3.598619	-1.130186	-1.266458	C	3.042602	-0.152921	-1.765983
C	3.305795	-0.864697	2.579341	C	3.135434	-2.885379	0.967511
H	3.809552	-0.153364	3.263575	H	3.923577	-3.087616	1.718424
H	3.569990	-1.888604	2.928179	H	3.000986	-3.815283	0.371680
H	2.212128	-0.729693	2.695805	H	2.182303	-2.694489	1.509599
C	6.824453	0.865467	-0.628953	C	6.623561	0.482892	-0.511330
H	7.448749	0.359160	-1.394012	H	6.970927	0.962811	-1.448618
H	7.424570	0.961450	0.298353	H	7.372052	-0.279470	-0.213782
H	6.627965	1.894484	-1.003224	H	6.625568	1.264071	0.280541
C	2.902850	-1.786659	-2.434618	C	2.118356	0.348629	-2.853035
H	3.561342	-1.804477	-3.325279	H	2.589655	1.169603	-3.428077
H	1.982252	-1.222683	-2.695917	H	1.159611	0.723436	-2.440101
H	2.606239	-2.833005	-2.209236	H	1.861258	-0.457656	-3.574156
C	-1.717246	0.610087	-0.266973	C	-1.443493	0.555736	1.294978
H	-2.329501	-0.292521	-0.451271	H	-2.146869	-0.051407	1.902817
C	-2.396713	1.895164	-0.315587	C	-1.868374	1.857542	0.792163
C	-3.758366	2.124003	-0.574155	C	-3.131667	2.458172	0.906455
H	-4.425505	1.268981	-0.768521	H	-3.949315	1.912928	1.403604

C	-4.274090	3.447445	-0.584183	C	-3.351841	3.764459	0.393577
H	-5.344850	3.604532	-0.790332	H	-4.350964	4.218651	0.488933
C	-3.455045	4.549301	-0.336743	C	-2.323787	4.488624	-0.209461
H	-3.871377	5.569352	-0.345704	H	-2.503356	5.509495	-0.582908
C	-2.062634	4.366264	-0.067105	C	-1.014584	3.924692	-0.330797
C	-1.125603	5.407870	0.203781	C	0.123561	4.593688	-0.873246
H	-1.460846	6.457625	0.216009	H	0.026005	5.620708	-1.259857
C	0.203626	5.079496	0.449877	C	1.350560	3.937630	-0.876819
H	0.951351	5.858160	0.662620	H	2.256678	4.429855	-1.260818
C	0.611601	3.719163	0.425882	C	1.455753	2.615191	-0.375680
H	1.658121	3.430016	0.613610	H	2.417995	2.081274	-0.357654
C	-1.557940	3.029267	-0.065379	C	-0.820352	2.597153	0.157293
N	-0.313468	-2.474558	0.261742	N	-0.903758	-1.877442	-0.958587
N	1.802888	-1.875238	0.238597	N	1.297447	-1.704800	-1.021580
N	-0.245297	2.726828	0.174901	N	0.395272	1.944310	0.102121
Cl	0.183202	0.683910	2.445649	Cl	0.144230	-1.808183	2.523905
Cl	0.996209	1.014818	-2.056580	Cl	1.784206	1.118580	2.652993
Ru	0.104860	0.600166	0.082669	Ru	0.338077	0.105463	1.088507

16-trans <sup>+</sup>				16-cis <sup>+</sup> t			
-1919.75354200				-1919.76007037			
C	-0.327651	-1.609202	-0.181582	C	-0.250486	-1.144673	0.419015
C	-1.473425	-3.661319	-0.316953	C	0.305798	-2.747916	2.054019
H	-2.139483	-4.042139	-1.116605	H	0.574189	-2.368466	3.064582
H	-1.810051	-4.106176	0.644320	H	0.788105	-3.737266	1.925543
C	0.022578	-3.923949	-0.599302	C	-1.215978	-2.784845	1.815340
H	0.440711	-4.720412	0.044929	H	-1.546692	-3.716870	1.306046
H	0.217097	-4.202391	-1.658708	H	-1.805727	-2.677374	2.747661
C	-3.355002	-1.305817	1.216212	C	2.836978	-2.463753	-0.173326
C	-4.616855	-0.685956	1.315137	C	4.227068	-2.317814	-0.341019
H	-5.035318	-0.507021	2.319500	H	4.737662	-2.953550	-1.083355
C	-5.359181	-0.297735	0.180741	C	4.984225	-1.397170	0.416461
C	-4.801542	-0.540090	-1.091884	C	4.307171	-0.597326	1.359942
H	-5.365543	-0.248157	-1.993392	H	4.880497	0.125243	1.964143
C	-3.543454	-1.154362	-1.250491	C	2.917330	-0.700188	1.568625
C	-2.827096	-1.522395	-0.082915	C	2.191542	-1.634565	0.783551
C	-2.595807	-1.709607	2.458051	C	2.057521	-3.454450	-1.005688
H	-3.177046	-1.471363	3.369312	H	2.732244	-4.040588	-1.658200
H	-1.616942	-1.188389	2.528578	H	1.312303	-2.945178	-1.654268
H	-2.386026	-2.800806	2.477852	H	1.495257	-4.175564	-0.374937
C	-6.728937	0.323743	0.327394	C	6.482091	-1.304565	0.243367
H	-6.788664	0.977368	1.220956	H	6.779313	-1.405982	-0.820197
H	-7.505657	-0.462652	0.450219	H	6.990808	-2.123394	0.797853
H	-7.008579	0.922010	-0.562468	H	6.885380	-0.347834	0.629838
C	-2.969723	-1.384686	-2.631086	C	2.227489	0.164629	2.599053
H	-3.687482	-1.077709	-3.415871	H	2.931359	0.896871	3.039361
H	-2.719749	-2.451929	-2.810762	H	1.818148	-0.438534	3.437920
H	-2.034170	-0.804889	-2.787175	H	1.376113	0.727395	2.161339
C	1.989638	-2.226268	-0.360272	C	-2.729727	-1.077156	0.647569
C	2.954713	-2.862169	0.468391	C	-3.523344	-1.618182	-0.400376
C	4.282786	-2.402768	0.412546	C	-4.796492	-1.051338	-0.621365
H	5.028796	-2.895139	1.058514	H	-5.413515	-1.454903	-1.441304
C	4.694397	-1.321229	-0.399991	C	-5.312736	-0.015930	0.181635
C	3.718761	-0.691309	-1.188448	C	-4.522906	0.446438	1.257677
H	4.010028	0.138701	-1.853060	H	-4.929029	1.222728	1.927736
C	2.368891	-1.126328	-1.198255	C	-3.240322	-0.071417	1.518251
C	2.569759	-3.955521	1.435765	C	-3.092648	-2.821463	-1.205202
H	3.362465	-4.106653	2.193186	H	-3.429324	-2.740586	-2.257085
H	2.417723	-4.933174	0.928558	H	-3.554912	-3.742276	-0.785819
H	1.631335	-3.699961	1.969830	H	-1.996179	-2.959409	-1.217591
C	6.138591	-0.878710	-0.418227	C	-6.674401	0.575049	-0.098566
H	6.794113	-1.679624	-0.821583	H	-7.068056	1.135464	0.772067
H	6.504038	-0.653033	0.605507	H	-7.410223	-0.209971	-0.366852
H	6.286863	0.023084	-1.043801	H	-6.630589	1.279788	-0.957571
C	1.407549	-0.522243	-2.202015	C	-2.455575	0.390412	2.726545
H	1.965117	0.065196	-2.958924	H	-2.893991	1.309014	3.163145
H	0.619392	0.305730	-1.903184	H	-1.390964	0.590897	2.490124
H	0.786846	-1.285195	-2.710873	H	-2.466486	-0.380302	3.528382
C	-1.011087	1.279790	-0.351804	C	1.522600	0.534144	-1.118500
H	-2.031514	0.883503	-0.535188	H	2.327962	-0.160472	-1.431003
C	-0.846124	2.719618	-0.314311	C	1.860874	1.913519	-0.809762
C	-1.864608	3.677791	-0.460504	C	3.095891	2.556719	-0.989945
H	-2.898263	3.347830	-0.650711	H	3.951591	1.993399	-1.393892

C	-1.569217	5.061490	-0.351273	C	3.234616	3.932735	-0.666237
H	-2.379697	5.797151	-0.468296	H	4.206143	4.427318	-0.818730
C	-0.272190	5.501072	-0.088709	C	2.159823	4.666713	-0.165456
H	-0.057900	6.577612	0.003515	H	2.282231	5.733294	0.080769
C	0.796925	4.563668	0.073875	C	0.882418	4.050882	0.035822
C	2.147974	4.908304	0.373044	C	-0.282855	4.715598	0.518761
H	2.433471	5.966379	0.484923	H	-0.242924	5.785587	0.776293
C	3.086245	3.894224	0.534100	C	-1.465859	3.992177	0.641273
H	4.133590	4.121822	0.781218	H	-2.390327	4.470316	0.996796
C	2.689937	2.539892	0.383361	C	-1.501068	2.617298	0.300594
H	3.411373	1.718031	0.516633	H	-2.433048	2.034179	0.377362
C	0.491081	3.174067	-0.056104	C	0.765095	2.666370	-0.281453
N	-1.551186	-2.177787	-0.233778	N	0.783226	-1.802358	1.012885
N	0.613898	-2.599991	-0.304473	N	-1.425020	-1.618468	0.929483
N	1.435416	2.187792	0.079768	N	-0.416212	1.956972	-0.143074
Cl	0.681022	0.114064	2.242167	Cl	-0.602901	-1.156354	-2.982211
Ru	0.507893	0.216164	-0.068667	Ru	-0.290381	0.105282	-1.092892

17-trans			17-cis				
-2058.16201024			-2058.15686487				
C	0.000335	-0.783146	0.019850	C	0.000700	-0.612988	0.231726
C	0.772945	-3.007270	0.087041	C	-0.767687	-2.635704	1.248358
H	1.173760	-3.461120	1.018764	H	-1.268904	-3.496924	0.757563
H	1.233790	-3.539588	-0.771733	H	-1.123632	-2.596795	2.300953
C	-0.770662	-3.008804	0.037448	C	0.765198	-2.687729	1.146520
H	-1.171553	-3.497110	-0.876709	H	1.257608	-2.810209	2.133649
H	-1.230603	-3.508973	0.915733	H	1.129361	-3.507619	0.487885
C	3.151098	-0.985232	-1.223554	C	-3.341396	-0.561273	1.255399
C	4.495757	-0.568136	-1.209277	C	-4.698548	-0.359962	0.920704
H	5.020807	-0.455207	-2.172833	H	-5.363477	0.085670	1.679653
C	5.187209	-0.304290	-0.009294	C	-5.228850	-0.712991	-0.332940
C	4.504283	-0.497916	1.206349	C	-4.361960	-1.312924	-1.270805
H	5.036408	-0.329007	2.157535	H	-4.759409	-1.628432	-2.250450
C	3.157877	-0.915085	1.254965	C	-3.000124	-1.527481	-0.992049
C	2.481180	-1.118450	0.023492	C	-2.485027	-1.107448	0.266492
C	2.455199	-1.277331	-2.530125	C	-2.861800	-0.250999	2.653027
H	3.174968	-1.260492	-3.371700	H	-3.443734	0.581909	3.095086
H	1.662046	-0.522786	-2.732317	H	-1.792476	0.034977	2.674490
H	1.964177	-2.273796	-2.526996	H	-3.004154	-1.132384	3.318276
C	6.623868	0.167773	-0.036025	C	-6.677723	-0.448390	-0.675252
H	7.078758	0.157139	0.974363	H	-7.105557	-1.259051	-1.300264
H	6.694812	1.207511	-0.423302	H	-6.783126	0.496310	-1.252970
H	7.248257	-0.464623	-0.701527	H	-7.302354	-0.346845	0.234710
C	2.476655	-1.136529	2.583282	C	-2.110806	-2.203430	-2.012161
H	3.200261	-1.040208	3.416144	H	-2.686811	-2.490025	-2.913631
H	2.019549	-2.146804	2.652196	H	-1.641083	-3.124458	-1.605164
H	1.660068	-0.396947	2.742928	H	-1.275477	-1.547526	-2.336823
C	-2.480132	-1.120010	0.012799	C	2.482445	-1.108290	0.259230
C	-3.139705	-0.964860	-1.236066	C	3.352293	-0.609231	1.262626
C	-4.486367	-0.549983	-1.223858	C	4.707713	-0.406275	0.926374
H	-5.004768	-0.421269	-2.188930	H	5.382531	0.002035	1.697468
C	-5.187438	-0.310083	-0.025589	C	5.224461	-0.711940	-0.346146
C	-4.513840	-0.527161	1.192617	C	4.344954	-1.264592	-1.299784
H	-5.053969	-0.379680	2.142960	H	4.731460	-1.539998	-2.295718
C	-3.167846	-0.941280	1.243093	C	2.982785	-1.481154	-1.019051
C	-2.436864	-1.235468	-2.543753	C	2.880316	-0.353081	2.673730
H	-3.148718	-1.182707	-3.390520	H	3.519037	0.401119	3.174324
H	-1.967087	-2.242080	-2.563180	H	2.942774	-1.283772	3.282007
H	-1.626895	-0.492860	-2.721880	H	1.834121	0.009161	2.701919
C	-6.619800	0.174766	-0.046735	C	6.672342	-0.440149	-0.687203
H	-7.178463	-0.155770	0.852344	H	7.054153	-1.147691	-1.451043
H	-7.162050	-0.185932	-0.944311	H	7.324120	-0.510734	0.207029
H	-6.661616	1.286349	-0.065873	H	6.796493	0.585224	-1.100377
C	-2.493184	-1.185731	2.570465	C	2.086638	-2.119894	-2.058111
H	-3.223256	-1.119551	3.400651	H	2.606570	-2.207439	-3.032157
H	-1.689261	-0.437047	2.750553	H	1.152001	-1.543406	-2.215812
H	-2.020353	-2.189967	2.617792	H	1.776208	-3.144825	-1.757758
C	1.348684	2.670396	-0.008259	C	-1.380047	1.425546	-1.595372
H	1.943039	2.759812	-0.936389	H	-1.912773	2.391532	-1.677545
C	-0.001889	3.501859	-0.041126	C	-0.020922	1.424355	-2.417727
H	0.010250	4.086848	-0.980811	H	-0.030176	2.382980	-2.974507
N	1.108462	-1.565207	0.036351	N	-1.099917	-1.372408	0.554654

N	-1.107266	-1.566020	0.034258	N	1.099661	-1.370783	0.562240
Cl	0.032264	1.299884	-2.418734	Cl	0.039442	1.686768	2.109045
Cl	-0.034234	1.356469	2.396739	Cl	-0.006638	3.819782	-0.357718
Ru	-0.000630	1.228244	-0.009550	Ru	0.001960	1.402139	-0.179203
H	1.913234	2.787007	0.935361	H	-2.013685	0.542073	-1.778699
C	-1.351640	2.668276	-0.044802	C	1.353998	1.435249	-1.623004
H	-1.941114	2.782972	0.883682	H	1.990888	0.556690	-1.818046
H	-1.921324	2.757888	-0.988264	H	1.877712	2.405352	-1.714528
H	-0.014669	4.118002	0.878486	H	-0.024039	0.524641	-3.062885

17-trans <sup>+</sup>			17-cis <sup>t</sup>				
-1597.73007616			-1597.74702201				
C	0.000039	-0.791645	-0.068973	C	0.003437	-0.568116	0.257474
C	0.775712	-2.997872	-0.147750	C	-0.764299	-2.763591	0.810474
H	1.204573	-3.524473	0.729390	H	-1.264535	-3.498112	0.144110
H	1.212057	-3.451081	-1.062022	H	-1.121074	-2.954109	1.846129
C	-0.775861	-2.997698	-0.149995	C	0.768699	-2.791487	0.701152
H	-1.209587	-3.448536	-1.066733	H	1.260442	-3.124908	1.638655
H	-1.207476	-3.526418	0.724477	H	1.133942	-3.448805	-0.119315
C	3.015217	-0.653287	-1.377777	C	-3.339474	-0.741419	1.264994
C	4.334748	-0.164158	-1.394959	C	-4.696512	-0.473013	0.980715
H	4.775373	0.136567	-2.359971	H	-5.362334	-0.202959	1.817658
C	5.112262	-0.064997	-0.221230	C	-5.225609	-0.545991	-0.320132
C	4.527674	-0.463991	0.998352	C	-4.357581	-0.927759	-1.365020
H	5.118839	-0.395162	1.926329	H	-4.754061	-1.023472	-2.390134
C	3.209622	-0.955258	1.077995	C	-2.995807	-1.196960	-1.138217
C	2.460596	-1.032551	-0.125934	C	-2.481967	-1.059643	0.181931
C	2.224541	-0.771231	-2.661678	C	-2.861163	-0.741436	2.697078
H	2.814504	-0.411598	-3.526395	H	-3.444021	-0.024547	3.308753
H	1.282053	-0.180500	-2.632082	H	-1.792058	-0.466365	2.781019
H	1.930525	-1.820895	-2.876363	H	-3.003403	-1.746208	3.155184
C	6.542935	0.416144	-0.274887	C	-6.674406	-0.214197	-0.598201
H	6.834774	0.941916	0.656043	H	-7.101192	-0.870212	-1.384554
H	6.717621	1.097168	-1.131356	H	-6.780035	0.833268	-0.957349
H	7.238644	-0.443400	-0.394029	H	-7.299803	-0.312772	0.311561
C	2.620971	-1.361839	2.408448	C	-2.105235	-1.635083	-2.279861
H	3.381432	-1.301980	3.210130	H	-2.680351	-1.719621	-3.222550
H	2.234588	-2.402906	2.396996	H	-1.635174	-2.622218	-2.081909
H	1.774962	-0.700189	2.693262	H	-1.270122	-0.923937	-2.453775
C	-2.460527	-1.032334	-0.126020	C	2.485509	-1.056295	0.179117
C	-3.014945	-0.652439	-1.377765	C	3.354239	-0.786305	1.267653
C	-4.334528	-0.163412	-1.394884	C	4.709772	-0.514538	0.984646
H	-4.775006	0.137829	-2.359803	H	5.383714	-0.282851	1.826552
C	-5.112266	-0.064984	-0.221252	C	5.227706	-0.536638	-0.323415
C	-4.527854	-0.464555	0.998234	C	4.349316	-0.869742	-1.375012
H	-5.119195	-0.396290	1.926140	H	4.736776	-0.922365	-2.406625
C	-3.209774	-0.955720	1.077821	C	2.987086	-1.142753	-1.149158
C	-2.224229	-0.769820	-2.661702	C	2.881006	-0.842578	2.700299
H	-2.812967	-0.406720	-3.525807	H	3.518813	-0.214582	3.353138
H	-1.933245	-1.819892	-2.878604	H	2.943656	-1.883018	3.092278
H	-1.280041	-0.181920	-2.630629	H	1.834535	-0.495621	2.805450
C	-6.542991	0.416007	-0.274882	C	6.675655	-0.196584	-0.596100
H	-7.238586	-0.443637	-0.393965	H	7.058547	-0.721400	-1.494882
H	-6.717766	1.097008	-1.131348	H	7.326800	-0.459112	0.262117
H	-6.834891	0.941748	0.656048	H	6.799398	0.894062	-0.776916
C	-2.621198	-1.362827	2.408143	C	2.092182	-1.541376	-2.302831
H	-3.382140	-1.304959	3.209516	H	2.612919	-1.415288	-3.272210
H	-1.776352	-0.700139	2.694005	H	1.157260	-0.944894	-2.332573
H	-2.233090	-2.403230	2.395799	H	1.782246	-2.607216	-2.232221
C	1.301476	2.619718	-0.487037	C	-1.377352	1.817473	-1.085194
H	1.659859	2.539696	-1.536697	H	-1.910696	2.778007	-0.956360
C	0.000234	3.498461	-0.313767	C	-0.017600	1.995395	-1.887009
H	0.000554	4.200787	-1.173793	H	-0.027105	3.051961	-2.222610
N	1.111601	-1.549558	-0.089086	N	-1.096890	-1.380076	0.407004

N	-1.111591	-1.549465	-0.088948	N	1.102680	-1.378986	0.416736
Cl	-0.000472	1.371484	2.252531	Cl	-0.006575	3.886971	0.643551
Ru	0.000027	1.208966	-0.008222	Ru	0.003590	1.488170	0.293423
H	2.113251	2.837883	0.232268	H	-2.010227	0.994467	-1.456355
C	-1.300955	2.619822	-0.487958	C	1.356706	1.834367	-1.107610
H	-2.113284	2.838082	0.230690	H	1.994363	1.019363	-1.488001
H	-1.658506	2.539741	-1.537900	H	1.879805	2.801500	-0.986064
H	-0.000093	4.041709	0.648121	H	-0.019591	1.257038	-2.711963

18-trans				18-trans <sup>+</sup>			
-1828.90314270				1482.37911979			
Ru	0.108072	0.420041	-0.289014	Ru	0.366466	0.393001	0.085571
O	0.264515	2.798988	-0.394118	O	0.480894	2.677669	0.339054
O	1.998771	0.066146	1.173636	N	1.307977	-2.277158	-0.340071
O	0.005881	0.626082	1.939174	N	-0.913812	-2.347843	-0.277717
N	0.952635	-2.301277	-0.823862	C	0.165563	-1.517022	-0.178666
N	-1.248557	-2.310619	-0.526005	C	0.983026	-3.638678	-0.816233
C	-0.133956	-1.489326	-0.494456	C	-0.488658	-3.766167	-0.394799
C	0.514973	-3.609665	-1.344456	C	2.596103	-1.658574	-0.363049
C	-0.893232	-3.723018	-0.763294	C	3.719394	-2.279524	0.250573
C	2.240515	-1.783666	-1.177941	C	4.949633	-1.593894	0.226710
C	3.417639	-2.482674	-0.808138	C	5.107754	-0.308698	-0.338532
C	4.662354	-1.958487	-1.212547	C	3.970870	0.299489	-0.895101
C	4.772141	-0.753288	-1.933081	C	2.715809	-0.355961	-0.949619
C	3.585841	-0.058623	-2.237047	C	3.629139	-3.607985	0.968279
C	2.312062	-0.547663	-1.879720	C	6.457855	0.369484	-0.346626
C	3.378800	-3.727118	0.051370	C	1.545409	0.293555	-1.611362
C	6.126880	-0.223014	-2.351096	C	-2.258807	-2.023445	0.109361
C	1.056139	0.216458	-2.168893	C	-3.318583	-2.298704	-0.795897
C	-2.594943	-2.031615	-0.107933	C	-4.638738	-2.023563	-0.384509
C	-3.614013	-1.983535	-1.096518	C	-4.937720	-1.483183	0.880607
C	-4.944572	-1.770505	-0.682597	C	-3.858995	-1.200495	1.744407
C	-5.288933	-1.618266	0.674209	C	-2.522329	-1.463321	1.391189
C	-4.256640	-1.698596	1.630359	C	-3.067792	-2.851800	-2.181556
C	-2.911725	-1.915057	1.271161	C	-6.364566	-1.233730	1.310194
C	-3.293152	-2.148887	-2.565425	C	-1.417749	-1.115042	2.362283
C	-6.723924	-1.404082	1.103347	C	-1.199374	0.918774	-0.772003
C	-1.844584	-2.012691	2.332166	C	-1.446313	2.335205	-0.968310
C	-1.560243	0.900875	-0.953379	C	-2.533944	2.838871	-1.731792
C	-1.917278	2.307222	-1.112564	C	-2.727655	4.217206	-1.878873
C	-3.192156	2.731335	-1.565246	C	-1.835531	5.114647	-1.260181
C	-3.503114	4.091456	-1.704625	C	-0.746821	4.652905	-0.493158
C	-2.533328	5.056626	-1.381134	C	-0.557002	3.271513	-0.356479
C	-1.255722	4.675177	-0.924581	C	1.204501	3.429085	1.388876
C	-0.949283	3.308960	-0.799599	C	2.446050	2.616054	1.723827
C	1.332476	3.713002	0.034086	C	0.287247	3.667603	2.585595
C	2.662112	3.008163	-0.199024	H	1.623565	-4.415442	-0.361959
C	1.092975	4.136866	1.483139	H	1.110436	-3.686972	-1.921518
C	1.237345	0.322998	2.154267	H	-1.099381	-4.317225	-1.134081
C	1.774377	0.240049	3.602368	H	-0.606262	-4.268598	0.592110
C	2.016386	-1.258854	3.914253	H	5.820183	-2.076462	0.701949
C	0.764108	0.831420	4.603679	H	4.057399	1.297094	-1.357048
C	3.119350	0.997863	3.679705	H	2.701606	-3.687998	1.572322
H	1.175929	-4.436866	-1.023483	H	4.489026	-3.737766	1.653449
H	0.507240	-3.589027	-2.459809	H	3.648258	-4.471183	0.267205
H	-1.611486	-4.211661	-1.451940	H	7.159537	-0.151822	-1.032795
H	-0.909364	-4.288183	0.198669	H	6.925819	0.355243	0.659776
H	5.579284	-2.500477	-0.923414	H	6.388022	1.423519	-0.679706
H	3.644329	0.893053	-2.792050	H	1.075046	-0.333426	-2.396347
H	2.562649	-3.672604	0.801036	H	1.783794	1.295911	-2.020956
H	4.335728	-3.853408	0.596184	H	-5.462272	-2.231664	-1.087850
H	3.225920	-4.657024	-0.542040	H	-4.065597	-0.767491	2.737457
H	6.634434	-0.915068	-3.057939	H	-2.106744	-2.494682	-2.604441
H	6.804530	-0.103785	-1.478417	H	-3.879696	-2.556525	-2.874954
H	6.043131	0.762830	-2.850692	H	-3.040899	-3.964241	-2.186230

H	0.404656	-0.342473	-2.876164	H	-6.749560	-2.085730	1.912516
H	1.275355	1.204942	-2.626432	H	-7.040866	-1.116830	0.440311
H	-5.735769	-1.717300	-1.449701	H	-6.450934	-0.326470	1.941666
H	-4.503256	-1.598609	2.701132	H	-0.892187	-0.167499	2.051960
H	-2.355052	-1.625724	-2.841996	H	-0.640435	-1.901665	2.438584
H	-4.113537	-1.756912	-3.198675	H	-1.820186	-0.923989	3.376330
H	-3.158088	-3.219209	-2.839723	H	-1.948904	0.235256	-1.225501
H	-7.133843	-2.310024	1.601657	H	-3.223171	2.121421	-2.205097
H	-7.380067	-1.173360	0.240485	H	-3.571597	4.599453	-2.472317
H	-6.810170	-0.571413	1.832452	H	-1.984022	6.200057	-1.372345
H	-1.232937	-1.084849	2.355930	H	-0.068527	5.377876	-0.022249
H	-1.146436	-2.853608	2.138609	H	1.512818	4.392955	0.930348
H	-2.294999	-2.162226	3.333196	H	2.173860	1.627665	2.156229
H	-2.385944	0.213008	-1.229060	H	3.047970	3.153819	2.483541
H	-3.941291	1.958589	-1.803394	H	3.080537	2.447447	0.832769
H	-4.499064	4.401541	-2.057109	H	-0.631430	4.217901	2.301610
H	-2.766003	6.129052	-1.478333	H	0.817769	4.268027	3.352050
H	-0.523100	5.453651	-0.672405	H	-0.010427	2.703990	3.049199
H	1.276991	4.597828	-0.636925				
H	2.711838	2.046050	0.350609				
H	3.488162	3.662953	0.146390				
H	2.815872	2.800295	-1.275555				
H	0.107907	4.629735	1.606813				
H	1.878589	4.851336	1.804526				
H	1.117631	3.254590	2.152653				
H	1.072202	-1.839893	3.858122				
H	2.427130	-1.375510	4.940018				
H	2.737685	-1.698296	3.196288				
H	0.569482	1.904250	4.399342				
H	1.156584	0.744718	5.639454				
H	-0.209816	0.305532	4.554151				
H	3.838391	0.597870	2.937705				
H	3.561740	0.896872	4.693782				
H	2.985752	2.081528	3.477314				

19-trans				19-trans <sup>+</sup>		
-1803.38947224				-1522.89704599		
Ru	7.785128	3.915335	6.098253	Ru	-0.079781	0.264588
O	6.261266	2.613778	4.930062	O	-0.854038	2.450413
O	9.391504	3.832228	4.361723	N	-0.326783	-2.566145
O	7.800048	5.288590	4.368646	N	1.825163	-2.047575
O	9.094858	5.135380	2.619372	C	0.566870	-1.538013
N	9.577831	4.188471	8.316259	C	0.302178	-3.854109
N	9.228843	6.202116	7.534453	H	-0.064429	-4.671406
N	8.782353	4.765934	3.746062	H	0.101023	-4.137714
C	8.921403	4.902950	7.354124	C	1.792553	-3.530968
C	10.199316	5.053669	9.330370	H	2.461452	-4.020745
H	11.109287	4.740773	9.565740	H	2.123054	-3.824237
H	9.647624	5.104489	10.151329	C	-1.744926	-2.203823
C	10.237811	6.392943	8.596910	C	-2.211031	-2.218589
H	9.989337	7.139808	9.198046	H	-2.148169	-3.256322
H	11.134379	6.566830	8.214121	H	-1.524182	-1.591439
C	9.033387	2.862649	8.602584	C	-3.658312	-1.694855
C	7.926355	2.979238	9.660728	H	-3.974355	-1.716097
H	8.313471	3.298362	10.513349	C	-4.589782	-2.597083
H	7.249530	3.637167	9.362600	H	-5.639841	-2.241345
C	7.260471	1.615799	9.875898	H	-4.577117	-3.636436
H	6.541886	1.696514	10.566688	C	-4.130874	-2.578413
C	8.324860	0.626290	10.348340	H	-4.798294	-3.225214
H	7.912449	-0.261577	10.495191	C	-2.682252	-3.121263
H	8.707606	0.934204	11.207884	H	-2.640593	-4.165345
C	9.435728	0.509951	9.301658	H	-2.345160	-3.144450
H	10.120470	-0.149473	9.615674	C	-4.195921	-1.127215
C	10.103576	1.887839	9.101355	H	-5.238753	-0.746883
H	10.484526	2.209703	9.956133	H	-3.908108	-1.093055
H	10.835432	1.818583	8.438824	C	-3.253459	-0.213924
C	8.817230	0.014698	7.989419	H	-3.301719	0.826291
H	8.394833	-0.869432	8.132411	C	-3.701950	-0.243997
H	9.525162	-0.089684	7.305098	H	-4.732190	0.164666
C	7.759205	1.022642	7.494166	H	-3.045779	0.409916
H	7.365665	0.700030	6.633261	C	-1.830406	-0.765128
C	6.655130	1.149444	8.547430	H	-1.590076	-0.824888
H	6.209912	0.274033	8.672605	C	3.038592	-1.286299
H	5.975960	1.801145	8.242493	C	3.261522	-0.319903
C	8.474517	2.365155	7.261973	C	4.475369	0.393354
H	9.302887	2.085143	6.776253	H	4.644571	1.135935
C	9.000045	7.290775	6.633147	C	5.480328	0.181142
C	9.907636	7.519468	5.591685	C	5.216538	-0.757852
C	9.734280	8.660941	4.812831	H	5.969535	-0.919805
H	10.332264	8.823866	4.092308	C	4.013920	-1.490071
C	8.709059	9.572474	5.058414	C	2.231179	-0.006343
C	7.822473	9.306413	6.092613	H	2.694260	0.504584
H	7.109216	9.912525	6.256487	H	1.465936	0.777406
C	7.949689	8.173411	6.897910	H	1.694686	-0.897803
C	11.072746	6.597970	5.331689	C	6.796249	0.920445
H	11.342025	6.668969	4.391911	H	7.196562	1.126226
H	10.808175	5.674976	5.526771	H	6.702802	1.884634
H	11.824441	6.850828	5.906950	H	7.562849	0.318280
C	8.616872	10.836016	4.240407	C	3.788534	-2.434090

H	7.780847	11.302620	4.452058	H	4.390195	-2.122147	3.049331
H	8.632742	10.610063	3.286556	H	4.097927	-3.475803	1.934337
H	9.377162	11.417215	4.450923	H	2.724226	-2.462614	2.483289
C	6.990723	7.948206	8.033565	C	-0.110940	0.816156	1.290699
H	6.525378	8.786498	8.239088	H	0.190584	0.191144	2.157675
H	7.486007	7.648015	8.824676	C	-0.556339	2.160156	1.615983
H	6.336884	7.264368	7.778335	C	-0.623548	2.648835	2.947749
C	6.222816	4.371575	6.951135	H	-0.326816	1.979471	3.771178
H	6.234395	4.959999	7.696625	C	-1.054873	3.954122	3.213069
C	4.958068	3.812050	6.462237	H	-1.101569	4.323811	4.248290
C	3.710960	4.155587	7.009126	C	-1.424578	4.792700	2.144984
H	3.667471	4.808035	7.698895	H	-1.763086	5.821159	2.345469
C	2.540190	3.558943	6.558473	C	-1.368535	4.343670	0.809905
H	1.703961	3.794113	6.943077	H	-1.660622	5.026379	0.000595
C	2.602775	2.625735	5.549582	C	-0.940042	3.033675	0.553889
H	1.802904	2.212194	5.247596	C	-1.003844	3.274508	-1.914206
C	3.820682	2.275720	4.960362	H	-1.858381	3.958310	-1.725320
H	3.849610	1.639216	4.255727	C	-1.376696	2.332050	-3.050696
C	4.989239	2.872116	5.418279	H	-0.577471	1.581509	-3.230656
C	6.397719	1.680072	3.803599	H	-1.506237	2.912773	-3.985870
H	5.762587	0.919256	3.935697	H	-2.325587	1.799974	-2.843955
C	7.814586	1.139978	3.802351	C	0.273966	4.071843	-2.164762
H	8.444567	1.875881	3.651982	H	0.538955	4.709007	-1.297987
H	7.910655	0.475821	3.087956	H	0.139369	4.734283	-3.043811
H	8.004709	0.719960	4.666547	H	1.127609	3.394568	-2.373672
C	6.057474	2.380351	2.506567				
H	5.149374	2.745313	2.560246				
H	6.108159	1.738865	1.766978				
H	6.693983	3.109030	2.352566				

20-trans				20-trans <sup>+</sup>			
-1327.48836413				-1098.83166389			
Ru	-0.229209	1.014014	0.262639	Ru	-0.316815	1.024344	0.148942
O	1.240278	2.327770	-0.629538	N	-0.829882	-1.528849	-1.096662
O	-0.339138	3.291295	0.592142	N	1.302945	-1.412589	-0.525096
N	-0.973042	-1.573224	-0.744818	C	0.156835	-0.691787	-0.579299
N	1.205877	-1.626947	-0.322986	C	-0.341995	-2.916231	-0.985262
C	0.093626	-0.822371	-0.287647	H	-0.793695	-3.462402	-1.822456
C	-0.629810	-2.989427	-0.904831	H	-0.562124	-3.151173	0.083058
H	-1.064808	-3.425989	-1.827990	C	1.123192	-2.734852	-1.156965
H	-0.995258	-3.590233	-0.038686	H	1.691652	-3.419151	-0.497174
C	0.911819	-2.936467	-0.944558	H	1.404786	-2.558719	-2.216366
H	1.392219	-3.766797	-0.387231	C	-2.146373	-1.198741	-0.544739
H	1.302971	-2.961473	-1.988507	C	-2.366304	-1.877044	0.795289
C	-2.306172	-1.055212	-0.414633	H	-1.522749	-1.516863	1.456656
C	-2.786703	-1.610200	0.955036	H	-2.554082	-2.945429	0.623173
H	-2.002768	-1.397685	1.712004	C	-3.637309	-1.330162	1.394465
H	-2.914530	-2.714363	0.892608	H	-3.791484	-1.839919	2.357639
C	-4.119121	-0.946387	1.363546	C	-4.794605	-1.633356	0.488856
H	-4.451049	-1.362862	2.340440	H	-4.862862	-2.712949	0.333871
C	-5.185257	-1.239093	0.284127	H	-5.686631	-1.180491	0.936397
H	-5.363706	-2.335242	0.206555	C	-4.547596	-0.952225	-0.825165
H	-6.156332	-0.775798	0.567020	H	-5.393541	-1.165413	-1.492666
C	-4.710177	-0.676016	-1.075106	C	-3.303173	-1.501420	-1.467779
H	-5.477299	-0.882938	-1.853650	H	-3.135687	-0.955303	-2.418632
C	-3.380865	-1.363369	-1.486743	H	-3.436042	-2.590551	-1.537646
H	-3.035317	-0.990247	-2.476077	C	-4.479186	0.530499	-0.622711
H	-3.539991	-2.461987	-1.585379	H	-4.245144	1.012808	-1.586337
C	-4.505819	0.852082	-0.941649	H	-5.409117	0.856685	-0.141992
H	-4.197825	1.287836	-1.917987	C	-3.343858	0.823282	0.326520
H	-5.469334	1.336270	-0.664787	H	-3.204427	1.918533	0.468154
C	-3.426260	1.148732	0.138023	C	-2.099177	0.294799	-0.300657
H	-3.269926	2.245246	0.221766	H	-1.957341	0.731429	-1.349887
C	-2.117723	0.480666	-0.318739	C	-3.522390	0.139683	1.653491
H	-1.881730	0.853495	-1.361432	H	-2.559371	0.321287	2.200379
C	-3.896666	0.576829	1.493400	H	-4.442436	0.504327	2.119489
H	-3.135981	0.786583	2.275524	C	2.622943	-0.986029	-0.232517
H	-4.839084	1.077090	1.808878	C	3.311232	-1.718818	0.751811
C	2.568282	-1.198463	-0.155940	C	4.648724	-1.407765	1.010595
C	3.257835	-1.563285	1.030327	H	5.183112	-1.982751	1.791859
C	4.608472	-1.190143	1.164063	C	5.292689	-0.386225	0.301998
H	5.146021	-1.469888	2.086048	C	4.581632	0.321833	-0.673842
C	5.288305	-0.474467	0.157792	H	5.075959	1.145475	-1.225564
C	4.578435	-0.141455	-1.011129	C	3.239875	0.050725	-0.969194
H	5.093948	0.408881	-1.816506	C	2.587781	-2.778854	1.510226
C	3.224901	-0.490639	-1.195289	H	3.045343	-3.745803	1.272315
C	2.562493	-2.321889	2.137461	H	1.493797	-2.745188	1.407617
H	3.258282	-2.530433	2.973690	H	2.830971	-2.662949	2.574607
H	2.152922	-3.294498	1.790114	C	6.724055	-0.050257	0.549424
H	1.705105	-1.742544	2.540141	H	6.693082	0.794042	1.242884
C	6.730169	-0.054951	0.341851	H	7.224721	0.314894	-0.349516
H	6.796276	0.921831	0.870472	H	7.284458	-0.849535	1.037959
H	7.249423	0.065132	-0.630561	C	2.492023	0.768165	-2.014282
H	7.297738	-0.790375	0.948055	H	1.562573	0.259902	-2.321948
C	2.505154	-0.081964	-2.458758	H	3.111321	1.162935	-2.819543
H	1.761490	-0.834906	-2.788363	H	2.017148	1.662321	-1.507395

H	3.221959	0.081733	-3.287985	C	0.050311	0.501945	1.862420
H	1.958145	0.869590	-2.285494	H	0.702829	-0.351087	2.061770
C	-0.201841	0.614297	2.044554	H	-0.306666	1.288135	2.539841
C	0.694409	3.397918	-0.130860				
C	1.329771	4.737572	-0.427987				
H	0.122850	-0.330543	2.534108				
H	-0.459832	1.449278	2.739686				
H	1.471548	4.856989	-1.521130				
H	0.709486	5.562071	-0.031691				
H	2.337060	4.775054	0.036164				

21-trans				21-trans <sup>+</sup>			
-1856.28951131				-1797.39038337			
Ru	-2.009851	-1.384862	-0.199009	Ru	-1.358531	-1.939038	-0.233480
Cl	-2.646147	-0.774037	2.059792	S	1.241299	-0.876167	1.501520
S	0.931465	-1.274733	1.250990	O	1.026293	0.020948	2.660918
O	1.056171	-0.504521	2.519662	O	1.275523	-2.347288	1.667480
O	0.576417	-2.719849	1.294032	N	-0.172489	-0.567579	0.407870
N	-0.101356	-0.502357	0.145058	N	-2.667430	-0.248921	-0.275598
N	-2.441737	0.691900	-0.445396	C	-0.605852	0.871056	0.442649
C	-0.155126	0.965449	0.364614	C	-1.858413	1.006228	-0.452173
C	-1.212318	1.519688	-0.620644	C	0.455395	1.872559	-0.005287
C	1.176525	1.686244	0.152282	C	1.058980	1.770351	-1.277748
C	1.858343	1.612059	-1.081413	C	1.976984	2.740634	-1.709189
C	3.057910	2.313645	-1.282006	C	2.296379	3.828581	-0.875979
C	3.595594	3.101475	-0.247927	C	1.700102	3.936797	0.392118
C	2.929584	3.174164	0.987385	C	0.786905	2.960975	0.826863
C	1.729499	2.469495	1.184926	C	-2.687830	2.257747	-0.215744
C	-1.507357	3.003871	-0.459699	C	-3.221590	2.547269	1.061596
C	-2.014053	3.513459	0.757862	C	-4.029694	3.678960	1.256423
C	-2.298663	4.881742	0.896196	C	-4.308614	4.539686	0.179187
C	-2.078774	5.762366	-0.178455	C	-3.776942	4.264648	-1.092099
C	-1.572581	5.266776	-1.392054	C	-2.973266	3.128629	-1.288445
C	-1.290677	3.896627	-1.529854	C	2.744219	-0.401375	0.642792
C	2.581724	-1.245268	0.477006	C	-2.442189	-3.653967	0.650872
C	-3.323076	-3.146135	0.005874	C	-3.004679	-3.454245	-0.648018
C	-3.839912	-2.351214	-1.056926	C	-2.162107	-3.365610	-1.792857
C	-2.936981	-1.920320	-2.093656	C	-0.743630	-3.512252	-1.634471
C	-1.579447	-2.381817	-2.143120	C	-0.178541	-3.828740	-0.354165
C	-1.096926	-3.198142	-1.067855	C	-1.023562	-3.857404	0.793040
C	-1.956015	-3.595000	0.001354	H	-0.870560	1.107001	1.496770
H	-0.504177	1.189099	1.399893	H	-1.519758	0.990088	-1.508667
H	-0.850873	1.328703	-1.653107	H	0.822420	0.916795	-1.934470
H	1.455447	0.976764	-1.886752	H	2.444719	2.649591	-2.701947
H	3.580192	2.241058	-2.249498	H	3.011021	4.593820	-1.217357
H	4.537018	3.652410	-0.403712	H	1.944773	4.786800	1.048152
H	3.348500	3.780657	1.806408	H	0.325650	3.044322	1.823735
H	1.216615	2.511194	2.158530	H	-3.001920	1.895524	1.925019
H	-2.183125	2.836761	1.612561	H	-4.437481	3.894726	2.256196
H	-2.690816	5.263384	1.852244	H	-4.938876	5.429247	0.333583
H	-2.300352	6.835739	-0.068117	H	-3.987319	4.938488	-1.937100
H	-1.392857	5.950438	-2.236977	H	-2.553986	2.920450	-2.286638
H	-0.884556	3.513198	-2.480460	H	-3.406900	-0.288710	-0.994123
H	-3.138188	0.923063	-1.169179	H	-3.170692	-0.201982	0.627300
H	-2.874087	0.886395	0.481619	H	-0.574863	-3.973135	1.789796
H	-1.538609	-4.131139	0.863348	H	0.907195	-3.929265	-0.226158
H	-0.030115	-3.453118	-0.999219	H	-3.088900	-3.641703	1.541087
H	-3.956578	-3.354667	0.880960	H	-0.085240	-3.374355	-2.505951
H	-0.901594	-2.039822	-2.938653	H	-4.083373	-3.257445	-0.748036
H	-4.873296	-1.975566	-1.020109	H	-2.583788	-3.115178	-2.777440
H	-3.293716	-1.215040	-2.863079	C	3.490095	0.677775	1.146314
C	3.667213	-0.762694	1.224424	C	4.717154	0.986821	0.543045
C	4.961404	-0.834937	0.684415	C	5.210348	0.240076	-0.552079
C	5.195251	-1.389341	-0.593110	C	4.430695	-0.839383	-1.032094
C	4.082806	-1.866316	-1.324055	C	3.206959	-1.174879	-0.437146

C	2.784515	-1.801457	-0.797168	H	3.110645	1.254517	2.001966
H	3.481449	-0.332533	2.219763	H	5.310052	1.827779	0.937272
H	5.811297	-0.449287	1.271954	C	6.549340	0.565641	-1.167125
C	6.598007	-1.495357	-1.148280	H	4.799261	-1.437371	-1.881072
H	4.239577	-2.297926	-2.326809	H	2.625035	-2.031483	-0.807718
H	1.927512	-2.165809	-1.383571	H	6.639910	0.166127	-2.196306
H	6.595902	-1.616950	-2.250192	H	6.730368	1.659032	-1.197519
H	7.205646	-0.600762	-0.900388	H	7.372200	0.119438	-0.566352
H	7.130403	-2.374175	-0.721242				

22-trans				22-trans <sup>+</sup>			
-1868.8246824				-1408.45855804			
Ru	0.002829	1.015920	-0.251370	Ru	-0.000754	0.997884	-0.273185
Cl	0.016007	0.867442	-2.637319	N	-1.092254	-1.894115	-0.388269
N	-1.082881	-1.926812	-0.120863	N	1.088671	-1.894359	-0.383636
N	1.090207	-1.926070	-0.120273	C	-0.001460	-1.054541	-0.262090
C	0.003297	-1.057684	-0.088921	C	-0.684055	-3.214731	-0.613474
C	-0.678195	-3.265566	-0.168042	H	-1.397591	-4.026042	-0.782304
H	-1.402086	-4.086013	-0.199058	C	0.681510	-3.214925	-0.610645
C	0.686519	-3.265039	-0.167421	H	1.395784	-4.026288	-0.776394
H	1.410985	-4.085033	-0.197247	C	-2.470480	-1.473768	-0.377381
C	-2.481986	-1.570193	-0.056152	C	-3.390506	-2.092230	0.504867
C	-3.108946	-1.533329	1.214075	C	-2.980385	-3.147840	1.509088
C	-2.335714	-1.844730	2.474376	H	-3.659020	-3.132420	2.384586
H	-2.953657	-1.667139	3.376434	H	-1.943809	-3.004807	1.873426
H	-1.417290	-1.228321	2.550721	H	-3.038276	-4.172694	1.082658
H	-2.004683	-2.905663	2.496833	C	-4.741043	-1.685532	0.437899
C	-4.484575	-1.237403	1.269272	H	-5.464106	-2.162355	1.120195
H	-4.978978	-1.201098	2.254792	C	-5.192366	-0.696699	-0.456147
C	-5.242406	-0.999131	0.104939	C	-6.653514	-0.322658	-0.538428
C	-6.709589	-0.641004	0.192045	H	-7.167514	-0.922612	-1.321213
H	-7.266960	-0.974177	-0.706855	H	-6.791734	0.744195	-0.805841
H	-6.847139	0.460230	0.270549	H	-7.181344	-0.513183	0.416939
H	-7.190080	-1.092470	1.083910	C	-4.235511	-0.079155	-1.290374
C	-4.591995	-1.097345	-1.140780	H	-4.559198	0.708263	-1.991303
H	-5.174377	-0.953086	-2.066336	C	-2.877867	-0.446260	-1.267814
C	-3.217972	-1.396446	-1.255314	C	-1.890126	0.273643	-2.151321
C	-2.573448	-1.559167	-2.607990	H	-2.407068	0.842645	-2.950131
H	-3.322254	-1.453002	-3.416932	H	-1.152573	-0.394952	-2.631358
H	-2.096274	-2.557368	-2.710651	H	-1.352630	1.143933	-1.602421
H	-1.769730	-0.805444	-2.767215	C	2.466718	-1.473195	-0.372901
C	2.488910	-1.568090	-0.054394	C	2.876939	-0.455293	-1.273779
C	3.228262	-1.403379	-1.252788	C	1.890886	0.260028	-2.163254
C	2.587114	-1.575413	-2.605907	H	2.409719	0.822266	-2.965575
H	3.337963	-1.475536	-3.413757	H	1.348344	1.130890	-1.622231
H	1.784993	-0.821296	-2.771536	H	1.153826	-0.411935	-2.639837
H	2.108888	-2.573646	-2.703003	C	4.235713	-0.094293	-1.300777
C	4.601649	-1.102346	-1.136614	H	4.562158	0.684640	-2.009877
H	5.186607	-0.965039	-2.061606	C	5.190217	-0.704556	-0.458320
C	5.248028	-0.992350	0.110236	C	6.652094	-0.334009	-0.543454
C	6.714460	-0.631417	0.198129	H	7.186041	-0.546289	0.403785
H	7.189654	-1.061302	1.103332	H	6.791816	0.738016	-0.789071
H	6.850898	0.471482	0.250921	H	7.158270	-0.918175	-1.343056
H	7.277569	-0.985424	-0.689224	C	4.735574	-1.680526	0.447815
C	4.486930	-1.221425	1.274292	H	5.456898	-2.151573	1.135977
H	4.978293	-1.176465	2.260971	C	3.383826	-2.084321	0.517034
C	3.111883	-1.520002	1.217324	C	2.970977	-3.132458	1.528012
C	2.334633	-1.823030	2.477113	H	1.931861	-2.990309	1.885068
H	1.416858	-1.205075	2.546459	H	3.644409	-3.107479	2.407333
H	2.949952	-1.640469	3.379986	H	3.035357	-4.160482	1.110104
H	2.002990	-2.883667	2.504723	C	0.605762	3.079466	0.303710
C	0.693011	3.084043	-0.109274	C	1.214625	2.048633	1.162722
C	1.162391	2.279602	1.031289	C	-0.813697	2.962210	0.411709
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C	0.002602	1.839190	1.788558	C	-1.126241	1.861648	1.340942
C	-1.176511	2.247982	1.044378	C	0.307265	0.328233	2.937217
C	0.018724	1.248855	3.168523	H	0.350990	0.842971	3.922554
H	-0.008756	2.053214	3.939357	H	-0.538794	-0.384967	2.973550
H	-0.855696	0.594328	3.353401	H	1.243701	-0.251594	2.824443
H	0.933685	0.653322	3.355830	C	2.680227	1.918023	1.448162
C	2.596151	2.133794	1.445062	H	2.976545	2.624442	2.256042
H	2.923695	3.007545	2.055111	H	2.951227	0.897290	1.780042
H	2.755371	1.219445	2.048234	H	3.297666	2.156282	0.560219
H	3.266741	2.068074	0.565536	C	1.362909	4.110515	-0.484418
C	1.574276	3.782655	-1.103542	H	1.586669	4.996208	0.150502
H	1.825889	4.812521	-0.763358	H	2.333981	3.723088	-0.851251
H	2.527264	3.236096	-1.251646	H	0.787207	4.469603	-1.359967
H	1.084079	3.858538	-2.093717	C	-1.836533	3.838140	-0.252970
C	-1.650814	3.731393	-1.090582	H	-2.113793	4.679309	0.420221
H	-1.915591	4.760809	-0.759072	H	-1.459373	4.281419	-1.195343
H	-1.178940	3.802793	-2.089998	H	-2.770021	3.285819	-0.479034
H	-2.595882	3.165413	-1.214387	C	-2.494509	1.510868	1.842711
C	-2.601347	2.073057	1.477459	H	-2.792175	2.191894	2.671524
H	-2.949063	2.957110	2.060909	H	-3.260975	1.599634	1.047429
H	-3.279809	1.955731	0.609148	H	-2.536397	0.474169	2.228784
H	-2.726081	1.176460	2.113772				

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Cl	0.241399	1.244118	2.128130	Cl	-0.028547	0.830184	2.370688
Cl	0.127117	0.109695	-2.331846	Cl	-0.061126	-0.312494	-2.327031
P	2.552719	0.069397	-0.002711	P	2.352870	0.468778	0.025885
C	-0.686202	-2.851532	0.256653	C	2.598565	2.328198	-0.255280
C	0.181068	-1.712877	0.563576	C	1.790054	2.819756	-1.477822
H	1.007792	-1.995550	1.260743	C	2.088989	4.297334	-1.791826
C	3.346518	-0.662743	-1.512505	C	1.840462	5.198923	-0.571426
C	2.839446	-1.877202	-2.025480	C	2.614952	4.699555	0.658924
C	4.465345	-0.066414	-2.132761	C	2.315349	3.220400	0.973714
C	3.451712	-2.490988	-3.130008	C	3.288702	-0.312377	-1.426172
H	1.952505	-2.338440	-1.564226	C	4.528293	0.424164	-1.985455
C	5.070653	-0.679377	-3.244740	C	5.043829	-0.268910	-3.264582
H	4.867341	0.882909	-1.746170	C	5.349548	-1.757794	-3.033501
C	4.567016	-1.892727	-3.743785	C	4.131187	-2.488276	-2.446054
H	3.044267	-3.436268	-3.522260	C	3.623614	-1.798455	-1.165857
H	5.941525	-0.202677	-3.722625	C	3.282398	0.168759	1.644607
H	5.040392	-2.370564	-4.616464	C	3.098289	-1.237786	2.251752
C	3.167905	1.814302	0.006979	C	3.689894	-1.301513	3.672883
C	4.086467	2.302606	0.958881	C	5.170937	-0.887481	3.693957
C	2.650839	2.692144	-0.975596	C	5.367237	0.500507	3.063223
C	4.484428	3.651588	0.927813	C	4.774420	0.572578	1.640459
H	4.492067	1.629812	1.729930	H	3.680348	2.435996	-0.500685
C	3.058597	4.035493	-1.005475	H	1.979398	2.186185	-2.369002
H	1.929056	2.316755	-1.720834	H	0.704129	2.701971	-1.260605
C	3.973915	4.519338	-0.052471	H	1.475039	4.630169	-2.656947
H	5.200188	4.024370	1.677910	H	3.152688	4.394473	-2.111757
H	2.653673	4.708957	-1.777636	H	0.750866	5.203331	-0.338026
H	4.288188	5.575113	-0.073643	H	2.112158	6.251850	-0.802714
C	3.476440	-0.784936	1.371163	H	2.379009	5.325054	1.547090
C	4.619657	-1.576530	1.112846	H	3.708253	4.821341	0.475894
C	3.018061	-0.655904	2.704159	H	2.926369	2.901611	1.843379
C	5.293027	-2.218987	2.166663	H	1.256747	3.096718	1.290311
H	4.987713	-1.694685	0.082840	H	2.496232	-0.291029	-2.211754
C	3.699078	-1.298318	3.752524	H	4.294898	1.482799	-2.221354
H	2.125163	-0.043593	2.912333	H	5.341950	0.439371	-1.226546
C	4.836498	-2.081430	3.488700	H	4.270714	-0.173810	-4.061175
H	6.181956	-2.832362	1.948423	H	5.946070	0.261568	-3.640158
H	3.331463	-1.185464	4.785122	H	6.208126	-1.851437	-2.328342
H	5.366059	-2.586393	4.312563	H	5.673654	-2.238153	-3.982331
C	-0.738072	-3.937868	1.178940	H	4.378422	-3.550252	-2.229435
C	-1.525053	-5.066384	0.917249	H	3.309754	-2.503948	-3.198022
C	-2.247696	-5.156629	-0.289054	H	4.413684	-1.868934	-0.384592
C	-2.177757	-4.110036	-1.227219	H	2.736317	-2.333879	-0.771602
C	-1.415783	-2.964282	-0.957239	H	2.725264	0.859469	2.319297
H	-0.149577	-3.877767	2.109665	H	3.592144	-2.004189	1.616292
H	-1.566408	-5.888821	1.649393	H	2.019617	-1.486437	2.282801
H	-2.855778	-6.050577	-0.501608	H	3.106135	-0.623391	4.336309
H	-2.725152	-4.184659	-2.179910	H	3.566379	-2.326126	4.086256
H	-1.340212	-2.151610	-1.693812	H	5.565754	-0.898975	4.733191
				H	5.770030	-1.635812	3.124665
				H	4.870274	1.267191	3.701174

H	6.445898	0.769406	3.035169
H	5.344958	-0.115413	0.976678
H	4.914820	1.594268	1.228781
C	0.024952	-1.748611	0.787744
H	-0.133871	-1.774431	1.895679
C	0.425935	-5.503181	0.797608
C	0.596689	-5.803869	-0.565999
C	0.584173	-4.763939	-1.516891
C	0.409172	-3.432622	-1.116305
C	0.232242	-3.106365	0.256738
C	0.243019	-4.172974	1.201613
H	0.433059	-6.309512	1.548431
H	0.737621	-6.848001	-0.888712
H	0.713608	-4.996556	-2.586051
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Ru	-0.229244	0.878736	0.091096	Ru	-0.156675	0.742073	0.131304
Cl	-0.972340	1.556755	-2.007499	Br	-1.147584	1.656863	-1.920001
N	-1.798072	-1.551861	0.152394	N	-1.705467	-1.715792	0.219965
C	-0.519565	-1.026598	0.092993	C	-0.437189	-1.171320	0.106727
C	-1.805921	-2.995101	0.445091	C	-1.677214	-3.156283	0.529461
C	-3.038441	-0.830419	0.026820	C	-2.967659	-1.044885	0.043201
C	-3.601070	-0.672565	-1.271184	C	-3.496562	-0.943414	-1.274037
C	-4.822348	0.014823	-1.389421	C	-4.744795	-0.320068	-1.447422
C	-5.506345	0.525683	-0.267297	C	-5.487911	0.182772	-0.359737
C	-4.959064	0.285203	1.006355	C	-4.967254	0.003546	0.934740
C	-3.743534	-0.407791	1.185730	C	-3.725273	-0.624223	1.168239
C	-2.923649	-1.239000	-2.496178	C	-2.755890	-1.509987	-2.462058
C	-6.787953	1.310506	-0.433667	C	-6.800927	0.898032	-0.584599
C	-3.273917	-0.745417	2.581347	C	-3.279487	-0.895795	2.585699
H	-2.099835	-3.176964	1.503966	H	-1.916971	-3.329257	1.603310
H	-2.533240	-3.524196	-0.204649	H	-2.427175	-3.702515	-0.078761
H	-5.255323	0.151301	-2.394662	H	-5.151243	-0.228026	-2.468615
H	-5.500095	0.636076	1.901302	H	-5.550513	0.351952	1.803791
H	-2.025590	-0.639252	-2.755961	H	-1.841590	-0.918157	-2.677343
H	-2.591775	-2.286893	-2.339454	H	-2.440254	-2.560955	-2.289693
H	-3.608489	-1.223141	-3.366642	H	-3.391926	-1.489999	-3.368569
H	-7.429125	0.883114	-1.1232153	H	-7.378777	0.441267	-1.414347
H	-6.571923	2.362843	-0.721947	H	-6.628790	1.962443	-0.857963
H	-7.377065	1.340618	0.504878	H	-7.435018	0.890694	0.324767
H	-3.598854	-1.771654	2.866124	H	-3.562202	-1.927063	2.896107
H	-3.712824	-0.050633	3.324204	H	-3.770267	-0.200216	3.294725
H	-2.172948	-0.686314	2.679736	H	-2.184673	-0.785891	2.711653
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C	-0.349247	-3.394550	0.169897	C	-0.230574	-3.538104	0.189835
C	1.779609	-2.106671	0.029736	C	1.871212	-2.233512	-0.067958
C	2.577109	-2.122157	1.202853	C	2.738636	-2.272456	1.054000
C	3.975586	-2.204032	1.053357	C	4.125937	-2.349661	0.818267
C	4.590695	-2.277827	-0.213419	C	4.665075	-2.399673	-0.483247
C	3.765296	-2.254365	-1.356244	C	3.772053	-2.361426	-1.573612
C	2.361382	-2.171552	-1.1263068	C	2.376346	-2.283378	-1.393962
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C	6.092686	-2.407155	-0.338621	C	6.156990	-2.522610	-0.700824
C	1.508188	-2.088918	-2.508068	C	1.451294	-2.195414	-2.586073
H	-0.226348	-3.909345	-0.811087	H	-0.143465	-4.055617	-0.793795
H	0.075181	-4.057697	0.951340	H	0.237205	-4.191912	0.954000
H	4.603888	-2.207923	1.959992	H	4.807232	-2.369860	1.685590
H	4.226818	-2.299176	-2.357163	H	4.171526	-2.391183	-2.601438
H	1.376084	-1.065805	2.674884	H	1.652241	-1.247171	2.632511
H	1.224917	-2.839211	2.759639	H	1.474266	-3.018902	2.670318
H	2.713747	-2.050263	3.367058	H	3.013724	-2.275147	3.205194
H	6.454068	-2.060640	-1.327690	H	6.460460	-2.135866	-1.694494
H	6.411475	-3.467083	-0.225908	H	6.479948	-3.586065	-0.650392
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H	0.732409	-2.883099	-2.538920	H	0.669995	-2.984256	-2.569610
H	2.126702	-2.189016	-3.421109	H	2.013563	-2.298788	-3.534383
H	0.970026	-1.117812	-2.560925	H	0.917390	-1.220936	-2.607576
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C	2.296402	2.302019	-0.099191	C	2.387844	2.154835	-0.209560
C	3.672019	2.349348	-0.463688	C	3.743525	2.164164	-0.645449
C	1.665447	3.518573	0.290405	C	1.828643	3.377537	0.260901
C	4.381194	3.558138	-0.449417	C	4.502976	3.341754	-0.618238
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C	2.377088	4.723311	0.304034	C	2.590188	4.551175	0.287087
H	0.607793	3.510908	0.601968	H	0.786368	3.398407	0.618701
C	3.736431	4.749047	-0.066799	C	3.929081	4.539228	-0.152476
H	5.444619	3.574019	-0.737163	H	5.550036	3.327799	-0.960835
H	1.871711	5.652806	0.610268	H	2.139535	5.486221	0.655640
H	4.293477	5.699435	-0.053578	H	4.525269	5.465417	-0.128966

5-14e				6-14e			
-1312.94687244				-2446.26985409			
Ru	-0.112886	0.594684	0.144159	Ru	-0.089904	-1.219864	-0.119774
I	-1.330275	1.834892	-1.894134	Cl	0.822396	-1.770165	-2.178615
N	-1.582680	-1.925807	0.154313	N	1.851970	0.847079	0.455677
C	-0.336416	-1.331230	0.029574	C	0.504344	0.565031	0.280581
C	-1.496547	-3.377655	0.392775	C	2.047683	2.112575	1.187941
C	-2.879477	-1.312372	0.022952	C	2.987536	0.068282	0.016814
C	-3.435349	-1.197257	-1.283008	C	3.462862	0.248303	-1.319207
C	-4.721283	-0.647649	-1.417742	C	4.596336	-0.483754	-1.721640
C	-5.478544	-0.232020	-0.302197	C	5.258000	-1.347667	-0.838201
C	-4.926061	-0.420243	0.976723	C	4.802249	-1.483224	0.477646
C	-3.642781	-0.976162	1.170492	C	3.669245	-0.778296	0.938529
C	-2.679991	-1.683278	-2.497122	C	2.830850	1.254499	-2.284864
C	-6.838889	0.402692	-0.483204	H	6.140265	-1.913460	-1.178137
C	-3.169062	-1.269645	2.574367	C	3.268398	-0.894143	2.410166
H	-1.686806	-3.608153	1.465988	H	2.210831	1.914082	2.271895
H	-2.253850	-3.918672	-0.210834	H	2.927851	2.661998	0.801265
H	-5.147449	-0.544004	-2.429646	H	4.970000	-0.374772	-2.750941
H	-5.515495	-0.138617	1.865696	H	5.337464	-2.150860	1.170460
H	-1.730265	-1.126314	-2.630928	H	1.775001	1.391985	-1.970160
H	-2.424427	-2.762258	-2.416209	C	3.544432	2.624375	-2.183915
H	-3.282350	-1.548508	-3.416472	C	2.810627	0.782820	-3.751114
H	-7.394523	-0.054221	-1.327796	C	4.211506	-0.046732	3.297383
H	-6.741729	1.487436	-0.709023	C	3.229696	-2.351627	2.910958
H	-7.459878	0.311386	0.430526	H	2.237735	-0.494240	2.511160
H	-3.612583	-2.222668	2.940685	N	-0.189477	1.709397	0.631058
H	-3.486771	-0.473688	3.277255	C	0.721785	2.832475	0.937772
H	-2.068889	-1.351739	2.642998	C	-1.593733	2.006534	0.518485
N	0.585368	-2.361815	-0.016068	C	-2.434634	1.840345	1.656953
C	-0.055866	-3.694090	-0.021651	C	-3.789476	2.214995	1.537300
C	1.993318	-2.328530	-0.303882	C	-4.298113	2.745439	0.343929
C	2.921615	-2.469365	0.761100	C	-3.453221	2.913612	-0.761795
C	4.294683	-2.506942	0.446472	C	-2.090745	2.553249	-0.701807
C	4.764130	-2.431131	-0.880380	C	-1.913037	1.302670	2.988826
C	3.813045	-2.312754	-1.913535	H	-5.359507	3.033553	0.276288
C	2.427791	-2.266425	-1.654848	C	-1.211587	2.755350	-1.938322
C	2.458717	-2.576902	2.194261	H	0.774098	3.536538	0.074711
C	6.243740	-2.513393	-1.184067	H	0.358649	3.397275	1.818996
C	1.444393	-2.114213	-2.792682	H	-4.459731	2.088902	2.401901
H	0.008135	-4.149812	-1.037178	H	-3.859554	3.332823	-1.696236
H	0.459678	-4.376407	0.684303	H	-0.916893	0.855578	2.795724
H	5.021047	-2.602286	1.271228	C	-1.742001	2.446879	4.014529
H	4.156537	-2.256152	-2.960269	C	-2.800869	0.181187	3.563029
H	1.804684	-1.726305	2.477717	C	-1.069157	4.253508	-2.287708
H	1.871173	-3.505340	2.366480	C	-1.723338	1.949522	-3.151415
H	3.321003	-2.598133	2.888687	H	-0.200387	2.365025	-1.699953
H	6.481464	-2.102143	-2.185523	Cl	-0.196665	-1.907511	2.100220
H	6.594687	-3.568895	-1.169345	C	-1.860900	-0.953338	-0.563021
H	6.845991	-1.963231	-0.432243	H	-2.305322	0.060415	-0.601235
H	0.651691	-2.890793	-2.766275	C	-2.794608	-2.040271	-0.850886
H	1.956599	-2.188942	-3.771608	C	-4.178516	-1.735539	-0.992228
H	0.925854	-1.131984	-2.753427	C	-2.392067	-3.399890	-0.983692
I	0.086415	0.780798	2.814943	C	-5.118160	-2.745288	-1.240575

C	1.652783	0.825896	-0.354732	H	-4.504367	-0.686987	-0.895316
H	2.223786	-0.024043	-0.780381	C	-3.333527	-4.405073	-1.233523
C	2.425459	2.064879	-0.268908	H	-1.324347	-3.663484	-0.907547
C	3.783865	2.041682	-0.696712	C	-4.699722	-4.083482	-1.360241
C	1.900665	3.293663	0.223544	H	-6.184798	-2.488889	-1.342804
C	4.581671	3.192081	-0.633003	H	-3.001760	-5.450399	-1.335522
H	4.203597	1.096587	-1.078558	H	-5.437212	-4.877845	-1.557168
C	2.699871	4.440792	0.284512	H	-1.038494	2.076231	-4.015677
H	0.852357	3.343395	0.559028	H	-1.779669	0.866352	-2.923607
C	4.042217	4.395370	-0.142024	H	-2.731069	2.288162	-3.473258
H	5.630561	3.152375	-0.967669	H	-0.376916	4.391338	-3.144796
H	2.275235	5.381938	0.667951	H	-2.046301	4.696910	-2.574800
H	4.667525	5.301074	-0.091263	H	-0.678170	4.843139	-1.432290
				H	3.055291	3.373303	-2.842485
				H	3.544751	3.029764	-1.151471
				H	4.605657	2.538006	-2.500962
				H	2.227998	1.496680	-4.370376
				H	3.831006	0.738919	-4.188311
				H	2.341738	-0.215934	-3.842034
				H	-2.331778	-0.247048	4.472796
				H	-3.807187	0.552256	3.853429
				H	-2.926279	-0.643774	2.834092
				H	-1.303711	2.062629	4.959738
				H	-1.078905	3.252767	3.635836
				H	-2.719375	2.914531	4.261604
				H	3.883827	-0.077621	4.358250
				H	5.251917	-0.434601	3.254879
				H	4.245977	1.016531	2.981176
				H	2.833988	-2.387079	3.947125
				H	2.569152	-2.977657	2.279715
				H	4.240597	-2.811832	2.929560

7-14e				13-14e		
-1979.58274394				-2403.61746704		
Ru	0.079657	0.468600	-1.401147	Ru	-0.575390	-0.644645
Cl	0.234259	2.758165	-0.989250	Cl	-0.948628	-0.122524
Cl	1.162148	-1.339852	-2.377836	Cl	-1.069601	-2.107213
C	-0.082662	-0.060496	0.451648	O	3.517581	-1.440873
C	-1.596014	0.297463	-2.059731	N	-2.458845	1.377407
H	-1.695233	0.630987	-3.125683	N	-0.438583	2.278437
H	-2.512532	-0.097116	-1.580690	C	-1.130357	1.091300
N	1.010283	-0.207016	1.283146	C	-3.546044	0.442959
N	-1.204944	-0.243198	1.227568	C	-5.478117	-0.722690
C	0.624959	-0.326957	2.701746	C	-3.798591	-0.109745
C	-0.875739	-0.637954	2.612350	C	1.750805	2.364687
H	1.208243	-1.127624	3.200679	C	1.261291	-0.587274
H	0.823662	0.627222	3.240675	C	-5.719316	-1.336395
H	-1.483821	-0.059500	3.337416	C	3.266979	-2.084219
H	-1.098202	-1.718433	2.771118	C	-1.298507	3.393851
C	2.404480	-0.205411	0.916290	C	-4.414772	0.182393
C	-2.582248	-0.266255	0.823638	C	1.773320	-2.308218
C	3.015678	-1.445585	0.581181	C	-4.261912	0.881729
C	4.383375	-1.447826	0.252633	C	2.088713	-1.657031
C	5.159367	-0.271262	0.267779	C	-2.934404	0.239539
C	4.538288	0.924449	0.673642	C	1.551416	3.001849
C	3.173117	0.984407	1.023487	C	3.726432	-3.729288
C	-3.355341	0.917710	0.941970	C	4.070575	-3.115874
C	-4.717636	0.857177	0.590218	C	2.925119	3.312613
C	-5.322946	-0.333327	0.135982	C	2.579091	-3.329848
C	-4.523468	-1.489283	0.036130	C	-2.712931	2.823216
C	-3.154474	-1.483547	0.374552	C	3.727657	3.170847
C	2.233345	-2.737472	0.593127	C	0.719065	3.176396
H	4.858597	-2.405054	-0.020148	C	1.138032	1.819737
C	6.613715	-0.296599	-0.144922	C	-6.837876	-2.338815
H	5.136469	1.849101	0.735625	C	4.895085	-0.697589
C	2.594186	2.271350	1.563025	C	3.119639	2.697809
C	-2.728294	2.210971	1.405319	C	4.576626	-1.883765
H	-5.325183	1.774160	0.673885	C	4.138799	-3.129212
C	-6.786706	-0.355926	-0.244850	C	5.202034	3.506565
H	-4.976170	-2.429496	-0.321222	C	-4.879512	-0.997447
C	-2.312963	-2.728746	0.212011	C	0.976638	2.516617
H	-3.481364	3.021288	1.457219	H	-6.145553	-0.944495
H	-2.271310	2.110823	2.413302	H	-1.072359	3.660642
H	-1.915525	2.531569	0.718241	H	-1.115374	4.296641
H	-2.913940	-3.562943	-0.199226	H	-4.877653	0.386105
H	-1.457844	-2.548114	-0.473707	H	-4.606688	1.938258
H	-1.883728	-3.073058	1.177583	H	-3.210443	0.886865
H	-7.140073	-1.384523	-0.456488	H	-3.405430	-0.098838
H	-7.422006	0.065207	0.562653	H	-1.944750	-0.256795
H	-6.974411	0.257430	-1.152631	H	-2.753764	1.332098
H	1.511384	-2.764427	-0.249635	H	3.380631	3.684209
H	2.910700	-3.607709	0.489697	H	-3.212697	3.214104
H	1.656260	-2.864775	1.533333	H	-3.377310	3.030372
H	3.255810	3.128102	1.328079	H	0.248772	2.218261
H	1.594997	2.492312	1.138990	H	-0.108938	3.901747
H	2.500332	2.228907	2.671401	H	1.337458	3.551318

H	7.176030	0.560778	0.276574	H	0.773701	0.779737	-2.390539
H	7.114825	-1.232547	0.177231	H	1.875610	1.813987	-3.360254
H	6.710721	-0.242069	-1.251680	H	0.263754	2.416975	-2.869580
				H	-7.619235	-2.223308	-0.172579
				H	-6.450383	-3.378905	-0.876774
				H	-7.321592	-2.244484	-1.944650
				H	3.727475	2.583629	-2.123841
				H	5.761725	2.770517	0.629901
				H	5.379062	4.504392	0.466302
				H	5.653785	3.507337	-0.999521
				H	-5.070546	-1.438965	-2.848941
				H	0.890063	-1.958024	2.782278
				H	4.368875	-4.533046	2.432617
				H	4.968185	-3.455738	0.285442
				H	2.315688	-3.807511	3.699894
				H	4.007583	-0.424646	-3.277604
				H	5.724816	-0.953775	-3.359990
				H	5.193055	0.185481	-2.071269
				H	5.479231	-2.113426	-1.150227
				H	3.868436	-3.961535	-1.860059
				H	4.956799	-3.478784	-3.203293
				H	3.252717	-2.897864	-3.166153
				H	1.783829	0.145257	-0.200092

14-14e				15-14e			
-2608.10131196				-2552.86214051			
Ru	0.594992	-0.596841	-0.136046	Ru	-0.508949	0.588053	0.182310
Cl	0.802022	-1.168797	-2.391194	Cl	-0.727794	0.580850	2.538273
Cl	1.059326	-1.253320	2.044386	Cl	-1.137401	1.115059	-2.024211
O	-3.274237	-0.013288	1.793496	O	3.754761	-0.974117	0.066304
N	2.856461	1.214949	-0.301729	O	5.706648	0.127186	0.008827
N	0.996320	2.338729	-0.734012	O	2.123546	5.295474	-0.316846
C	1.480357	1.107322	-0.352806	N	-2.311016	-1.752355	0.129093
C	3.795007	0.227379	0.166983	N	-0.240238	-2.494200	0.256884
C	5.393854	-1.551026	-0.239628	C	-0.989647	-1.345360	0.124715
C	4.115225	0.208337	1.552132	C	-2.478343	-3.184655	0.438930
C	-1.014673	3.298700	0.311206	H	-2.854039	-3.314232	1.479042
C	-1.175847	-0.126753	0.032311	H	-3.212916	-3.653480	-0.248083
C	5.685785	-1.642708	1.134028	C	-1.056075	-3.727457	0.265375
C	-3.312501	-1.072861	0.953584	H	-0.920944	-4.284116	-0.690943
C	2.065394	3.351844	-0.858802	H	-0.742112	-4.400170	1.090019
C	4.470812	-0.616379	-0.753893	C	-3.489958	-0.955330	-0.102364
C	-2.186347	-2.259166	-0.872369	C	-4.246545	-0.450820	0.989324
C	4.277756	-0.494408	-2.247497	C	-5.403789	0.304381	0.702774
C	-2.215554	-1.163820	0.020732	H	-5.981230	0.718549	1.546658
C	3.481488	1.185690	2.513601	C	-5.852421	0.524481	-0.611902
C	-0.985945	2.819601	-2.116555	C	-5.131067	-0.073931	-1.664587
C	-4.282253	-3.125244	0.050502	H	-5.491342	0.041657	-2.700796
C	-4.328566	-2.057126	0.954590	C	-3.962927	-0.824453	-1.438980
C	-2.287709	3.350162	-2.205411	C	-3.903874	-0.769295	2.425542
C	-3.211305	-3.214347	-0.851429	H	-4.319152	-1.761645	2.713421
C	3.343526	2.502255	-0.828836	H	-2.811142	-0.779883	2.604707
C	-2.969923	3.860174	-1.081671	H	-4.350291	-0.022861	3.112139
C	-0.281002	2.293751	-3.343856	C	-7.071330	1.374574	-0.892545
C	-0.354464	3.240160	1.670408	H	-7.666412	0.970801	-1.737592
C	6.643641	-2.687492	1.660501	H	-7.733991	1.448864	-0.006729
C	-4.237542	1.620114	3.230377	H	-6.776137	2.410304	-1.171319
C	-2.314579	3.825226	0.164574	C	-3.251616	-1.484377	-2.595835
C	-4.242979	0.137957	2.866129	H	-2.303056	-0.949659	-2.817113
C	-3.874697	-0.771559	4.040822	H	-2.997557	-2.543299	-2.378499
C	-4.367274	4.423004	-1.220265	H	-3.881198	-1.463778	-3.507232
C	5.050571	-0.737425	2.008264	C	1.179207	-2.674109	0.150964
C	-0.362370	2.791816	-0.841626	C	1.940905	-2.846663	1.335451
H	5.908703	-2.222874	-0.946894	C	3.317626	-3.121061	1.205665
H	2.013359	4.077313	-0.014369	H	3.918635	-3.250271	2.121708
H	1.947463	3.926047	-1.800427	C	3.941622	-3.241890	-0.052749
H	4.642742	-1.402324	-2.766762	C	3.154211	-3.053564	-1.207784
H	4.856825	0.365423	-2.653472	H	3.624474	-3.133082	-2.202742
H	3.213830	-0.353136	-2.522829	C	1.774924	-2.772796	-1.134379
H	3.946959	1.111022	3.515854	C	1.298023	-2.712377	2.695190
H	2.397343	0.977458	2.625027	H	2.055636	-2.777767	3.500558
H	3.587357	2.235682	2.166081	H	0.755303	-1.747333	2.793323
H	-2.781562	3.369960	-3.191652	H	0.550913	-3.516075	2.876057
H	3.780944	2.365164	-1.843534	C	5.406169	-3.607828	-0.160701
H	4.132672	2.922184	-0.171790	H	5.858723	-3.228986	-1.099698
H	-0.012591	1.221656	-3.230254	H	5.993468	-3.213956	0.693920
H	0.667761	2.839174	-3.539099	H	5.540148	-4.712367	-0.161245

H	-0.918581	2.401661	-4.242853	C	0.967131	-2.528724	-2.387530
H	-0.142218	2.191274	1.969714	H	0.074983	-3.187686	-2.444053
H	-1.001920	3.694640	2.445300	H	0.586238	-1.484757	-2.423455
H	0.617390	3.777732	1.689493	H	1.576415	-2.707147	-3.295030
H	7.377899	-2.997652	0.889848	C	1.320832	0.478817	-0.015758
H	6.094412	-3.601546	1.977334	H	1.803607	-0.512053	-0.117860
H	7.202493	-2.322001	2.546190	C	2.302396	1.565102	-0.085472
H	-2.827577	4.223056	1.056267	C	1.758626	2.877929	-0.178537
H	-5.091294	3.633724	-1.517219	H	0.663060	2.971599	-0.202607
H	-4.411542	5.207788	-2.004859	C	2.580808	4.018850	-0.235186
H	-4.726241	4.870047	-0.271899	C	3.990017	3.68147	-0.207565
H	5.291129	-0.765866	3.084271	H	4.619867	4.768823	-0.253993
H	-1.374917	-2.347473	-1.611525	C	4.542116	2.592824	-0.123795
H	-5.061090	-3.900198	0.030911	H	5.634169	2.470306	-0.105853
H	-5.163013	-2.000009	1.666532	C	3.730036	1.433689	-0.060598
N	-3.171596	-4.344566	-1.806786	C	4.359788	0.108019	0.013008
H	-3.238270	1.924792	3.603253	C	6.361245	-1.153158	0.080600
H	-4.983157	1.820155	4.026172	C	0.719462	5.520624	-0.343437
H	-4.487883	2.242527	2.348689	H	0.224801	5.142456	0.578936
H	-5.249848	-0.129754	2.471641	H	0.583515	6.616694	-0.405217
H	-3.845470	-1.838551	3.742640	H	0.242533	5.043004	-1.228021
H	-4.618836	-0.663965	4.856606	H	6.074626	-1.686218	1.009360
H	-2.875570	-0.499284	4.438138	H	7.444265	-0.934310	0.075248
H	-1.512369	0.892282	0.302924	H	6.086199	-1.781915	-0.790093
O	-4.099649	-5.161254	-1.760957				
O	-2.217804	-4.401956	-2.587617				

16-14e			
-2380.12990298			
C	-1.159515	1.040975	0.021396
C	-1.407106	3.389397	-0.210190
H	-1.270170	3.795513	-1.239268
H	-1.186731	4.208735	0.504260
C	-2.794396	2.766562	-0.002050
H	-3.218995	3.014323	0.997382
H	-3.532131	3.073783	-0.771594
C	1.552024	2.828983	1.251982
C	2.919254	3.165051	1.218088
H	3.426514	3.404784	2.168050
C	3.653335	3.204049	0.014799
C	2.984185	2.883031	-1.181925
H	3.542225	2.892377	-2.133057
C	1.618471	2.535660	-1.204425
C	0.913386	2.510284	0.025640
C	0.794962	2.794028	2.558546
H	1.454953	3.068211	3.404713
H	0.372974	1.785265	2.755793
H	-0.061029	3.503373	2.558868
C	5.115343	3.592269	0.016325
H	5.679539	3.045794	0.800736
H	5.243069	4.677127	0.225016
H	5.595916	3.381895	-0.959762
C	0.943030	2.144448	-2.498948
H	1.647664	2.212574	-3.350205
H	0.071599	2.793089	-2.732150
H	0.563221	1.101360	-2.452292
C	-3.597471	0.388599	-0.246928
C	-4.360098	-0.013060	0.883543
C	-5.426547	-0.913069	0.677924
H	-6.009134	-1.245291	1.553786
C	-5.777102	-1.383716	-0.600973
C	-5.049378	-0.900388	-1.707133
H	-5.332413	-1.223698	-2.722989
C	-3.969503	-0.011391	-1.560777
C	-4.107993	0.546620	2.264029
H	-4.558245	-0.102456	3.040773
H	-4.573257	1.552325	2.372812
H	-3.027643	0.639096	2.488170
C	-6.894939	-2.384939	-0.785974
H	-7.451892	-2.208086	-1.728997
H	-7.617409	-2.354950	0.054492
H	-6.492259	-3.420679	-0.836871
C	-3.238796	0.505955	-2.776687
H	-3.810031	0.290286	-3.700946
H	-2.245312	0.018960	-2.866573
H	-3.068438	1.601654	-2.724174
C	1.307144	-0.565274	0.136916
H	1.773782	0.290045	-0.386518
C	2.222445	-1.652906	0.477014
C	1.942251	-2.604774	1.476933
H	1.013729	-2.500346	2.061563

C	2.841882	-3.655309	1.781722
H	2.581347	-4.372271	2.576168
C	4.043860	-3.781296	1.094726
H	4.743527	-4.601403	1.325536
C	4.388907	-2.843585	0.075824
C	5.604478	-2.923148	-0.665876
H	6.316334	-3.736717	-0.448252
C	5.868967	-1.980869	-1.648787
H	6.795718	-2.013747	-2.242451
C	4.908534	-0.955495	-1.878730
H	5.102484	-0.189586	-2.653206
C	3.481985	-1.763914	-0.243646
N	-0.498748	2.246622	0.018871
N	-2.510857	1.323597	-0.098908
N	3.765197	-0.847444	-1.214304
Cl	-0.786056	-0.653499	2.665604
Cl	-1.033003	-1.943566	-1.582206
Ru	-0.517369	-0.751531	0.343857

<b>PPh<sub>3</sub></b>				<b>PCy<sub>3</sub></b>			
-1035.92206281				-1046.78814573			
P	-0.001003	-0.000719	-1.223816	P	-0.229587	-0.055192	-1.051402
C	1.211296	-1.152405	-0.408549	C	-1.838662	-0.101953	-0.036338
C	0.391831	1.624092	-0.408518	C	-2.720081	1.122420	-0.381874
C	-1.605014	-0.472923	-0.408550	C	-4.088759	1.079091	0.325367
C	-1.710888	-1.326786	0.711763	C	-4.843471	-0.225687	0.026099
C	-2.971977	-1.657460	1.240295	C	-3.983997	-1.449538	0.380577
C	-4.142539	-1.136434	0.662282	C	-2.615638	-1.408619	-0.326122
C	-4.048539	-0.286612	-0.455219	C	0.576306	1.564431	-0.455141
C	-2.791016	0.033089	-0.992443	C	0.575237	1.951158	1.041139
H	-0.799452	-1.737219	1.174269	C	1.119933	3.380856	1.244721
H	-3.038180	-2.326309	2.113776	C	2.524032	3.547921	0.638597
H	-5.129007	-1.396726	1.078242	C	2.544937	3.145566	-0.846183
H	-4.961488	0.120547	-0.919007	C	1.993384	1.722542	-1.053501
H	-2.725016	0.683263	-1.881229	C	0.737013	-1.517918	-0.311991
C	1.369684	-2.431572	-0.993576	C	1.940015	-1.897633	-1.209383
C	2.277049	-3.359202	-0.456259	C	2.566749	-3.238212	-0.780594
C	3.057410	-3.015160	0.662720	C	2.961917	-3.231902	0.706320
C	2.920205	-1.741686	1.241748	C	1.771112	-2.848929	1.601786
C	2.001747	-0.816294	0.713295	C	1.150370	-1.502482	1.174319
H	0.774760	-2.699592	-1.883033	H	-1.603918	-0.070304	1.054270
H	2.384374	-4.352450	-0.921324	H	-2.198030	2.067724	-0.121410
H	3.777567	-3.737979	1.078450	H	-2.876065	1.148872	-1.485949
H	3.531645	-1.463890	2.115613	H	-4.696933	1.960016	0.024043
H	1.899420	0.177671	1.176674	H	-3.935830	1.169831	1.425911
C	-0.291745	2.140833	0.714727	H	-5.100549	-0.260029	-1.057951
C	0.052749	3.398517	1.242594	H	-5.808996	-0.253201	0.576685
C	1.087046	4.153056	0.662272	H	-4.516160	-2.390115	0.118438
C	1.773403	3.648381	-0.457429	H	-3.826065	-1.479147	1.483741
C	1.420728	2.399667	-0.994755	H	-2.019024	-2.295182	-0.021821
H	-1.100767	1.555026	1.179030	H	-2.764779	-1.499008	-1.427645
H	-0.491217	3.789400	2.117809	H	-0.065491	2.313031	-0.981557
H	1.354850	5.137633	1.077963	H	-0.446403	1.873384	1.470303
H	2.580670	4.236502	-0.923008	H	1.207849	1.240424	1.615735
H	1.948301	2.018309	-1.885368	H	0.424757	4.108028	0.764086
				H	1.131973	3.633509	2.327743
				H	3.242045	2.906317	1.200596
				H	2.879435	4.593926	0.764169
				H	3.576370	3.219637	-1.255156
				H	1.925411	3.864613	-1.430685
				H	2.681123	0.996477	-0.562817
				H	1.983374	1.461973	-2.134455
				H	-0.007982	-2.340812	-0.437473
				H	2.715167	-1.100467	-1.150592
				H	1.619386	-1.938485	-2.272706
				H	1.831747	-4.057109	-0.960381
				H	3.449443	-3.468834	-1.416472
				H	3.369789	-4.222194	1.005014
				H	3.786010	-2.497242	0.862308
				H	0.994083	-3.645956	1.540170
				H	2.084812	-2.803928	2.667903
				H	1.902186	-0.697702	1.335938
				H	0.282685	-1.256838	1.824271

PMe <sub>3</sub>				POMe <sub>3</sub>			
-461.011948569				-686.687922057			
C	-0.304998	1.617519	0.281181	P	0.037550	-0.064434	-0.739464
P	0.000731	-0.001154	-0.607897	O	-0.764179	1.370529	-0.587878
C	1.554321	-0.544508	0.282715	C	-0.855559	2.075639	0.661379
C	-1.250284	-1.071525	0.282129	O	1.423874	0.371712	0.093212
H	1.807792	-1.582164	-0.018719	C	2.439350	-0.610473	0.283153
H	2.399777	0.106532	-0.022502	O	-0.613017	-1.010254	0.507227
H	1.456123	-0.507472	1.389808	C	-1.675804	-1.903559	0.178167
H	-1.109394	-2.130920	-0.017192	H	-1.687887	2.801008	0.566258
H	-1.173533	-0.999155	1.389159	H	-1.066295	1.380162	1.501224
H	-2.274236	-0.772383	-0.024316	H	0.086893	2.621444	0.874497
H	-1.292221	2.024470	-0.021443	H	-1.600046	-2.794344	0.835578
H	-0.285986	1.513383	1.388200	H	-2.668864	-1.428378	0.342137
H	0.466475	2.356106	-0.020690	H	-1.626954	-2.243871	-0.882937
				H	3.346544	-0.086877	0.646075
				H	2.135773	-1.369373	1.037775
				H	2.696242	-1.138806	-0.665331

<b>PF<sub>3</sub></b>				<b>Py</b>			
<b>-640.983475065</b>				<b>-248.165897258</b>			
F	0.567701	1.287195	-0.286354	N	0.000000	0.000000	1.428342
P	0.000341	-0.000373	0.515670	C	0.000000	1.149104	0.728703
F	-1.398829	-0.151538	-0.286294	C	0.000000	1.207164	-0.677213
F	0.830561	-1.135036	-0.286802	C	0.000000	0.000000	-1.395645
				C	0.000000	-1.207164	-0.677213
				C	0.000000	-1.149104	0.728703
				H	0.000000	2.082557	1.322346
				H	0.000000	2.179584	-1.194727
				H	0.000000	0.000000	-2.497641
				H	0.000000	-2.179584	-1.194727
				H	0.000000	-2.082557	1.322346

<b>tBuCOO<sup>-</sup></b>				<b>CH<sub>2</sub>Cl<sub>2</sub></b>			
<b>-346.447844077</b>				<b>-78.5402487159</b>			
C	0.543287	0.015894	0.000064	C	0.000000	0.000000	-0.003569
C	-1.076378	0.028855	-0.000038	C	0.000000	0.000000	1.338569
O	-1.600634	-1.119933	-0.000180	H	0.938223	0.000000	-0.584148
O	-1.622814	1.163521	0.000041	H	0.938223	0.000000	1.919148
C	1.105386	1.444097	-0.000185	H	-0.938223	0.000000	1.919148
C	1.001335	-0.752590	1.253919	H	-0.938223	0.000000	-0.584148
C	1.001572	-0.752867	-1.253610				
H	2.223800	1.457597	-0.000319				
H	0.741203	2.003269	-0.887089				
H	0.741179	2.003725	0.886398				
H	2.106712	-0.922494	-1.273092				
H	0.480330	-1.732698	-1.278453				
H	0.728520	-0.202119	-2.181680				
H	2.106506	-0.922004	1.273907				
H	0.727877	-0.201820	2.181861				
H	0.480237	-1.732503	1.278672				

NOOO <sup>-</sup>				MeCOO <sup>-</sup>			
-280.374584112				-228.572004981			
O	-0.762935	-1.141494	0.003052	O	-0.762935	-1.141494	0.003052
O	-0.753281	1.146388	0.003033	O	-0.753281	1.146388	0.003033
N	-0.226320	0.000173	-0.013451	C	-0.226320	0.000173	-0.013451
O	1.366478	-0.004754	-0.005407	C	1.366478	-0.004754	-0.005407
				H	1.777970	-0.930023	-0.468386
				H	1.780734	0.893818	-0.516251
				H	1.730081	0.024534	1.049111

Cl <sup>-</sup>	Br <sup>-</sup>	I <sup>-</sup>
-460.359025202	-2574.23478508	-11.5757464121