

Mechanism of Enyne Metathesis Catalyzed by Grubbs Ruthenium-Carbene Complexes: A DFT Study

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Validation of the Used Methodology

The used quantum-chemical methodology was validated both structurally and energetically. We compared Grubbs η^3 -vinylcarbene complex **30** as well as first- and second-generation Grubbs catalysts with their non-simplified quantum-chemical models after completed geometry optimization at the B3LYP/LACVP* level of theory. The bond lengths of ruthenium σ -bonds differed by 0.01-0.03 Å (Ru=C) to 0.05-0.07 Å (Ru-Cl and Ru-P). Bond angles deviate generally by 1° to 4°, *cis*-bond angles at ruthenium up to 6°. The experimental stability of structure **30** was reproduced theoretically by the predicted higher relative energies of alternative isomeric structures with a different vinylcarbene coordination mode.

The additional basis set flexibility in the single-point calculations generally provided only minor differences in relative energies. An exception is the alkyne insertion step with an overestimation of the Gibbs free reaction energy of about -20 kJ mol⁻¹ at the B3LYP/LACVP* level of theory compared to the relative energies obtained at the triple-zeta single point level of theory. Since this step is clearly irreversible anyway, basis set effects are too small to affect the conclusions made in this study.

Energy Data of Model Complexes

#	E _{total} (B3LYP/LACVP*) [a.u.]	zero point energy [kcal mol ⁻¹]	ΔG correction (1 atm, 298.15 K) [kcal mol ⁻¹]	E _{total} single point (B3LYP/LACV3P**+ // B3LYP/LACVP*) [a.u.]	G _{relativ} [kJ mol ⁻¹]
1	-1820.80898599054	186.348	-31.8389	-1821.0505596428	0.00
2	-1820.80351036481	185.906	-31.8215	-1821.0454076654	11.75
3	-1820.80655197381	186.144	-32.2335	-1821.0485781081	2.70
4	-1359.67797140408	113.816	-25.8772	-1359.8494754356	41.45
5	-1437.02078382863	132.508	-27.801	-1437.2204100741	53.72
5b	-1437.01700557720	132.023	-28.2545	-1437.2158343285	61.81
5c	-1437.00774403212	131.460	-27.6761	-1437.2072656970	84.37
6	-1436.99925233420	131.441	-28.3510	-1437.1982527331	105.13
7	-1437.08470091891	135.224	-27.8845	-1437.2778606425	-86.10
8	-1437.07746709805	134.615	-27.5964	-1437.2715547072	-70.89
9	-1437.08781170019	135.291	-28.0525	-1437.2810969742	-95.02
10	-1898.21800270158	207.595	-34.4819	-1898.4811924313	-136.79
11	-1515.68462386883	169.245	-31.1882	-1515.9030139988	-62.71
12	-1515.68242986910	169.680	-29.8372	-1515.9011901635	-50.45
13	-1515.69313266453	171.034	-29.5749	-1515.9111820756	-69.92
14	-1515.67576761276	169.373	-29.4724	-1515.8943297496	-32.20
15	-1515.67703531990	168.995	-30.5923	-1515.8954738829	-41.47
16	-1438.27649782179	148.076	-28.5190	-1438.4736642797	71.14
16b	-1438.27542264353	148.231	-28.2271	-1438.4722500575	76.73
16c	-1438.27444712135	148.015	-28.5150	-1438.4720655149	75.10
17	-1438.27544335741	148.142	-28.1646	-1438.4724583287	76.07
18	-1438.29396858164	150.049	-27.5881	-1438.4897145715	41.15
19	-1514.43004540308	153.870	-29.8382	-1514.6511288672	-80.28
20	-1514.40788769442	153.132	-30.0054	-1514.6282590094	-24.02
21	-1514.49240934618	156.293	-30.0257	-1514.7077740373	-219.64
22	-1515.66623459488	170.532	-28.9813	-1515.8824784466	5.82
23	-1515.69722565730	171.975	-28.6769	-1515.9132506259	-67.66
23 isomer	-1515.70026218678	172.243	-28.2845	-1515.9159988206	-72.11
24	-1436.96679018513	132.268	-28.6711	-1437.1620699703	202.25
25	-1437.04608091480	135.144	-27.2323	-1437.2405333788	14.30
26	-1437.02996870700	134.128	-27.2745	-1437.2262660658	47.33
27	-1437.06140649924	134.897	-28.0171	-1437.2571085872	-33.54
28	-1437.06037626873	134.517	-27.8333	-1437.2551069752	-29.10
29	-1437.08240083031	134.786	-28.6202	-1437.2748894217	-83.21

#	E_{total} (B3LYP/LACVP*) [a.u.]	zero point energy [kcal mol ⁻¹]	ΔG correction (1 atm, 298.15 K) [kcal mol ⁻¹]	E_{total} single point (B3LYP/LACV3P**+/ / B3LYP/LACVP*) [a.u.]	G_{relativ} [kJ mol ⁻¹]
30	-2749.58373437400	-	-	-	0.00
31	-2749.57975149422	-	-	-	10.46
6-Me ₂ 2,4-isomer	-1515.64896829230	167.552	-30.8783	-1515.86800571300	105.84
6-Me ₂ 2,3-isomer	-1515.64517972774	167.926	-30.4534	-1515.86365933040	120.59
6-Me ₁ 4-isomer	-1476.32595375442	149.646	-29.9565	-1476.53461867241	108.66
6-Me ₁ 3-isomer	-1476.32390628683	149.995	-29.6240	-1476.53192527591	118.58
ethene	-78.58581299934	32.15	-13.0998	-78.6154688406	-
ethyne	-77.32383605858	16.645	-11.9523	-77.3563641018	-
propene	-117.90519708326	50.265	-15.6864	-117.94546243195	-
propyne	-116.65077344182	34.902	-14.5650	-116.69255106368	-
butadiene	-155.98884509371	53.656	-16.1768	-156.0406785745	-
PMe ₃	-461.09394380789	71.176	-17.7357	-461.1643713828	-

#	E _{total} (B3LYP/LACVP*) [a.u.]	zero point energy [kcal mol ⁻¹]	ΔG correction (1 atm, 298.15 K) [kcal mol ⁻¹]	E _{total} single point (B3LYP/LACV3P**+/ /B3LYP/LACVP*) [a.u.]	G _{relativ} [kJ mol ⁻¹]
1(1 st)	-1975.88847166297	162.2890	-31.7578	-1976.11468653858	0.00
2(1 st)	-1975.88813151471	162.0840	-31.1178	-1976.11437864389	2.63
3(1 st)	-1975.89215855923	162.4150	-31.1959	-1976.11907030806	-8.63
4(1 st)	-1514.75786228876	89.9580	-25.0677	-1514.91438177615	43.30
5(1 st)	-1592.09687307077	108.8050	-26.7416	-1592.28073849459	69.28
5b(1 st)	-1592.10030819870	108.2360	-27.2561	-1592.28412159578	55.86
5c(1 st)	-1592.09089607882	107.7760	-26.9731	-1592.27492127515	79.28
6(1 st)	-1592.06909939260	107.9520	-27.7751	-1592.25242775452	135.72
7(1 st)	-1592.16489995622	111.3390	-27.1885	-1592.34279478571	-84.92
8(1 st)	-1592.15736126352	110.7820	-26.9518	-1592.33605698379	-68.57
9(1 st)	-1592.16695128820	111.4120	-27.4037	-1592.34504408304	-91.42
10(1 st)	-2053.29843334021	183.8840	-34.0842	-2053.54631284610	-136.62
11(1 st)	-1670.76336896567	145.5890	-30.2758	-1670.96650693468	-55.88
12(1 st)	-1670.75406429838	146.2490	-28.8841	-1670.95742465988	-23.45
13(1 st)	-1670.75947132179	147.2340	-28.7037	-1670.96248697646	-31.87
14(1 st)	-1670.74832510588	145.9170	-28.6436	-1670.95194669936	-9.45
15(1 st)	-1670.76014876362	145.3310	-29.3265	-1670.96392974099	-46.22
16(1 st)	-1593.35878853056	124.1680	-27.8137	-1593.54066516553	66.84
16b(1 st)	-1593.35950687144	124.4800	-27.1981	-1593.54119700386	69.33
16c(1 st)	-1593.35092413834	124.3790	-27.3672	-1593.53276072822	90.35
17(1 st)	-1593.34718710783	124.2280	-27.8966	-1593.52834055031	99.10
18(1 st)	-1593.36035920703	126.2680	-26.9384	-1593.54100557746	78.40
19(1 st)	-1669.50710212785	130.1570	-28.9977	-1669.71272136109	-69.00
20(1 st)	-1669.47943128794	129.6160	-28.8488	-1669.68376043257	5.40
21(1 st)	-1669.57180791306	132.5260	-29.1468	-1669.77163408490	-214.38
22(1 st)	-1670.74296185315	146.8400	-27.9684	-1670.94391912250	18.31
23(1 st)	-1670.77966449980	148.3110	-27.6741	-1670.97988019348	-68.72
24(1 st)	-1592.04508735929	108.6610	-27.5695	-1592.22482654014	231.64
25(1 st)	-1592.12170996184	111.4280	-26.3389	-1592.30079497634	48.91
26(1 st)	-1592.10159468225	110.3300	-26.6369	-1592.28245278121	91.23
27(1 st)	-1592.13256789395	111.5190	-26.4197	-1592.31216114172	19.11
28(1 st)	-1592.13108351891	111.1080	-26.3091	-1592.30964330472	24.47
29(1 st)	-1592.15854817675	111.2920	-26.9657	-1592.33676252696	-48.71
32(1 st)	-1592.12216341698	111.0320	-26.8438	-1592.30147521896	23.72
33(1 st)	-1592.12123640578	111.0870	-26.0298	-1592.30070024246	29.39

#	E_{total} (B3LYP/LACVP*) [a.u.]	zero point energy [kcal mol ⁻¹]	ΔG correction (1 atm, 298.15 K) [kcal mol ⁻¹]	E_{total} single point (B3LYP/LACV3P**+// B3LYP/LACVP*) [a.u.]	G_{relativ} [kJ mol ⁻¹]
34	-1632.35351418786	207.6940	-34.2951	-1632.61009056754	84.38
35	-1632.34952626776	207.5480	-34.2735	-1632.60573246362	91.58
36	-1632.34962941537	207.458	-34.8388	-1632.60610624379	95.31
37	-1632.36956129061	209.6740	-33.3363	-1632.62439919470	59.11
37 isomer	-1632.36897627495	209.665	-33.3701	-1632.62379572879	60.51
38	-1632.35663720410	207.7720	-33.8031	-1632.61263299837	80.09
39	-1632.35616085137	207.7200	-34.2407	-1632.61229380984	78.94
40	-2014.89026978239	246.1380	-37.6941	-2015.19072498756	3.81
41	-1553.76253053123	173.6350	-31.6506	-1553.99292437271	37.11
42	-1553.76932896141	173.8140	-30.2386	-1553.99577270910	36.29
43	-1553.75163818300	174.0510	-29.7885	-1553.97672237394	89.18
44	-1553.82573558051	176.0010	-30.2018	-1554.04724387048	-89.55
45	-1553.81746450152	175.5940	-29.4339	-1554.03968568985	-68.19
46	-1553.82928855312	176.0770	-30.1641	-1554.05103092071	-99.01
47	-2014.95382928290	248.3890	-36.4520	-2015.24557568513	-125.58
48	-1632.42064235329	209.9930	-33.3375	-1632.66804574173	-54.15
49	-1632.41790215646	210.4810	-32.0919	-1632.66521556836	-39.47
50	-1632.42827706071	211.8270	-31.6827	-1632.67447210367	-56.43
51	-1632.41190443332	210.2080	-31.4973	-1632.65855994932	-20.65
52	-1632.41362902454	209.7740	-32.6890	-1632.66068931044	-33.04
48-Me	-1671.73906171882	227.868	-33.8188	-1671.99756190206	(80.49 to 47 + H ₂ CCHMe)
49-Me	-1671.73179213884	228.240	-32.9609	-1671.98969027319	(106.30 to 47 + H ₂ CCHMe)
50-Me	-1671.74338289830	229.476	-32.6171	-1672.00002184853	(85.79 to 47 + H ₂ CCHMe)
51-Me	-1671.73303686978	227.959	-33.0831	-1671.99024192975	(103.16 to 47 + H ₂ CCHMe)
48-OMe	-1746.94370779028	230.652	-35.1732	-1747.22668111048	(78.70 to 47 + H ₂ CCHOMe)
49-OMe	-1746.93495070713	231.054	-33.8697	-1747.21757762898	(109.73 to 47 + H ₂ CCHOMe)
50-OMe	-1746.94788157391	232.356	-33.9420	-1747.22950307572	(83.57 to 47 + H ₂ CCHOMe)
51-OMe	-1746.94450597064	231.525	-34.2132	-1747.22582690556	(88.69 to 47 + H ₂ CCHOMe)
53	-1632.36100512177	207.6140	-33.8030	-1632.61682380962	68.43
54	-1632.34186012352	206.7400	-34.4570	-1632.59661420172	115.10
55	-1632.41618581518	209.7720	-33.4764	-1632.66624329565	-50.93
56	-1632.41329186332	209.3760	-33.1463	-1632.66332767007	-43.55
57	-1632.41734780096	210.1290	-33.3865	-1632.66737437887	-52.03
58	-2093.54606215040	282.8320	-39.0053	-2093.86613761994	-85.24
59	-1632.42938112073	211.0760	-31.7745	-1632.67629555649	-64.74
60	-1632.41703583699	211.2140	-30.9066	-1632.66440931810	-29.32
61	-1632.41940573088	211.8920	-30.6546	-1632.66595970335	-29.50
62	-1632.40494239376	210.4090	-30.5741	-1632.65190472135	1.53
63	-1632.41068264879	209.5030	-32.4332	-1632.65845062266	-27.23
H ₂ C=CHOMe	-193.10697760122	53.210	-17.4656	-193.17347990695	
hept-1-en-6-yne	-272.66522365250	92.4270	-20.8088	-272.75395413453	-
1-vinyl cyclo pentene	-272.72704965945	94.6300	-19.2112	-272.80710177523	-

Cartesian Coordinates of Model Complexes

Intermolecular Enyne Metathesis

1

C	-0.4758870748	0.3400137769	-2.4394668634
N	-0.9214236553	0.6560441856	-1.0710246635
C	-0.0834145410	0.1542587913	-0.1456013644
N	0.9809945840	-0.3787566817	-0.7802551630
C	0.9881910430	-0.0557974218	-2.2135371173
Ru	-0.1636766473	0.0940271287	1.9348409763
P	0.4176764445	-0.5256191671	4.1894055457
C	-0.9313683142	-1.2484292883	5.2117878156
C	2.2012536124	-0.7936145950	-0.1067978575
C	-2.2957135756	1.0676062467	-0.8620750625
C	-1.5885514275	1.0884918881	2.4512910756
Cl	1.3862488810	2.0062425100	1.9805014119
Cl	-1.4511784617	-2.0005181234	1.7902924617
C	1.6766530369	-1.8758432813	4.1366302332
C	1.1826542181	0.7557763297	5.2653594370
H	1.6760613652	0.7794126802	-2.4106090465
H	1.3015190451	-0.9175225894	-2.8108385147
H	-1.0723383202	-0.4920598871	-2.8414553291
H	-0.5948111229	1.2051546228	-3.0987948031
H	2.7358408720	-1.5022602892	-0.7475812360
H	2.8455890429	0.0606322514	0.1310400914
H	1.9453640450	-1.3165673654	0.8201975777
H	-2.5111371483	1.9500873419	-1.4750878103
H	-2.9927983513	0.2628097504	-1.1337677168
H	-2.4358709551	1.3163980599	0.1886787027
H	-2.5746355738	0.6344852836	2.6157091553
H	-1.4906647895	2.1658160347	2.6354906814
H	-0.5413758130	-1.6932403795	6.1341375039
H	-1.6498361571	-0.4626734909	5.4662725622
H	-1.4443722252	-2.0051263948	4.6116538268
H	1.9438042455	-2.2078165897	5.1463911070
H	1.2606730378	-2.7183122698	3.5755332008
H	2.5804129963	-1.5208959002	3.6306399471
H	1.5584571752	0.3211385382	6.1985433131
H	1.9921753180	1.2401719778	4.7133218748
H	0.4358376859	1.5216716317	5.4962589581

2

C	0.764597	-0.497175	-2.334128
C	-0.610985	0.169369	-2.466296
N	-0.902297	0.568053	-1.079029
C	-0.030299	0.047500	-0.187741
N	0.901344	-0.638948	-0.878329
C	-2.217143	1.113364	-0.780398
Ru	-0.094094	0.209435	1.935027
Cl	-2.049818	-1.244732	1.860476
C	2.045700	-1.362617	-0.354731
P	-0.018031	-0.034050	4.344287
C	0.812090	1.301434	5.307285
C	-0.699502	1.920766	2.066652

Cl	2.263516	0.863899	2.113425
C	-1.621246	-0.269033	5.224499
C	0.946662	-1.540627	4.795612
H	1.576667	0.130978	-2.725986
H	0.820555	-1.474075	-2.827042
H	-1.383241	-0.527983	-2.820394
H	-0.604162	1.038367	-3.132847
H	2.063330	-2.370307	-0.789330
H	2.982772	-0.848314	-0.599413
H	1.980648	-1.434631	0.728766
H	-2.251781	2.196040	-0.958482
H	-2.957561	0.633617	-1.432510
H	-2.482447	0.882632	0.249209
H	-0.280937	2.637489	2.785387
H	-1.487356	2.332462	1.425305
H	-1.469572	-0.534819	6.276784
H	-2.202342	0.657348	5.167967
H	-2.188705	-1.051899	4.714591
H	1.005695	-1.672053	5.882145
H	0.467908	-2.420771	4.354308
H	1.955836	-1.444237	4.384142
H	0.920771	1.024232	6.361752
H	1.794074	1.489538	4.865015
H	0.221660	2.221521	5.243744

3

C	-0.0197596250	0.0594176327	-0.1993546541
Ru	-0.0087861739	0.1206853005	1.9328033293
N	0.9188697310	-0.4473854969	-1.0252252345
N	-1.0225495331	0.5443570794	-0.9804440707
C	0.6487796115	-0.1845466233	-2.4450904985
C	2.1820510974	-1.0723331541	-0.6755762941
C	-0.8104800789	0.2755384237	-2.4120249755
C	-2.3915896372	0.8307082678	-0.5746010767
H	1.3282034068	0.5958707149	-2.8167090888
H	0.8067435627	-1.0871612948	-3.0450922849
H	-1.5041947349	-0.5096472853	-2.7465307087
H	-0.9961113548	1.1724560662	-3.0125024104
H	2.3098558889	-1.9716255548	-1.2910168023
H	3.0253919957	-0.3942850811	-0.8543445711
H	2.1855049893	-1.3455716806	0.3757968279
H	-2.6940270070	1.8227963535	-0.9340215691
H	-3.0682365616	0.0821301508	-1.0083781153
H	-2.4813242757	0.7812597151	0.5064967220
C	-0.6876808659	1.8149750983	1.9231613383
H	-0.9959602672	2.3568349726	2.8265468487
H	-0.7786860435	2.3978329213	0.9995439235
Cl	2.3526896572	0.5576122056	2.1504093728
Cl	-1.7819826748	-1.5092780954	1.9081191095
P	-0.0954008716	0.0313300573	4.3582521719
C	0.4884424864	-1.5856028951	5.0273758695
C	0.9006883278	1.2667945715	5.3004443016
C	-1.7825409624	0.1997832742	5.0899968784
H	-1.7716928566	0.0647747573	6.1774427032
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H	0.4035782057	-1.6284090188	6.1192520203

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4

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N	-1.0790240852	-0.0098872698	-0.6674469424
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Cl	1.8150952294	-1.0232193325	2.8559553438
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H	1.4953718978	-0.3465800359	-2.5704174053
H	-0.7497894472	-1.1957404057	-2.3901512775
H	-1.2474294504	0.4795619781	-2.7205971957
H	3.1865136654	0.0710898863	-0.6770306611
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5

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6

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Ru	-0.1427337661	0.1163937061	1.8876989676
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H	2.8465967103	1.5316717552	-0.4392299074

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H	-2.5466274546	-0.5620683842	0.3015310435
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Cl	1.8290732177	-1.5616595241	2.0338344760
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H	1.1878062890	2.7325630519	-0.6504768265
H	2.1265806628	1.6837309252	0.4414164471
H	2.6021929553	1.8246697848	-1.2601609752
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H	-2.1668489092	-1.3210161481	0.6137237278
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C	1.1334087712	0.9738596446	-3.0659924331
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H	-0.7876873562	-1.5185163425	2.6262368066
H	-1.4478784804	0.1230313661	2.3985430032
H	2.0517345806	1.5044683664	-0.6854043648
H	2.9771859662	0.3384573038	0.2945293105

H	2.4059316595	1.8712779182	1.0156782082
H	-2.4029373717	-2.2362944760	0.7162343538
H	-1.8904499687	-1.8138562345	-0.9207029114
H	-2.8771721060	-0.6546867541	0.0108395025
C	1.1236565023	2.4184158084	-3.2666833484
H	-2.2029909557	-0.4596538605	-3.8148711915
H	-0.9878463108	-1.8674719725	-3.9588074338
H	0.6240629762	-0.3524185665	-5.0197767948
H	-0.5765164089	1.0506415673	-4.8555882646
C	2.2326379205	3.0684594857	-3.6659680844
H	0.2077336718	2.9547750936	-3.0360080436
H	2.2527794029	4.1502717445	-3.7690072253
H	3.1558772143	2.5369871430	-3.8896861644

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C	-0.0799570514	-0.2009539570	-0.1280319837
N	0.7625145360	0.3799509844	0.7372907935
C	0.4955971135	-0.0679755384	2.1138537045
C	-0.9261519178	-0.6371298389	1.9859268128
N	-1.0164111968	-0.8933252945	0.5386852382
C	2.0391046850	0.9785787550	0.3767864975
C	-2.2453070579	-1.4025228509	-0.0544458533
Ru	0.0464517545	-0.0896564826	-2.1424406410
C	1.1033493686	0.9571258250	-3.4478579733
C	0.2084157144	0.0826510844	-4.4086599488
C	-0.9942410905	-0.7205193388	-3.7387000680
C	-1.0718135655	-2.1679810091	-3.9781555441
C	-2.2419466216	-2.8121605750	-4.1183944550
Cl	1.7570610839	-1.8290627296	-2.1031678723
Cl	-1.5697505207	1.7456026272	-1.9795346938
H	0.5658752675	0.7671506095	2.8166854320
H	1.2238940657	-0.8386993453	2.4037796891
H	-1.0760401160	-1.5586952378	2.5555402731
H	-1.6908997691	0.0940338147	2.2842693531
H	1.9564694280	1.4244518754	-0.6159459479
H	2.8407929702	0.2301471403	0.3644046828
H	2.2787071592	1.7677035453	1.0964768883
H	-2.6031761586	-2.2453213304	0.5449235848
H	-2.0434802302	-1.7623210269	-1.0654348734
H	-3.0162414457	-0.6237466146	-0.1002647427
H	2.1601823936	0.6969790349	-3.5035268629
H	0.8780307355	2.0222112977	-3.4882291755
H	-0.2866447023	0.7864270387	-5.0816409099
H	-1.9422127198	-0.1913297146	-3.8451576162
H	0.8463093468	-0.6322699736	-4.9283906140
H	-0.1331836900	-2.7157078581	-4.0021879742
H	-2.2828333150	-3.8865297551	-4.2735991850
H	-3.1926214766	-2.2832845251	-4.0847172674

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N	0.8513941139	0.3452550085	0.7632567630
C	0.5816037338	-0.1196244189	2.1345858394
C	-0.8634906040	-0.6137672341	2.0201027473
N	-0.9861474772	-0.8319003220	0.5705895647
C	-0.0282673996	-0.1748978825	-0.1130822495

C	-2.2503187173	-1.3003971955	0.0217790001
Ru	0.0089596199	-0.0855535857	-2.1697243341
C	0.2761267755	-0.0206128947	-4.5397662521
C	-0.8851524621	-0.6957718918	-4.1360692265
C	2.1736475605	0.8610863031	0.4441769977
Cl	1.8949275780	-1.6641903817	-2.1359339763
Cl	-1.8910167113	1.4709407868	-2.0547568821
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H	0.7073534272	0.6939421957	2.8551067918
H	1.2756939223	-0.9318021071	2.3951199105
H	-1.0521086322	-1.5380520745	2.5743523539
H	-1.5879703737	0.1469752190	2.3456368301
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H	2.9047138834	0.0506881995	0.3390975072
H	2.4834943978	1.5412932113	1.2436846854
H	-2.5911452137	-2.1564810107	0.6139142662
H	-2.1122466088	-1.6301832372	-1.0089348998
H	-3.0087676724	-0.5094959016	0.0363509689
H	2.1639150865	1.0927329438	-2.9823152328
H	0.7047555926	2.2621063042	-2.9930000324
H	0.1672740453	0.9488261433	-5.0163527480
H	-1.8310990640	-0.1631572879	-4.2021405312
C	-0.9594402234	-2.1483860203	-3.9438265372
H	1.1958527782	-0.5683350622	-4.7192722674
C	-2.1239361335	-2.7863223331	-3.7309942521
H	-0.0220638788	-2.6982496167	-3.9606395311
H	-2.1611163153	-3.8636718926	-3.5993839054
H	-3.0701339601	-2.2502882146	-3.6964004420

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C	-0.0393226142	-0.1783851913	-0.1515554605
N	0.8452194331	0.2925592293	0.7504708558
C	0.5581680730	-0.2119214070	2.1041647682
C	-0.8904310277	-0.6855423499	1.9637986319
N	-1.0148990649	-0.8384801336	0.5068106593
C	2.1829010506	0.7897379144	0.4658094084
C	-2.2901463717	-1.2756396173	-0.0415913440
Ru	0.0179744574	-0.0593372616	-2.2037029670
C	1.0412624096	1.4263304599	-2.4638707171
C	0.3452781382	-0.1224741277	-4.6618680729
C	-0.8325211051	-0.7311504701	-4.2993545473
C	-0.9291092751	-2.1445320838	-3.9208178039
C	-2.0953121074	-2.7248104088	-3.5853919052
Cl	1.9695151124	-1.5641358786	-2.1589339790
Cl	-1.9918530974	1.3591680185	-2.1382212230
H	0.6868706042	0.5773891115	2.8506600587
H	1.2411059806	-1.0391501116	2.3454047303
H	-1.0904908338	-1.6317315831	2.4755353883
H	-1.6097672672	0.0660136355	2.3207101884
H	2.1419448853	1.5140395034	-0.3484878232
H	2.8597194838	-0.0223747263	0.1793836403
H	2.5561711545	1.2963175414	1.3607732777
H	-2.6017464833	-2.1842011481	0.4860239429
H	-2.1850296383	-1.5049761779	-1.1007016218
H	-3.0556888684	-0.4995042701	0.0687227071
H	2.1130332562	1.3450933641	-2.6838916759
H	0.6020033391	2.4309602308	-2.4778903928

H	0.3280876013	0.8785759594	-5.0803756318
H	-1.7639996715	-0.1784399860	-4.3914170171
H	1.2824304118	-0.6689423035	-4.6903145778
H	-0.0032301247	-2.7140456221	-3.9022705604
H	-2.1456087360	-3.7754827128	-3.3147206378
H	-3.0290280937	-2.1666250651	-3.5857208536

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C	-0.6415896830	0.0237346069	2.2951621524
N	-0.9329769560	-0.2799258954	0.8893229949
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C	0.8620088218	0.3157707530	2.2570786224
Ru	-0.0146871478	-0.0020043259	-1.9835621299
Cl	-2.1700077796	1.0797842913	-2.0946326570
C	2.5195742179	0.5605362905	0.4152127213
C	-2.2494654245	-0.7952835303	0.5523501814
C	0.9881118650	1.5204047654	-2.0964498713
Cl	1.4603844961	-1.8910795682	-1.8928836834
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H	1.4599648742	-0.5193747597	2.6487859648
H	-0.9014808639	-0.8240912467	2.9379150097
H	-1.2303333059	0.8932970113	2.6188921809
H	2.9201826551	1.5603303329	0.6242827840
H	2.6235147010	0.3262478514	-0.6412158531
H	3.1035003694	-0.1738918210	0.9851498510
H	-2.4731797805	-1.6349414984	1.2218151502
H	-2.2656634545	-1.1442999007	-0.4773095165
H	-3.0210971438	-0.0257176934	0.6632089148
H	1.4082538100	1.8809999111	-3.0410675792
H	1.1687277989	2.1722994872	-1.2357476812
C	0.2981141398	0.0243715392	-4.4985326795
C	-0.6655210591	-0.8874065864	-4.2320425777
H	0.0376327758	1.0459719805	-4.7592649040
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16b

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N	-1.1631005915	0.0610276746	-0.8142877542
C	-0.0798381953	0.1062538146	-0.0169154949
C	-2.5626639029	0.1620921566	-0.4368695274
Ru	-0.1266866458	0.2441171976	2.0396602373
Cl	0.3823525375	2.5674003279	1.6213199713
C	2.3742927401	0.4734946922	-0.4568888437
C	1.3871698033	-0.7428989234	2.2313572227
Cl	-1.6849369149	-1.6163998481	2.0823479484
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H	0.9502770263	1.0046856256	-2.6857447925
H	1.2399159000	-0.7478148934	-2.7630309830
H	-1.0921376626	-1.2378975162	-2.4775470019

H	-1.3801313319	0.4692084897	-2.8830152391
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H	2.4087686540	0.8026412102	0.5785426094
H	3.0928174487	-0.3392843450	-0.6204189514
H	-3.0596247623	0.8424996221	-1.1393643351
H	-3.0566581642	-0.8146257525	-0.4607182035
H	-2.6514343499	0.5656088799	0.5695349080
H	1.8858372068	-0.8271913747	3.2057371959
H	1.8279192173	-1.3484933388	1.4334242478
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H	-0.3224583833	-0.9791634697	4.6652474612
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16c

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C	1.5250656992	-0.4194530731	2.4514802889
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C	-1.1939220400	-0.0118202049	4.1393090862
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H	0.7072164507	-0.5324794625	-2.9577241811
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H	-1.7679327558	0.8594739671	-2.6235162448
H	2.5842020734	1.0590041549	-0.5512538690
H	2.4810011409	-0.5192593906	0.2656461947
H	2.7579197307	-0.4623285155	-1.4852536506
H	-3.3364084192	0.8745342289	-0.6014812101
H	-2.9908115407	-0.6912501401	0.2109761284
H	-2.5713661354	0.8555527674	0.9885116057
H	1.7016161712	-1.4915661627	2.5949143632
H	2.3710250714	0.2668155888	2.5719111903
H	-1.2426593846	2.1108351118	3.7869352952
H	-0.6894303219	-0.8416044397	4.6216180148
H	0.3073827777	1.4840709399	4.5411206813
H	-2.2305718092	-0.1930234019	3.8690070428

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C	0.6208772053	-0.2375018187	2.1225325564
C	-0.8610260845	-0.6189029591	2.0203752790
N	-1.0306879615	-0.7542192142	0.5656365056
C	-0.0340835520	-0.1512074669	-0.1091328283
N	0.9030127200	0.2593305067	0.7640731907
C	-2.3340563331	-1.0889911430	0.0106953892
Ru	-0.0348245740	-0.0392680633	-2.1565622863
Cl	1.5956292572	-1.8600795592	-2.1986801338
C	2.2617763480	0.6531363884	0.4238451209

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C	1.1651608221	1.1880381183	-2.8313032696
C	-0.8828627211	-0.7356756222	-4.0670763744
C	0.1367980528	0.0862601552	-4.5612241630
H	0.8197881393	0.5352782272	2.8707629889
H	1.2563608854	-1.1084575000	2.3376096107
H	-1.1044968152	-1.5542331239	2.5332708415
H	-1.5200032917	0.1746682658	2.4014868684
H	2.2483929927	1.2411929835	-0.4934338365
H	2.9031461256	-0.2235638253	0.2716079592
H	2.6610113572	1.2701120183	1.2349928510
H	-2.7274019723	-1.9664471017	0.5350041238
H	-2.2365195527	-1.3369140365	-1.0482004545
H	-3.0346446408	-0.2508079402	0.1008467832
H	2.2044001270	0.9133127375	-3.0413323970
H	0.8682875646	2.2256505407	-3.0130353558
H	-0.1169114571	1.0641154478	-4.9595451091
H	-1.9075405703	-0.3755753424	-4.0802998445
H	-0.7090134280	-1.8084338667	-4.0238956590
H	1.0808747857	-0.3566212368	-4.8609895643

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C	0.0000000000	0.0000000000	-1.3149168052
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N	-0.5669516485	-0.9406086246	-2.0837029531
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Ru	0.0000000000	0.0000000000	0.7080789311
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C	0.0000000000	0.0000000000	2.9890879365
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Cl	2.2540860569	-0.9235700264	0.6536420993
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H	0.2864136259	1.4016972915	-4.1390756525
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H	-0.2864136259	-1.4016972915	-4.1390756525
H	-1.5223712832	-0.1607768874	-3.8015934865
H	1.2568839904	2.2208932369	-0.5846791483
H	2.5375576263	1.5605929682	-1.6265921075
H	1.4327949384	2.8329196407	-2.2418909672
H	-1.4327949384	-2.8329196407	-2.2418909672
H	-1.2568839904	-2.2208932369	-0.5846791483
H	-2.5375576263	-1.5605929682	-1.6265921075
H	1.5942679754	1.4082433249	2.2648488343
H	-0.1085409289	2.1220220717	2.2558543515
H	-0.8430821157	0.3555345151	3.5827618679
H	-1.5942679754	-1.4082433249	2.2648488343
H	0.1085409289	-2.1220220717	2.2558543515
H	0.8430821157	-0.3555345151	3.5827618679

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C	0.5744920923	0.0933630497	-2.0329963120
C	-0.7222815984	-0.7096883364	-1.8852669341

N	-1.0066353459	-0.5409944131	-0.4536460354
C	0.0813815078	-0.1412568597	0.2293274953
N	1.0630092739	0.1409348296	-0.6428010008
C	-2.1993102698	-1.1356144629	0.1288709875
Ru	-0.0514690997	-0.0023132117	2.3060518027
C	1.7057425570	0.3307945996	2.7608012133
H	2.0110050414	1.3849969996	2.7510615842
C	2.2847754149	0.8756546629	-0.3560125138
C	-1.2465308485	0.6275328468	4.0080506441
C	-1.0961272168	-0.6040207105	4.1173699901
Cl	0.2265310947	-2.4794053967	2.1598450951
Cl	-0.2983801392	2.4101060314	1.7650288545
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H	1.3089572344	-0.3844874805	-2.6875005209
H	-0.5788264578	-1.7751748992	-2.1153978447
H	-1.5441243921	-0.3249478694	-2.4964736168
H	2.7313773879	0.5001766751	0.5637288396
H	2.9867763510	0.7082902510	-1.1781290918
H	2.0858641849	1.9488104967	-0.2507700942
H	-2.0866288053	-2.2179620968	0.2561698448
H	-2.3990220231	-0.6883792421	1.1058438569
H	-3.0529644763	-0.9187151684	-0.5215071026
C	2.6943111394	-0.6002009292	3.2638524517
H	-1.5271361175	1.6474435679	4.1850356830
H	-1.1288263375	-1.6157445122	4.4719635078
C	3.8904012667	-0.1626864918	3.7123862258
H	2.4516613523	-1.6577871801	3.2677733466
H	4.6438182807	-0.8488618432	4.0901296667
H	4.1444712781	0.8956249135	3.7170934264

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N	-1.0349580800	-0.8001810908	-0.5120148967
C	-0.0126186424	-0.1975359986	0.1214943678
N	0.9122375988	0.1670959253	-0.7867321871
C	0.4203867768	-0.0453312902	-2.1594907914
C	-0.7391434790	-1.0229940212	-1.9338851780
Ru	-0.0298050263	0.0892792995	2.1469173444
Cl	0.5515338717	-2.3043069153	2.3548283985
C	1.9895807171	1.1162496012	-0.5563916834
C	-2.0963331775	-1.5404626350	0.1541870234
Cl	-0.8653868382	2.3461661506	1.7564640608
C	1.5455550374	0.7804792562	2.9073505298
C	2.7187297639	0.0496840583	3.3620312155
C	3.8587401074	0.6989063064	3.6671151686
C	-0.9852068523	-0.1414740859	4.0525778043
C	0.0083554888	0.4878871381	4.4775088362
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H	1.2100020852	-0.4506605696	-2.7989272852
H	-0.4373068083	-2.0676851890	-2.0972451554
H	-1.6140944031	-0.8078201097	-2.5545075742
H	2.4113658794	0.9520034710	0.4344385658
H	2.7729271336	0.9431449427	-1.3009922776
H	1.6340077475	2.1517934309	-0.6299468697
H	-1.7857802710	-2.5625255754	0.3972247020
H	-2.3782441547	-1.0262504598	1.0774000015
H	-2.9748158156	-1.5587251728	-0.4987435250
H	1.6270130822	1.8749033245	2.9353112547

H	0.6072456631	1.0304148267	5.1805880097
H	-1.9193287650	-0.6531169035	4.1920027028
H	2.6518914758	-1.0329936479	3.4089087041
H	4.7558868488	0.1637157579	3.9667985463
H	3.9293335146	1.7838714810	3.6135504242

21

N	-0.3299118439000	-0.4159571402000	-1.2298651003000
C	-1.4833386345000	-1.0212781823000	-1.9033789750000
C	-2.1131344871000	-1.8488360176000	-0.7797756563000
N	-1.5001133949000	-1.2687175383000	0.4229099829000
C	-0.4299768338000	-0.4814609424000	0.1197437974000
C	-1.7953102485000	-1.9289724116000	1.6878689783000
Ru	0.7653446629000	0.4039128893000	1.4104413473000
Cl	1.1518441860000	2.5224697529000	0.4090765559000
C	0.5997341370000	0.3681407741000	-2.0263635376000
C	-0.5941078913000	0.8405321982000	2.5868781147000
C	-0.3699681591000	1.2618685408000	3.9442284713000
C	0.6905782609000	0.8890643528000	4.7186354349000
C	0.8739376650000	1.3194307698000	6.0867080760000
C	1.8917581031000	0.9037816518000	6.8630766826000
Cl	1.6584540474000	-1.6434017797000	2.2075936604000
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H	-1.8506194317000	-2.9145531223000	-0.8500166236000
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H	1.4767126764000	0.6278231540000	-1.4383599904000
H	0.9047497223000	-0.2312095879000	-2.8920400513000
H	0.1377193136000	1.2993098522000	-2.3757337632000
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H	1.4219247168000	0.1921795668000	4.3100451936000
H	-1.1347260310000	1.9038125582000	4.3899140427000
H	-1.6295666865000	0.8962866548000	2.2312558671000
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H	2.0060899353000	1.2471807830000	7.8868781960000
H	2.6386454029000	0.2060775909000	6.4915681940000

22

C	-0.1394114297	-0.3406274077	-0.1765528297
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C	-0.9041813534	-0.2585933586	2.0180817383
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Ru	-0.2005376049	-0.7690765516	-2.1644293876
Cl	1.5215928797	-2.3492050977	-2.0074584606
Cl	-1.8578750446	1.1238554694	-1.6876827089
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C	-1.1698735782	-0.4018878511	-4.0451770389
C	-0.9107686639	-1.7617949851	-4.5240246086
C	-1.8652642318	-2.7114682721	-4.6448278999

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H	1.2562540799	-0.3675892968	2.4399623993
H	-1.0451531639	-1.0106809932	2.8001238779
H	-1.6514781794	0.5368359909	2.1511904950
H	2.1468458439	0.6146574970	-1.0298648353
H	2.8708571786	0.3801412440	0.5759746898
H	2.1090229100	1.9417237009	0.1671030902
H	-3.0944317008	-0.7617294059	0.1807899109
H	-2.5553010225	-2.2338097289	1.0604804166
H	-2.1504742164	-2.0144318673	-0.6535526433
H	-2.2150532532	-0.1134133389	-4.0018405563
H	0.3410835211	0.4899873511	-5.3394039149
H	0.9316816850	1.6176180707	-2.6830982007
H	1.8609246717	0.2786247333	-3.4599104956
H	-0.6485071901	1.6547846651	-4.4153301684
H	0.1085067333	-2.0106961920	-4.8191716698
H	-1.6334338494	-3.7041861692	-5.0189627679
H	-2.9009617639	-2.5104762912	-4.3794973527

23

N	-1.0080399887	-0.9021708756	0.7297896408
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N	0.8265726032	0.2461201620	0.4418497514
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Ru	-0.4797887553	-0.7508324038	-2.2628758050
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C	-0.5613396548	-1.5691639838	-4.3399786924
C	-1.2673043083	-2.4105211812	-3.4425888789
C	2.0914846696	0.6762993763	-0.1327907852
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Cl	1.4326030141	-2.2840444493	-1.9686735541
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C	0.8289927915	0.5931868853	-3.2571943493
C	0.0531066532	0.8493746940	-4.5525797492
H	0.7842568874	1.1981425433	2.3443512650
H	1.4609560356	-0.4473253080	2.3317037247
H	-0.7731556599	-1.1943975285	2.8202238031
H	-1.4698985724	0.3745721183	2.3474963747
H	2.2248639106	0.2055074757	-1.1038927316
H	2.9082519475	0.3475880277	0.5208515538
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H	-3.1024165559	-0.8352370402	0.4391434304
H	-2.4551909308	-2.3209703427	1.2119597923
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H	-2.0474181608	0.0090058275	-4.3952660482
H	0.6650266525	0.7569187444	-5.4607702649
H	0.8889174753	1.4529503095	-2.5866552588
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H	-0.8442564872	-3.3755734278	-3.1823459293
H	-2.3443145808	-2.2933516529	-3.3243471620

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C	0.0794561846	-0.1973323478	0.0912602092
N	1.1917447348	-0.6797156947	-0.5060911314
C	1.1306719779	-0.5620190148	-1.9728805276
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Ru	-0.3103873649	-0.0256771704	2.1534579435
Cl	-2.4095582340	-1.2393893806	1.9243304421
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C	0.4790965061	-2.0125638824	2.4457483616
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C	0.8120529639	-0.3591082935	4.0072591234
C	-0.5677394448	-0.2693567379	4.3656920790
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H	1.4379543243	-1.4956672688	-2.4549924012
H	-0.9252367117	-1.0778040236	-2.5665002660
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H	2.8828452831	-1.8503749258	-0.0418373558
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H	2.4385801636	-0.6027030292	1.1663137323
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H	0.9823252010	-2.3484959653	1.5409606222
H	-0.3656013838	-2.6625879489	2.6680939663
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24

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C	-1.4846691931	-0.3799692332	-2.0771685645
N	-1.5228008345	0.0139329647	-0.6626928372
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C	1.7784768156	-1.4598044946	-0.6628926179
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H	0.1106634791	-1.6873263866	-2.8585226031
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H	2.5241707346	-0.8181137052	-1.1486201451
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C	-1.1707727049	0.1707098755	-2.0843096273
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H	-1.6025007264	0.9750077010	-2.6878068738
H	2.5063538668	-1.2953843485	-1.3644674322
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H	-3.1703130200	-0.3241174480	-0.2059725254
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N	-1.1003389812	0.8634765695	-1.0727574361
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Ru	0.6574053660	0.5689013811	1.3829290825
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C	-2.3413085430	1.0552937046	-0.3402752673
C	0.3198901436	2.7539077394	1.3494659830
C	-0.2547147099	2.5151912808	2.6809796774
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H	-2.8972516120	1.8952853448	-0.7716969003
H	-2.9677634456	0.1537888139	-0.3957450505
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H	1.1830520027	3.4164270834	1.2855762863
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N	0.9056987865	0.6365397980	-1.5056329818
C	0.2687165859	0.6010061286	-2.8295745137
C	-1.2167829991	0.4456476321	-2.4649749241
Ru	0.6281852620	0.6025351857	1.4661561136
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C	-2.4612493286	0.5173743515	-0.2846310129
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C	-0.6009267517	1.6062814469	2.3853442422
Cl	2.3681636802	-0.0704194598	2.9313249990
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H	-1.8698359084	1.1346938794	-3.0095581857
H	2.7654851287	-0.3184835435	-1.7311153738
H	2.7826079537	1.4495470907	-1.9817181364
H	2.6328233391	0.7779811199	-0.3371524892
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H	-2.6736463739	-0.5555994582	-0.2047787536
H	-2.3616769524	0.9296970793	0.7175492072
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H	2.1184041799	3.3204091002	1.3513770688
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28

N	1.0606826318	-0.1873698677	-1.1111974500
C	0.6344362188	-0.1556087234	-2.5222930596
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N	-1.1285117531	-0.1814480836	-0.9972933650
C	0.0051567238	-0.0810196022	-0.2771613836
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Ru	-0.0987193780	0.3432352675	1.7254220268
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C	1.4704317553	-0.2662777977	2.4140693742
C	0.9529690268	-1.5197171417	2.9301790000
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H	-1.1172098254	-1.4858983849	-2.6599650914
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H	-2.9065809377	-1.2589409861	-0.6532458480
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H	2.3388383346	0.2862390423	2.7774729426
H	0.8883402500	-1.6347909149	4.0155543690
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29

C	-0.0865145494	-0.0955649180	0.0296404217
N	1.0225606839	-0.2030576790	0.8012614561
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C	-0.7891355779	-0.8714060545	2.1345554150
N	-1.1428781470	-0.5454517265	0.7491163110
C	2.4123500483	-0.0896883660	0.3923723058
C	-2.5370425841	-0.6533625609	0.3541233955
Ru	-0.1631254689	0.5253429914	-1.8511145107
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C	1.4076856685	2.8667958261	-0.7434610845
C	0.6415559277	3.1973940683	0.3146370565
H	1.1559239939	-0.1855165473	2.9188408396
H	1.2106439107	-1.7953981064	2.1711097415
H	-1.1710202396	-1.8619674594	2.4059044754
H	-1.2349366224	-0.1368178177	2.8195293096
H	2.8990564031	0.7477407232	0.9065038227
H	2.4708305926	0.0508095029	-0.6833710253
H	2.9377389641	-1.0179292347	0.6496758323
H	-3.1506785359	0.0925898653	0.8740451126
H	-2.9014447261	-1.6558336702	0.6107036100
H	-2.6437220488	-0.4900030761	-0.7151082547
H	1.4293407952	2.1445858069	-2.7791652821
H	2.3537237387	3.3909819492	-0.8979752827
H	0.9593650827	3.9583613336	1.0223934487
H	-0.3370127777	2.7501212099	0.4567072741

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C	-1.2426844806	0.4577509873	-2.4769241367
N	-1.2138602133	0.5465837554	-0.9952296817
C	0.0463159626	0.5006057410	-0.5026531564
N	0.9051394228	0.3330101553	-1.5408020278
C	0.2066711340	0.0903986982	-2.8214380741
C	-2.4511042353	0.7969518539	-0.2990040733
Ru	0.8529036151	0.3433563628	1.3993017747
Cl	2.7129519260	-0.3998774240	2.7173843729
C	2.3415638383	0.5019246891	-1.5018933206
Cl	0.1688613584	-1.9740307257	1.2450893651
C	1.1500808139	2.8248152090	1.4983918966

C	0.5716592645	2.2769102705	2.6507188721
C	-0.3926922452	1.1953271915	2.4688935435
H	0.6320126209	0.7117857092	-3.6132532027
H	0.3175740519	-0.9618791972	-3.1086092092
H	-1.9602493300	-0.3005969086	-2.7967891012
H	-1.5516389949	1.4226985370	-2.8978887427
C	-1.5489475342	0.8990047569	3.2971935080
C	1.0262679348	2.6212739030	4.0354010241
C	2.4125223519	3.5909777255	1.4652380196
H	0.5230266100	2.9273099437	0.6227459727
C	2.4642317586	4.7859007189	0.7226451607
C	3.6216198439	5.5663101125	0.6973970432
C	4.7548420382	5.1542107140	1.4048925126
C	4.7219721454	3.9557115854	2.1276414317
C	3.5651198469	3.1772155405	2.1603767239
H	1.5805197719	5.1134446691	0.1787981426
H	3.6366675343	6.4944068064	0.1306462905
H	5.6586948090	5.7585590665	1.3878861073
H	5.6047657018	3.6220504557	2.6672079959
H	3.5509740734	2.2342266768	2.6995898238
C	1.1494444868	3.9790526166	4.3805967902
C	1.4672560455	4.3558326470	5.6857777917
C	1.6741222100	3.3794552211	6.6650576984
C	1.5531456370	2.0274149540	6.3302443685
C	1.2238783928	1.6470040527	5.0280977556
H	0.9915120717	4.7400692087	3.6214574068
H	1.5550240590	5.4104905175	5.9351845085
H	1.9278972571	3.6707064349	7.6815610611
H	1.7184823676	1.2616994727	7.0841315193
H	1.1559983064	0.5965101625	4.7695023787
C	-2.1999560308	1.9547907037	3.9748387416
C	-3.2777380051	1.6976782560	4.8179598961
C	-3.7173682877	0.3822108062	5.0095207832
C	-3.0833580945	-0.6704171914	4.3395210289
C	-2.0140601169	-0.4201153923	3.4820921998
H	-1.8425445783	2.9719968237	3.8456534013
H	-3.7641779388	2.5187055187	5.3382999340
H	-4.5466725285	0.1788985684	5.6829392125
H	-3.4206176643	-1.6927287992	4.4898603050
H	-1.5096725898	-1.2303260420	2.9650283657
C	3.1983169556	-0.5788875303	-1.2158832906
C	4.5788170603	-0.3359268233	-1.1976292780
C	5.1206876582	0.9208157292	-1.4692536518
C	4.2457513800	1.9603444826	-1.8054032704
C	2.8631558690	1.7728558702	-1.8364339633
C	2.7097691050	-1.9783024707	-0.9310965267
H	5.2434302300	-1.1631818951	-0.9557970808
C	6.6107403594	1.1546111122	-1.3841740096
H	4.6476792914	2.9451302587	-2.0340449987
C	1.9730202130	2.9203286590	-2.2553549385
H	1.0682244030	2.9849703339	-1.6443628130
H	2.5069367458	3.8698252067	-2.1656678069
H	1.6515416858	2.8213106629	-3.3022994913
H	6.8947711130	2.1069940059	-1.8447690680
H	6.9392753324	1.1826041955	-0.3363835208
H	7.1725529363	0.3527690152	-1.8785532593
H	3.3672844171	-2.7067954682	-1.4180257698
H	2.7177332733	-2.1796766096	0.1445722869
H	1.6863069216	-2.1439166181	-1.2706075261

C	-2.8356064322	2.1202139611	-0.0105772351
C	-4.0574439448	2.3370031517	0.6369417470
C	-4.9047815101	1.2835947516	0.9846490941
C	-4.5259828891	-0.0138730942	0.6233037019
C	-3.3179111058	-0.2827163454	-0.0260410567
C	-1.9948206882	3.3235644172	-0.3728463870
H	-4.3489047606	3.3588921770	0.8737453222
C	-6.1816694656	1.5354282406	1.7491473334
H	-5.1863595212	-0.8460912038	0.8573367837
C	-2.9865707895	-1.6985587697	-0.4304941430
H	-1.9868922347	-1.9866059138	-0.0912022942
H	-3.7125148298	-2.3971991033	-0.0022272271
H	-3.0226275529	-1.8238924235	-1.5216639186
H	-2.6301846326	4.1334794149	-0.7479071844
H	-1.4622381037	3.7114895513	0.5030367497
H	-1.2477112503	3.0978581607	-1.1386766653
H	-6.9182307960	0.7444439511	1.5723829087
H	-5.9809301092	1.5626603986	2.8284325552
H	-6.6342297343	2.4946814232	1.4742157745

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N	1.3450380081	-0.1701986658	-0.6431894286
C	1.1975110623	-0.8626858462	-1.9480898286
C	-0.2647751533	-1.3191848346	-1.9422013543
N	-0.7457090154	-0.8388703415	-0.6326808175
C	0.2109528115	-0.1865098612	0.0950361555
C	-2.1558068582	-0.9595893371	-0.3376775143
Ru	-0.3110890322	0.1838138462	2.0184287210
C	0.8721409094	1.3154922469	2.9230306200
C	0.5847096973	1.2610832593	4.3588701477
C	1.2550974557	2.0519092202	5.2549079486
C	2.5885352749	0.5370936614	-0.4778601931
Cl	0.7284606544	-1.9421639725	2.5384937803
Cl	-1.7999481087	2.0500190071	1.4760699541
H	1.4273017062	-0.1678208286	-2.7627056166
H	1.9038579002	-1.6970406321	-2.0026690221
H	-0.3711400868	-2.4070540435	-2.0073450487
H	-0.8556739622	-0.8678989545	-2.7467479211
C	1.8519621317	2.3210354191	2.4538124519
C	-0.4905267938	0.2925943234	4.7721898423
C	1.1100781272	2.2056349775	6.7028593989
H	2.0466867610	2.6695987519	4.8414488117
C	3.2281237877	2.1409681660	2.6825333690
C	4.1240300984	3.1837551167	2.4437996448
C	3.6601245043	4.4181803689	1.9771404888
C	2.2961128807	4.5941494463	1.7254936876
C	1.3936001981	3.5529647177	1.9548012954
H	3.5844099010	1.1889684561	3.0664013098
H	5.1843330398	3.0333496095	2.6314487842
H	4.3576317735	5.2351887293	1.8082665902
H	1.9279657096	5.5497576153	1.3593957767
H	0.3294999167	3.6870632836	1.7808792369
C	-0.1582086112	-0.8735969180	5.4889923699
C	-1.1495382117	-1.7562746532	5.9009282094
C	-2.4956195843	-1.4988393709	5.5991530352
C	-2.8388372897	-0.3499946102	4.8910347037
C	-1.8428303829	0.5523681395	4.4828566697

H	0.8844847120	-1.0824832889	5.7045804573
H	-0.8767414306	-2.6542983902	6.4489830330
H	-3.2671990100	-2.1948252766	5.9193970495
H	-3.8783227268	-0.1349655757	4.6580383817
H	-2.1208386252	1.4659834517	3.9690600280
C	2.1840039958	2.8194295701	7.3862921393
C	2.1485837535	3.0198925496	8.7638581781
C	1.0221910880	2.6310025081	9.4953467153
C	-0.0628437828	2.0463342583	8.8329674197
C	-0.0242607702	1.8317619256	7.4570765762
H	3.0571479705	3.1322185881	6.8180657336
H	2.9937106632	3.4847650976	9.2648977447
H	0.9850644471	2.7909080904	10.5699019575
H	-0.9494074764	1.7580756812	9.3919800453
H	-0.8824831298	1.3938216396	6.9647498433
C	2.6605049031	1.8631318284	-0.9532384406
C	3.9111371036	2.4797566368	-1.0108951040
C	5.0791134573	1.8157128345	-0.6155348685
C	4.9721189284	0.5042278473	-0.1483378055
C	3.7405127604	-0.1627220882	-0.0799717746
C	1.4251011357	2.5977987755	-1.4197546128
H	3.9739407032	3.5046209613	-1.3707251409
C	6.4137688692	2.5207369107	-0.6696793912
H	5.8697467752	-0.0266879318	0.1634274616
C	3.6865277553	-1.6006044778	0.3776110266
H	3.5496319089	-2.2859927225	-0.4710810771
H	4.6253898025	-1.8799960884	0.8667921710
H	2.8619611732	-1.7786356695	1.0745088610
H	7.2436839803	1.8220255892	-0.5219775349
H	6.5618299025	3.0267463710	-1.6312535647
H	6.4814699145	3.2893931918	0.1118589210
H	1.6652108270	3.6395161075	-1.6528063099
H	1.0026168937	2.1450198045	-2.3273933606
H	0.6390797493	2.5946679174	-0.6583170294
C	-2.6520178041	-2.1295320236	0.2773378563
C	-4.0277918135	-2.2094053258	0.5272416815
C	-4.9117028090	-1.1958295516	0.1466442347
C	-4.3986571579	-0.0960575960	-0.5475950125
C	-3.0336219568	0.0379702428	-0.8128581904
C	-1.7754802829	-3.3177986783	0.5930207061
H	-4.4150919720	-3.1005960558	1.0168985291
C	-6.3834399073	-1.2864902507	0.4747396336
H	-5.0754082171	0.6851010710	-0.8879696355
C	-2.5582212343	1.2032448002	-1.6489503912
H	-1.5537854910	1.5252820696	-1.3744126832
H	-2.5602134988	0.9385885609	-2.7168485437
H	-3.2233156213	2.0615888538	-1.5207437259
H	-6.9948619332	-0.7776381642	-0.2785422526
H	-6.7168879461	-2.3279066039	0.5413978518
H	-6.5980862344	-0.8119751278	1.4417850940
H	-2.3785395479	-4.1239644464	1.0228756268
H	-1.3056599289	-3.7115930017	-0.3185096421
H	-0.9711180266	-3.0793101164	1.2924918010

6-Me₁ 4-isomer

C1	-0.153337	0.592564	-2.175150
C2	-1.659785	0.470652	-1.921929
N3	-1.714617	0.524578	-0.453764
C4	-0.516736	0.245540	0.098734
N5	0.407730	0.176392	-0.877925
C6	-2.993785	0.403160	0.229010
Ru7	-0.270956	0.036982	2.113717
C18	0.576931	2.330023	2.169246
C9	1.847949	0.232877	-0.683967
C10	1.356986	-0.695070	2.551366
C11	0.156997	-0.235989	4.468633
C12	-0.954501	0.261092	4.226591
C13	-2.285519	0.850942	4.446259
C114	-1.371520	-2.144931	2.013984
H15	0.144034	1.628257	-2.394361
H16	0.204814	-0.054070	-2.981563
H17	-2.061989	-0.489201	-2.277712
H18	-2.241946	1.282718	-2.367745
H19	2.185386	1.260497	-0.501937
H20	2.122642	-0.383989	0.171217
H21	2.336386	-0.166454	-1.578135
H22	-3.713854	1.073583	-0.251541
H23	-3.365879	-0.627399	0.209224
H24	-2.888859	0.711924	1.271219
H25	2.238363	-0.067746	2.726981
H26	1.480175	-1.779042	2.654232
H27	0.986220	-0.624295	5.020937
H28	-2.494166	0.921261	5.520244
H29	-2.328635	1.857301	4.015611
H30	-3.058250	0.228611	3.982009

6-Me₁ 3-isomer

N1	-2.296842	0.847954	0.043375
C2	-1.029862	0.498942	0.319079
N3	-0.303750	0.534778	-0.813717
C4	-1.060631	1.158860	-1.912731
C5	-2.503927	1.103777	-1.389685
Ru6	-0.383769	0.153392	2.231699
C17	-1.464782	-2.043695	2.227470
C8	1.148698	0.499236	-0.886644
C9	-3.426820	0.759635	0.954307
C10	-0.718077	0.292849	4.329132
C11	0.423321	-0.194745	4.507021
C12	1.584859	-0.679815	5.276580
C113	0.522847	2.428282	2.183983
C14	1.284076	-0.601684	2.458506
H15	1.407115	-1.687665	2.517080
H16	-1.633239	0.681538	4.737252
H17	-0.716109	2.192273	-2.058957
H18	-0.918622	0.607650	-2.847415
H19	-3.080716	0.279155	-1.831478
H20	-3.052757	2.037265	-1.549094
H21	1.582704	1.481345	-0.663494
H22	1.527871	-0.225272	-0.165925
H23	1.439659	0.181539	-1.893011

H24	-3.758251	1.756845	1.268600
H25	-4.258635	0.249147	0.454686
H26	-3.148656	0.158696	1.823033
H27	2.186052	0.018139	2.483791
H28	2.481727	-0.086286	5.069868
H29	1.350667	-0.586516	6.343537
H30	1.804118	-1.731431	5.063907

6-Me₂ 2,4-isomer

N	-0.1485374234	0.4754793343	-0.7923267659
C	-0.8806790640	1.0292751331	-1.9440317856
C	-2.3346759374	0.9326873782	-1.4701428828
N	-2.1628566441	0.8410567229	-0.0134683107
C	-0.9075997016	0.4824924966	0.3225238734
C	-3.3311491785	0.7239890277	0.8439194665
Ru	-0.3463722993	0.1190651772	2.2577512930
C	0.4352929453	-0.2697655441	4.4517954531
C	-0.7555172790	0.0985973849	4.4182709658
C	-2.0896955272	0.4688237158	4.9204646221
C	1.3048295944	0.4814221507	-0.8206979880
Cl	0.5874153179	2.3751192387	2.3251427157
C	1.3438748455	-0.6428615739	2.4279618072
C	1.7340088775	-2.0879190883	2.4107461271
Cl	-1.6527822501	-1.9829617110	2.1645669458
H	-0.5724473542	2.0709306056	-2.1157282953
H	-0.6800576702	0.4503282894	-2.8505010253
H	-2.8340815388	0.0281331298	-1.8470677468
H	-2.9377995545	1.8048057414	-1.7405701733
H	1.7037276200	1.4881220090	-0.6445380272
H	1.6844317190	-0.1855489558	-0.0481203757
H	1.6382935203	0.1163133396	-1.7974353056
H	-4.0418329302	1.5158125873	0.5829966524
H	-3.8077560289	-0.2575564300	0.7419798626
H	-3.0410868555	0.8544860126	1.8875099920
H	2.1807865367	0.0661458710	2.5011317440
H	1.3723650993	-0.5278552688	4.9006333857
H	-2.1072528517	0.4279826008	6.0160084631
H	-2.3501424044	1.4866514365	4.6087625300
H	-2.8382605606	-0.2273346166	4.5273847064
H	2.4734322969	-2.3025798221	3.1970163581
H	0.8757587332	-2.7545264224	2.4958217531
H	2.2386854099	-2.2886230437	1.4524099679

6-Me₂ 2,3-isomer

N	-0.2986402949	0.5582459596	-0.8154991787
C	-1.0824929289	1.1255694912	-1.9256044658
C	-2.5084281306	1.0708953403	-1.3639248506
N	-2.2493572868	0.9936118028	0.0807398756
C	-0.9917425988	0.5881936018	0.3386011081
C	-3.3544882777	0.9169214703	1.0239819477
Ru	-0.3614423111	0.1616755257	2.2423534082
C	0.4036316348	-0.3233576682	4.4490846916
C	1.6202239801	-0.3813578851	5.2881741798
C	1.1464054467	0.4813507181	-0.9344323119
Cl	0.6453244962	2.3747670143	2.3953770874

C	1.3018080498	-0.6618275515	2.4671338536
C	1.6554348146	-2.1141759873	2.3791014078
Cl	-1.6600904385	-1.9415198723	1.9699646276
C	-0.8246814052	-0.0921382378	4.2893333872
H	-1.8092488013	0.0106988686	4.7090449885
H	-0.7562657449	2.1571058956	-2.1233756654
H	-0.9525728279	0.5353300146	-2.8375692671
H	-3.0497178263	0.1737035884	-1.6975347419
H	-3.1053705157	1.9543774165	-1.6091724067
H	1.5970431742	1.4822930809	-0.9522627060
H	1.5458166473	-0.0665106645	-0.0825101006
H	1.4046513315	-0.0500735938	-1.8567479027
H	-4.0900568622	1.6867039027	0.7684077141
H	-3.8222102755	-0.0738536596	1.0157197077
H	-2.9899936953	1.1205454463	2.0339804001
H	2.1528447714	0.0259053267	2.5592663512
H	2.4598753843	-2.3738816393	3.0820070378
H	0.7908315060	-2.7634429765	2.5172681363
H	2.0555101997	-2.2980928671	1.3695769467
H	2.2567531406	0.4887010034	5.0923114228
H	1.3210862312	-0.3564959095	6.3418446161
H	2.2081153603	-1.2887914232	5.1179558564

First-Generation Phosphane Complexes

1(1st)

C	-4.3984808855	1.2925042541	1.3430938347
P	-2.8031773110	1.0552609762	2.2279101426
C	-2.2316294051	-0.6084840033	1.6700090542
Ru	-2.8961123155	1.0503679597	4.6298501753
Cl	-4.9518446744	-0.2812970104	4.4508861816
P	-2.6135640676	0.3695401933	6.9184062779
C	-1.8460823049	1.6013113310	8.0485731224
C	-3.7488376737	2.6305627236	4.8928773810
Cl	-0.6301114972	1.9969847109	4.7486303973
C	-4.0917247051	-0.2381162610	7.8289039847
C	-1.4362544802	-1.0508127998	6.9543969363
H	-4.8447474608	2.6944406283	4.9037645208
H	-3.1903122248	3.5629387629	5.0480061791
H	-3.8103362778	-0.6646135322	8.7983976021
H	-4.7850643254	0.5938731540	7.9855695034
H	-4.6020528027	-0.9847581097	7.2154000699
H	-1.2534777692	-1.3880128806	7.9810537384
H	-1.8455008491	-1.8839772798	6.3739209443
H	-0.4931906795	-0.7315130728	6.5008697569
H	-1.5773437135	1.1460482820	9.0083910593
H	-0.9570305971	2.0080555820	7.5593149224
H	-2.5518261474	2.4196056532	8.2231144869
H	-4.7336976936	2.3258761927	1.4771558014
H	-5.1418629915	0.6270300431	1.7899652162
H	-4.2937816861	1.0835367697	0.2725322459
H	-1.2352420440	-0.8098259484	2.0763386118
H	-2.9285159585	-1.3630154660	2.0471216877
H	-2.1888518298	-0.6654053170	0.5763410654
C	-1.6444884096	2.2284874302	1.4136771412
H	-2.0013013133	3.2515296195	1.5675076018
H	-0.6638022416	2.1428443456	1.8881363121
H	-1.5698765392	2.0282129165	0.3388482654

2(1st)

C	-4.3609083044	0.7270657409	1.3034536508
P	-2.8011564883	1.0478021389	2.2270543334
C	-2.0898093314	2.5388449771	1.4152268146
C	-1.6768247234	-0.3164413112	1.7026231240
Ru	-2.9259183314	1.1051956069	4.6310482685
Cl	-0.6433800923	1.9894634982	4.5940220683
Cl	-4.8474706066	-0.4130784065	4.6173477223
P	-2.7783623696	0.6777820292	6.9964628566
C	-2.1953241341	-1.0491632060	7.2758479946
C	-3.8217709748	2.6809757997	4.7591570714
C	-1.6098673252	1.7107603951	7.9741598807
C	-4.3601951191	0.7655083552	7.9346965923
H	-4.8057720431	2.7543890431	5.2422573668
H	-3.4117618152	3.6192451788	4.3610669313
H	-4.2333351517	0.4122215527	8.9641784052
H	-4.7121974146	1.8020987076	7.9541783600
H	-5.1045280097	0.1559944943	7.4152399979
H	-2.1407104740	-1.2844556555	8.3448278455
H	-2.8915166639	-1.7349480952	6.7840520525

H	-1.2025117202	-1.1746181719	6.8318484038
H	-1.5140051893	1.3427647082	9.0018843255
H	-0.6366515257	1.7075340448	7.4764264694
H	-1.9710871215	2.7438009199	7.9921428788
H	-5.0352125049	1.5801093034	1.4289786166
H	-4.8495430071	-0.1509972588	1.7337572294
H	-4.1691784101	0.5716959189	0.2357801973
H	-0.6931229525	-0.1489232413	2.1510966884
H	-2.0715099452	-1.2721022353	2.0623019208
H	-1.5804979631	-0.3572101652	0.6116350044
H	-2.7787129140	3.3810153446	1.5378137011
H	-1.1475869755	2.7862494637	1.9114819356
H	-1.9212020709	2.3680467991	0.3460733761

3(1st)

C	-4.3618262145	1.1310600306	1.3074185586
P	-2.7599381302	1.0594387893	2.2190503071
C	-1.7607518034	2.4129872919	1.4636105160
C	-1.9654255569	-0.4758967688	1.5783463070
Ru	-2.8914507616	1.0239255443	4.6227411928
Cl	-0.5151266408	1.3469542667	4.7158385852
Cl	-4.5976767962	-0.6570781679	4.4679528016
P	-2.9110279350	0.7618965167	7.0160512036
C	-2.1789947484	-0.8559349459	7.5117478439
C	-3.7037570382	2.6602343158	4.6979221125
C	-1.9425668788	1.9923671852	7.9904613468
C	-4.5655254500	0.7563683046	7.8319133240
H	-3.9947662123	3.1446218798	5.6384456618
H	-3.9477018680	3.2520994784	3.8068327913
H	-4.4887136744	0.5416768826	8.9037430144
H	-5.0449775113	1.7316988963	7.6980064385
H	-5.1891803008	0.0015022001	7.3449855281
H	-2.1853872015	-0.9881755924	8.5996450281
H	-2.7538027687	-1.6606394362	7.0432639830
H	-1.1489641177	-0.9039699325	7.1453716107
H	-1.9304787497	1.7455502930	9.0580230458
H	-0.9207519852	2.0148783681	7.6015970186
H	-2.3775653633	2.9888129648	7.8602272265
H	-4.8677968971	2.0770090723	1.5270992282
H	-4.9982520655	0.3154958383	1.6618888718
H	-4.2169979830	1.0477017456	0.2244471872
H	-0.9596367203	-0.5551178602	2.0019529878
H	-2.5517476741	-1.3392456034	1.9075678614
H	-1.9016862737	-0.4741297926	0.4842756172
H	-2.2228027609	3.3800772869	1.6878708747
H	-0.7641942252	2.4001464245	1.9136229209
H	-1.6808569310	2.2996890326	0.3766529071

4(1st)

C	0.7405966775	2.3450174107	1.4585217902
P	-0.0057720653	1.5126627245	0.0000000000
C	0.7405966775	2.3450174107	-1.4585217902
C	-1.7642819791	2.0449149864	0.0000000000
Ru	0.1556486954	-0.7211996964	0.0000000000
Cl	-0.5725407134	-0.9257776895	-2.2321938508

Cl	-0.5725407134	-0.9257776895	2.2321938508
C	1.9684212231	-0.7751399230	0.0000000000
H	2.4161898811	-1.7808065512	0.0000000000
H	2.6807030859	0.0570078887	0.0000000000
H	1.8150174598	2.1419521070	1.4911103073
H	0.2864408732	1.9370947419	2.3649525905
H	0.5797446854	3.4279598621	1.4102835606
H	-2.2578938731	1.6433708094	-0.8895833254
H	-2.2578938731	1.6433708094	0.8895833254
H	-1.8399258661	3.1383508665	0.0000000000
H	1.8150174598	2.1419521070	-1.4911103073
H	0.2864408732	1.9370947419	-2.3649525905
H	0.5797446854	3.4279598621	-1.4102835606

5(1st)

C	-0.8835316709	0.3401093750	-1.0725444166
P	0.2842479113	-0.1879086124	0.2432781590
C	1.8901571034	-0.3279961228	-0.6390082543
Ru	-0.3489545829	-2.0367025084	1.6578342222
C	-0.4823210882	-2.8464677815	3.6775889472
C	-1.6399041480	-2.8364308071	3.2262761974
Cl	-2.5776485911	-1.9061483293	0.5952878979
Cl	2.0033067660	-1.8238226854	2.4365477838
C	0.1483808692	-3.2839785289	0.4277426000
H	1.1681903976	-3.6811493849	0.4182525953
H	-0.5778421148	-3.6958459699	-0.2793093481
H	-2.6975342784	-2.9498374684	3.0935984790
H	0.3781393773	-2.9704640633	4.3048318183
H	-1.8548358296	0.5750706843	-0.6338356183
H	-0.4791366770	1.2149240862	-1.5945972670
H	-1.0323355406	-0.4778723670	-1.7820145681
H	2.6606162297	-0.6384548061	0.0692460278
H	1.8007829476	-1.0856253471	-1.4239232593
H	2.1587018049	0.6312412364	-1.0955253302
C	0.4658840587	1.2969548827	1.3170260214
H	1.2313577559	1.0930156316	2.0702966993
H	0.7525906056	2.1718379580	0.7225389066
H	-0.4839229979	1.5051958625	1.8200949537

5b(1st)

C	-0.7806277108	-0.0792611601	-1.3688731377
P	0.3199763651	-0.3226507378	0.0874179399
C	0.3576477528	1.3232819616	0.9067911670
C	1.9917636029	-0.4950676378	-0.6646572969
Ru	-0.3150615613	-2.0123809488	1.5755075518
C	-0.1982340810	-3.2884389297	0.2812710241
C	-0.3862492715	-3.7497840785	3.2960183898
C	-1.5559095926	-3.5535562599	3.0098580681
Cl	-2.5252336280	-1.0596089159	1.4702977568
Cl	1.8681661865	-1.7658132037	2.5613410892
H	-0.4305310957	-4.3260677183	0.5474245430
H	0.0875835301	-3.1295992481	-0.7650584700
H	-2.6070496382	-3.4436104516	2.8529522162
H	0.6012059360	-3.9752928835	3.6364168397
H	-1.7974492700	0.1107239457	-1.0179990239

H	-0.4316366063	0.7595968625	-1.9813872538
H	-0.7911992182	-0.9860425209	-1.9818562708
H	2.7347076858	-0.5727581639	0.1322696573
H	2.0353797072	-1.4085199643	-1.2661104577
H	2.2173007074	0.3641937923	-1.3061095850
H	1.0701340505	1.2892797029	1.7360699503
H	0.6526832775	2.1090549804	0.2022658202
H	-0.6374969876	1.5424084281	1.3042267469

5c(1st)

C	0.8856988791000	2.6169316561000	1.4531664766000
P	0.1001612181000	1.8053796583000	0.0000000000000
Ru	0.1295917236000	-0.4953761450000	0.0000000000000
C	1.9585768444000	-0.5040440484000	0.0000000000000
C	0.8856988791000	2.6169316561000	-1.4531664766000
C	-1.6229985608000	2.4471458389000	0.0000000000000
Cl	-0.6146444409000	-0.5001703182000	-2.2629353289000
Cl	-0.6146444409000	-0.5001703182000	2.2629353289000
C	-0.8017530834000	-2.8878564524000	0.0000000000000
C	0.3876608662000	-3.1238018716000	0.0000000000000
H	2.5211885547000	-1.4437579102000	0.0000000000000
H	2.5965147476000	0.3879856825000	0.0000000000000
H	1.9516253893000	2.3712781191000	1.4862430481000
H	0.4172588342000	2.2335868901000	2.3630462910000
H	0.7720797651000	3.7055391623000	1.4009124729000
H	-2.1401250400000	2.0775981165000	-0.8901102369000
H	-2.1401250400000	2.0775981165000	0.8901102369000
H	-1.6316048688000	3.5430529588000	0.0000000000000
H	1.9516253893000	2.3712781191000	-1.4862430481000
H	0.4172588342000	2.2335868901000	-2.3630462910000
H	0.7720797651000	3.7055391623000	-1.4009124729000
H	1.4110699332000	-3.4236475558000	0.0000000000000
H	-1.8607182001000	-2.7513545980000	0.0000000000000

6(1st)

C	-1.5925207164	0.8058698621	-0.5920157689
P	-0.1182289972	0.0848072240	0.2363979635
Ru	-0.4539701973	-1.9623572102	1.4484264575
Cl	1.4170897318	-1.3771788531	2.9001073217
C	0.5896772519	1.4885617285	1.1901261141
C	1.0907412576	-0.1941898819	-1.1254892350
C	0.5053495246	-3.3149760128	0.6386698990
Cl	-2.4375258295	-2.4274863979	0.1073349042
C	-1.2668868828	-3.2472744584	2.9903240069
C	-0.5729590743	-4.1264914539	2.4461306656
H	1.2614069337	0.7328738810	-1.6845102765
H	1.5459341041	-3.5164401599	0.9144258552
H	0.0618551766	-3.9280420853	-0.1530548534
H	-1.9550006889	-2.8691276814	3.7227508694
H	-0.1074689216	-5.0735122793	2.2653279747
H	-1.3036321270	1.6587488564	-1.2166102601
H	-2.0773079353	0.0322447700	-1.1913660205
H	-2.3095244519	1.1398533874	0.1642770818
H	2.0357873751	-0.5428606042	-0.7003899671
H	0.7002142298	-0.9590690968	-1.8023852758

H	-0.1241305297	1.8103938648	1.9547173658
H	1.4952280614	1.1487656785	1.6971998819
H	0.8084061562	2.3318455707	0.5251670431

7(1st)

C	-3.8001474034	1.5630896900	1.1482598118
P	-2.4772978399	1.0720134893	2.3267272919
Ru	-3.0948069587	1.0108594610	4.4789116034
C	-3.5567793916	2.7820410393	4.6200477545
C	-1.0682587965	2.1922169299	1.9508202439
C	-1.9242599546	-0.5826538863	1.7455627837
Cl	-0.8763920463	0.8555548935	5.2861945286
Cl	-5.0792019563	-0.1882015618	4.0139647414
C	-3.9584517952	3.2661563689	5.9324709129
H	-3.6632542885	3.4758366313	3.7774264349
H	-4.1350572601	2.5810082230	1.3695446366
H	-4.6490953591	0.8869177672	1.2767584310
H	-3.4367320223	1.5217672518	0.1152495119
H	-1.0742717465	-0.9071298781	2.3530756211
H	-2.7424831074	-1.2970936770	1.8740365045
H	-1.6279676471	-0.5490860637	0.6908577790
H	-1.3417009265	3.2228232643	2.1961902326
H	-0.2183949092	1.9067820811	2.5759096308
H	-0.7949038518	2.1331593008	0.8911896862
C	-3.3721381955	2.9036319189	7.0925727177
H	-4.7991488776	3.9644218700	5.9550692332
H	-3.7394144430	3.2750265710	8.0450944430
H	-2.4932712944	2.2640654644	7.1070835095

8(1st)

C	-3.8774344908	1.4288038148	1.1356657021
P	-2.5195553016	1.0836813375	2.3259913807
C	-1.7837033237	-0.5001775343	1.7539279089
Ru	-3.1523298313	0.9540147676	4.4708129450
Cl	-4.9951358716	-0.4501278910	3.9935574248
C	-1.2403009878	2.3535852570	1.9650092916
C	-3.7750412457	2.6620102316	4.6041757547
C	-4.1815248092	3.0884956702	5.9558415256
C	-5.4542756354	3.1881376752	6.3679167973
Cl	-0.9425202487	1.0276883113	5.3029828319
H	-3.8807356413	3.3724997473	3.7741719230
H	-4.3243902193	2.4029893725	1.3559058302
H	-4.6480432087	0.6630996459	1.2548618974
H	-3.5017237700	1.4305438321	0.1062371130
H	-0.9113647922	-0.7299175915	2.3727308167
H	-2.5216511472	-1.2984738900	1.8750750330
H	-1.4809394417	-0.4352585996	0.7026713078
H	-1.6316047937	3.3479041122	2.2004422213
H	-0.3735674683	2.1672760871	2.6042171071
H	-0.9460246056	2.3222900304	0.9098304384
H	-3.3685843249	3.2929995322	6.6561357570
H	-5.6945106451	3.4858845416	7.3848876615
H	-6.2883202413	2.9612695088	5.7086729911

9(1st)

C	-3.8443917250	1.6154157435	1.1870645861
P	-2.4971427426	1.1091801563	2.3311478611
C	-1.9419994262	-0.5284915707	1.7085783786
Ru	-3.0764256740	0.9881639920	4.4877309133
Cl	-5.0775501482	-0.1892956558	4.0566863096
C	-1.1031386405	2.2486808082	1.9583756369
C	-3.5380031839	2.7656090024	4.6420325363
C	-4.0080509283	3.2806063576	5.9088179196
C	-4.3595032534	4.5703553266	6.0896429018
Cl	-0.8506566033	0.8030113648	5.2544905419
H	-3.4862530890	3.4985424468	3.8264383146
H	-4.1847985584	2.6241222608	1.4394719082
H	-4.6854600046	0.9290435827	1.3133454243
H	-3.4980786461	1.6022065596	0.1474109521
H	-1.0830970964	-0.8610244916	2.2986953742
H	-2.7548473348	-1.2502399118	1.8304635051
H	-1.6593633578	-0.4693819744	0.6512502370
H	-1.3798823846	3.2724523105	2.2273652322
H	-0.2419825030	1.9569208587	2.5648018125
H	-0.8454160344	2.2134882984	0.8937458975
H	-4.0777671599	2.5882412651	6.7484194541
H	-4.7088954471	4.9382052761	7.0498925930
H	-4.3034763662	5.2909825491	5.2768015616

10(1st)

C	1.5369398749	-0.0923009974	3.3267817379
P	-0.0044338914	-0.4244226557	2.3778704492
Ru	0.0664049234	-0.0872801016	-0.0002789371
C	0.4259485580	1.7214959041	0.0000653381
C	-0.5338052647	2.8125065810	0.0014194453
C	-0.1330925388	4.1006331986	-0.0019021716
C	-1.3144985349	0.4747622016	3.3083029717
C	-0.3659888086	-2.2034853880	2.7131296403
Cl	-2.4088136753	-0.1189494403	0.0055057525
Cl	2.4490071938	-0.6804681947	-0.0066666503
P	-0.0005299905	-0.4213040128	-2.3787911469
C	1.5247126878	-0.0365651248	-3.3338824754
C	-0.2981655383	-2.2110822900	-2.7117231523
C	-1.3453952315	0.4287286007	-3.3047498399
H	1.4833218213	2.0298524671	-0.0014107786
H	1.4464372732	-0.3888714181	-4.3686168025
H	1.6839139554	1.0466063299	-3.3335165307
H	2.3764790918	-0.5044625021	-2.8335939600
H	-0.3435697362	-2.4141768606	-3.7877313699
H	0.5125516062	-2.7982709822	-2.2692572224
H	-1.2440175810	-2.5069426529	-2.2477689104
H	-1.3932608603	0.0854273223	-4.3442672336
H	-2.2931262671	0.2332983277	-2.7960810622
H	-1.1651267752	1.5084553194	-3.2903387257
H	1.7362609938	0.9845461395	3.3208152540
H	2.3706210841	-0.5923614182	2.8260342275
H	1.4493986553	-0.4372323218	4.3633764838
H	-1.3232448952	-2.4644599403	2.2502834522
H	0.4231068202	-2.8204971785	2.2701380642
H	-0.4167489061	-2.4037877845	3.7896536140

H	-1.0937868304	1.5472817018	3.2927316263
H	-2.2708481774	0.3133086491	2.8035031812
H	-1.3707615341	0.1336060764	4.3483158331
H	-1.5906098185	2.5580907513	0.0051156676
H	-0.8452793048	4.9221669966	-0.0010145333
H	0.9225550325	4.3659278646	-0.0057519946

11(1st)

C	-4.0588391378	1.7358306583	1.3125396477
P	-2.5943122558	1.1453420865	2.2560391076
Ru	-2.8965308487	0.8458303090	4.5616818899
C	-3.5837730930	2.5406299719	4.8756427767
C	-1.2015250628	2.1787258923	1.6329223851
C	-2.2350999847	-0.5159385563	1.5405684441
Cl	-0.5413350291	1.2661611097	4.9455076391
Cl	-4.9508244967	-0.3508182332	4.0817396679
C	-3.2710407919	0.6645441583	7.0292734778
C	-2.8090823847	-0.5240725489	6.5615972936
C	-3.1213182231	3.8168205408	4.3760971068
H	-4.4525596754	2.6103000685	5.5445362323
H	-4.2923041566	2.7628914870	1.6100389091
H	-4.9095485496	1.0991644530	1.5693008844
H	-3.8756949454	1.7055028843	0.2327642801
H	-1.3097596774	-0.9057442792	1.9767843079
H	-3.0574083384	-1.1930200356	1.7879357238
H	-2.1204985916	-0.4566462673	0.4523017291
H	-1.4104544378	3.2394808353	1.7991310484
H	-0.2936457033	1.9165545180	2.1817913566
H	-1.0571780769	2.0150566086	0.5591843923
H	-1.7449741576	-0.7438574737	6.5716199339
H	-2.5908467941	1.4186175929	7.4130767288
H	-4.3374001477	0.8444787436	7.1290053396
H	-3.4950850477	-1.3188033213	6.2843715476
C	-3.7821137640	4.9653400395	4.6342839934
H	-2.1938871604	3.8422532058	3.8106553948
H	-3.4236412863	5.9260460909	4.2744344802
H	-4.7028313867	4.9708392812	5.2138116741

12(1st)

C	-1.4400890805	-0.6177973477	0.7639559602
P	0.0745703140	-0.0330811661	-0.1048507503
C	0.3284893506	1.6846072076	0.5004711786
C	1.4504055406	-1.0058147548	0.6264281571
Ru	-0.2497599076	-0.1360395153	-2.4828986394
Cl	-1.9916463617	1.5718428983	-2.1968616711
C	0.9402381723	0.8408932448	-3.5856785832
C	-0.4352281550	-0.0245563582	-4.7685174901
C	-1.3291237445	-0.9412636411	-4.1092628587
Cl	1.2383535388	-2.0622272636	-2.6313390280
C	0.9415345579	2.2856006373	-3.8020659420
C	2.0614615789	2.9260946043	-4.1803292392
H	-1.3254594568	-0.5260675519	1.8498733324
H	1.8592215036	0.3250737561	-3.8844352292
H	-2.3667920725	-0.6376879635	-3.9931645466
H	-1.1195030911	-2.0051240831	-4.1808534351

H	0.3515661537	-0.4704002684	-5.3720096082
H	-0.8668920262	0.9011518536	-5.1369719572
H	0.0248038635	2.8292737302	-3.5922735973
H	2.0907067010	4.0072702964	-4.2859649539
H	2.9859952881	2.3879820497	-4.3807590738
H	1.3407400881	-2.0538343143	0.3384664519
H	2.4004101673	-0.6519184091	0.2165025804
H	1.4605309729	-0.9078807244	1.7178996781
H	-1.6279335929	-1.6665969192	0.5130857905
H	-2.2873830454	-0.0145756284	0.4265769079
H	-0.4949855623	2.3018344533	0.1325477080
H	0.3677275476	1.7126287040	1.5952821856
H	1.2672865702	2.0770180465	0.0974092612

13(1st)

C	-0.7184308668	-0.9241232091	-0.9817967800
P	0.1432903698	0.0523731741	0.3110235868
C	1.5903142996	0.8120519461	-0.5306667675
H	2.2009387412	0.0423313068	-1.0161925605
Ru	-1.0644177569	1.7172876390	1.5063669933
Cl	-2.9950868585	1.2890020590	0.0693856758
C	-1.3822613443	3.6519965928	1.2646817750
C	-2.1515876738	3.3558036929	2.6143217404
C	-2.3829935274	1.8272824721	3.0131387840
C	-1.9413393940	1.3833236038	4.3401555267
C	-2.6081010902	0.4503188265	5.0394991769
Cl	0.9837876967	2.1637540601	2.7682914808
H	-0.5043322405	4.2814047937	1.4077706798
H	-2.0355663584	3.9319968366	0.4399772178
H	-3.1650889659	3.7308374176	2.4544156314
H	-3.3741720589	1.4787137236	2.7215204185
H	-1.6263062183	3.8463417193	3.4333340708
H	-1.0221797332	1.8143556887	4.7285367757
H	-2.2586155295	0.1119404337	6.0107460671
H	-3.5203672753	-0.0045163920	4.6585726936
H	-1.5664465613	-1.4495819014	-0.5357515857
H	-1.1167800884	-0.2477225628	-1.7411941947
H	-0.0288657855	-1.6438849429	-1.4377938518
H	1.2419505042	1.5216528371	-1.2871065976
H	2.1805455124	1.3499011756	0.2155395317
C	0.8456067779	-1.1898917317	1.4705340384
H	1.4418631646	-0.6625307110	2.2194273431
H	0.0329274794	-1.7205040179	1.9766271170
H	1.4641291707	-1.9162310268	0.9313183178

14(1st)

C	1.0268190092	0.0702924859	-1.0589111997
P	-0.1285348871	-0.2670561484	0.3323560484
C	-0.4466644711	-2.0786662533	0.2237650877
Ru	0.7790932767	0.2819656861	2.4796694243
Cl	-1.2586243022	1.5280179953	3.0130870163
C	-1.7126923083	0.5094467359	-0.1777657135
C	1.7869644529	1.8376140666	2.5365949602
C	1.9269328227	0.8459890290	4.4197053142
C	0.8633518661	-0.0833401757	4.6330185402

C	1.0415014112	-1.5369687040	4.7002627732
C	0.0360341725	-2.3570799549	5.0583124081
Cl	2.7503116461	-1.0441842184	1.8401345505
H	0.6417836306	-0.3571039697	-1.9931623398
H	2.8441800562	1.8429485859	2.2547447986
H	1.3328789719	2.8032971304	2.7739068307
H	1.8013971374	1.8319423215	4.8669852758
H	-0.0610542425	0.3106657856	5.0519791931
H	2.9446439197	0.4767965113	4.3115829923
H	2.0125622457	-1.9374988793	4.4185019936
H	0.1711040187	-3.4337961582	5.1015147682
H	-0.9461999690	-1.9698286361	5.3204457734
H	1.1448596906	1.1503312191	-1.1784582246
H	1.9967133097	-0.3664538990	-0.8131495699
H	-2.4989749488	0.2192698875	0.5223181724
H	-1.6171993351	1.5970965460	-0.1303709354
H	-1.9838838772	0.1995805556	-1.1938104167
H	-1.1818579488	-2.3712397660	0.9783808135
H	-0.8269434796	-2.3504363331	-0.7680318942
H	0.4905381134	-2.6043011574	0.4206902590

15(1st)

C	-4.3393233886	0.9521912877	1.3529168050
P	-2.7470942006	1.0167740794	2.2728746122
Ru	-2.8806851755	1.0358431877	4.5985504233
C	-3.8456016105	2.5882980074	4.5605797201
C	-1.8592969365	2.4344105006	1.5047960492
C	-1.8273064349	-0.4685580828	1.6949801559
Cl	-0.5644115635	1.6835355644	4.6397102594
Cl	-4.5702733606	-0.6749364216	4.4128947508
C	-2.7758154440	0.0624323562	6.9435408444
C	-2.7657694638	1.4187344993	7.0805404779
H	-4.1648798179	3.0789321790	5.4858926884
H	-4.1704178547	3.1076004311	3.6504928036
H	-4.9257784506	1.8520926625	1.5621561037
H	-4.9096560131	0.0858561552	1.6950294594
H	-4.1623156760	0.8864380929	0.2739284803
H	-0.8250744278	-0.4549299801	2.1330758873
H	-2.3520903977	-1.3647289143	2.0385959018
H	-1.7495629700	-0.4857858824	0.6019575618
H	-2.3984343125	3.3635931046	1.7153333746
H	-0.8636087825	2.5088997635	1.9480653115
H	-1.7828863668	2.3046403845	0.4195730915
H	-3.6878743818	1.9490178440	7.2925314258
H	-3.7258259040	-0.4644394159	6.9822787118
C	-1.5796169126	-0.7708537815	6.8230713699
H	-1.8398138184	1.9818372496	7.1369506402
C	-1.6393570103	-2.1064176356	6.6926637355
H	-0.6196508938	-0.2605623992	6.8376738922
H	-0.7396663847	-2.7102623876	6.6185571363
H	-2.5914159173	-2.6295986953	6.6476532230

16(1st)

C	-4.2779830884	1.3238834176	1.3253934314
P	-2.7242043268	1.0392964132	2.2689111777

C	-1.5419326141	2.2684890773	1.5782181180
C	-2.1096869664	-0.5843396328	1.6613475125
Ru	-2.9259737567	0.9966055864	4.5842588770
Cl	-0.5452524821	1.1493106359	4.7727866824
Cl	-4.8599863147	-0.3960236400	4.3597994482
C	-3.5486435917	2.7190429811	4.5811807560
H	-3.8161019535	3.2362078895	5.5079588211
H	-3.6908089760	3.3270173025	3.6794453187
H	-4.6736052388	2.3185612776	1.5537407640
H	-5.0167973367	0.5820031027	1.6387670921
H	-4.1026056078	1.2494421823	0.2465726204
H	-1.1361591909	-0.7879893831	2.1169154636
H	-2.8130579323	-1.3648640499	1.9659539740
H	-2.0101809383	-0.5868243635	0.5700911280
H	-1.8823028058	3.2816196404	1.8142873643
H	-0.5669696991	2.1177558136	2.0482690238
H	-1.4572962020	2.1648899165	0.4908406741
C	-3.2200634236	1.2537628744	7.0742394354
C	-2.7887080534	-0.0130329546	6.8689839969
H	-4.2805407822	1.4797387707	7.1363603171
H	-3.4919894348	-0.8321174634	6.7539775182
H	-1.7303377240	-0.2545030970	6.8971429613
H	-2.5189962654	2.0578383914	7.2778123409

16b(1st)

C	-4.2246414770	1.4457231835	1.2368737455
P	-2.7461215771	1.0360581440	2.2558083939
Ru	-3.0811589881	1.0539428970	4.5892134872
C	-3.5573132049	2.8130162872	4.5575765751
C	-1.4601379984	2.1942034623	1.6261266266
C	-2.2141728058	-0.6146595106	1.6468806472
Cl	-0.6841840950	0.9051267984	4.7415829897
Cl	-5.0304727563	-0.2774362540	4.1228812750
C	-4.0503336197	0.8399044579	6.8222389220
C	-2.7563451804	1.2136752005	7.0081761733
H	-3.8326554813	3.3262026193	5.4875736117
H	-3.6027879315	3.4471605101	3.6645961885
H	-4.5608274460	2.4622225397	1.4646045697
H	-5.0310587137	0.7528893382	1.4876313860
H	-3.9904336585	1.3795678340	0.1686381262
H	-1.2788632970	-0.8892078735	2.1429544820
H	-2.9814560961	-1.3499227825	1.9056139033
H	-2.0649802951	-0.6063907994	0.5613614885
H	-1.7414918421	3.2245433922	1.8657646397
H	-0.5112736543	1.9737568037	2.1201642645
H	-1.3500944593	2.0988507614	0.5402059099
H	-2.4644683394	2.2517561127	7.1326633827
H	-4.8631971857	1.5585136754	6.7886191580
H	-4.3442671106	-0.2042777828	6.8311849671
H	-1.9731171066	0.4809301043	7.1704624919

16c(1st)

C	-0.8486809727	0.2973887093	-1.1316299447
P	0.2961492273	-0.2018274570	0.2151181934
C	0.4636630420	1.3060649164	1.2590806164

C	1.9179961329	-0.3651820469	-0.6328122697
Ru	-0.3519254705	-2.0113576215	1.6544164236
C	0.0914201731	-3.2947870473	0.4538827589
C	-0.4181405546	-3.1096775662	3.7123500599
C	-1.7009571369	-3.0895064863	3.2267721881
Cl	-2.6112263397	-1.7915730946	0.6981076261
Cl	1.9812560661	-1.8068402005	2.4652972461
H	1.1086035763	-3.7018650256	0.4134692782
H	-0.6497671941	-3.6916815736	-0.2492759420
H	-2.4060092067	-2.3178419075	3.5212618658
H	-0.0643915994	-2.3550687697	4.4085057932
H	-1.8290190873	0.5321659394	-0.7134882517
H	-0.4408189690	1.1643383284	-1.6637049482
H	-0.9793202335	-0.5343798916	-1.8290023631
H	2.6727941825	-0.6570366464	0.1001096825
H	1.8451011278	-1.1448681425	-1.3977181327
H	2.1965597296	0.5803869392	-1.1108865543
H	1.2170511624	1.1174244213	2.0284978583
H	0.7625178916	2.1666894827	0.6501375014
H	-0.4938083018	1.5292947180	1.7409051447
H	0.2394192732	-3.9605763553	3.5716049227
H	-2.1240135552	-3.9219623751	2.6755122944

17(1st)

P	-0.0446871623	-0.1712902086	0.1333271125
C	0.9992406161	0.6929371323	-1.1130816337
H	0.6679348461	0.4527968261	-2.1296532250
Ru	0.6362180334	0.3136460012	2.3780498619
C	2.0479534735	1.4626092860	2.1668006195
C	1.5968178249	1.0135570075	4.4986021704
C	0.5174469388	0.1553100545	4.6266373089
H	0.6930863426	-0.9046804679	4.7886076812
Cl	2.1046864311	-1.6358304494	2.3925085995
Cl	-0.9536510187	2.1614579452	2.5060423183
H	3.0760439227	1.0924970214	2.0803868714
H	1.8999297959	2.5480611892	2.1327668726
H	1.4510723024	2.0842932186	4.6013322710
H	-0.4682835641	0.5617208389	4.8353342968
H	2.6083205779	0.6234721304	4.5518483973
H	0.9293210558	1.7727966289	-0.9546304767
H	2.0402072010	0.3820031183	-0.9879124397
C	-1.7626715498	0.3261458588	-0.2984548322
H	-2.4717528704	-0.2476904912	0.3062400256
H	-1.8984436212	1.3826337145	-0.0560720187
H	-1.9640433714	0.1429770259	-1.3600025837
C	0.0483320611	-1.9423340765	-0.3556906973
H	-0.6519382731	-2.5260728109	0.2497418496
H	-0.2030879969	-2.0648647825	-1.4153108734
H	1.0547352506	-2.3150758511	-0.1518608844

18(1st)

C	-0.7287268647	-0.9388844493	-0.9333603067
P	0.1751912846	0.0602844257	0.3119354532
C	0.8954395471	-1.1510121669	1.4898411640
C	1.5998055088	0.7955073609	-0.5847943949

Ru	-1.0222452793	1.7493422958	1.4921451161
Cl	1.0616083466	2.2438490065	2.6684337961
Cl	-3.0601480907	1.2055262149	0.2917738851
C	-1.3880270802	3.6732928956	1.2603880581
C	-2.1011142443	3.3681180844	2.6451038771
C	-2.0388954975	1.8768531031	3.1791007089
H	-1.4461715661	1.7686803540	4.0865275174
H	2.1938759996	0.0137844496	-1.0715393499
H	-0.5213015781	4.3258040039	1.3583106055
H	-2.0873278572	3.9244343654	0.4641256948
H	-3.1577892826	3.5953062333	2.4982499725
H	-3.0077981800	1.3795711295	3.1785801139
H	-1.6023021472	3.9867719639	3.3918212597
H	-1.5673092367	-1.4467837684	-0.4508078543
H	-1.1448141653	-0.2766655425	-1.6964984756
H	-0.0591723028	-1.6729029917	-1.3957379139
H	1.2347926510	1.4917898085	-1.3460964296
H	2.2102701450	1.3465999640	0.1349872670
H	1.5036317196	-0.6035031312	2.2143409205
H	0.0916536856	-1.6695802763	2.0214885897
H	1.5062260251	-1.8890985917	0.9580918306

19(1st)

C	-0.8555198997	0.4379394240	-1.0414368742
P	0.3075838335	-0.1774542697	0.2432570113
C	0.6031369046	1.2876747930	1.3192848353
C	1.8783005027	-0.3878304258	-0.6908698282
Ru	-0.3807525994	-2.0246362524	1.6416429754
C	0.1104782591	-3.2761202046	0.3678704679
C	-0.4749078938	-3.0061662955	3.5964378641
C	-1.6393207518	-2.9716178789	3.1667911985
Cl	-2.6631854696	-1.6079764993	0.7626114205
Cl	1.9954468963	-1.9008540447	2.3738226778
H	1.1767134806	-3.5356839171	0.3275705232
C	-0.7445464975	-4.0216305945	-0.5287237903
H	-2.7010609047	-3.0619436233	3.0522186505
H	0.4016544425	-3.1758791230	4.1892898482
H	-1.7990746785	0.7305830042	-0.5778759966
H	-0.4092703015	1.2900618287	-1.5669163704
H	-1.0717085377	-0.3615559507	-1.7550356544
H	2.6545350565	-0.7414504715	-0.0094997607
H	1.7291724316	-1.1325176448	-1.4791850866
H	2.1805900196	0.5606630772	-1.1484411830
H	1.3719442758	1.0328791618	2.0533931708
H	0.9270394507	2.1492190108	0.7243140916
H	-0.3212510052	1.5458725381	1.8460651581
C	-0.2338291892	-4.9884555087	-1.3204071665
H	-1.8034844398	-3.7831574468	-0.5507615466
H	-0.8595201062	-5.5581931110	-2.0025770913
H	0.8256059521	-5.2366099087	-1.3022513616

20(1st)

C	-0.5291744548	-1.0903196159	-1.1277770032
P	0.6734668761	-0.0657347503	-0.1823867380
C	2.2578313993	-0.9920242109	-0.2897007979

C	0.9452089942	1.4183986527	-1.2353462545
Ru	-0.1093081107	0.3337417660	2.0464577900
C	1.2968686886	0.8383866625	3.2084858166
C	2.2630737153	-0.0212076343	3.8743026756
C	3.4090324040	0.4845860114	4.3685145509
C	-0.4899980461	0.6941624013	4.2958688143
C	-1.3853857450	0.0295400046	3.7053329680
Cl	0.1748207633	-2.1362044762	2.2761080671
Cl	-0.6681695532	2.6293261625	1.5551941244
H	-0.1551144716	-1.2899226034	-2.1383636346
H	1.5001031481	1.9149765045	3.2756996041
H	-0.1826860538	1.3525275744	5.0874237739
H	-2.3280975088	-0.4873229062	3.7029595169
H	2.0548417273	-1.0863745641	3.9020691458
H	4.1697721294	-0.1535185746	4.8102883759
H	3.6258184073	1.5505516265	4.3283224779
H	1.7165716457	2.0489859102	-0.7844104510
H	1.2545479159	1.1262335009	-2.2454278966
H	0.0247465113	2.0053727658	-1.2743997954
H	-1.4863888967	-0.5642094358	-1.2003743785
H	-0.6786175073	-2.0317703591	-0.5928403078
H	2.1557522504	-1.9181552328	0.2804293684
H	2.5099748065	-1.2114416466	-1.3334384275
H	3.0581945368	-0.3920553508	0.1544395019

21(1st)

C	-3.6302500914	1.6577806744	1.0863723511
P	-2.4029972646	1.1127050130	2.3425844816
Ru	-3.1735113678	0.9424784444	4.4356664604
C	-3.5930312966	2.7299940763	4.6503260290
C	-0.9719659732	2.2470224571	2.1259907215
C	-1.7995196846	-0.5142205961	1.7323148206
Cl	-1.0116936670	0.7157789825	5.3856690280
Cl	-5.1694264689	-0.1496392073	3.7851028617
C	-3.9830839682	3.2213929232	5.9476799574
H	-3.6867572376	3.4353468482	3.8158475137
H	-3.9827785901	2.6654981004	1.3266610576
H	-4.4863402660	0.9790691092	1.1177768896
H	-3.1861961889	1.6620490958	0.0843892225
H	-1.0009221595	-0.8663194166	2.3920424902
H	-2.6225472765	-1.2342061476	1.7600589990
H	-1.4184117136	-0.4328571885	0.7079060103
H	-1.2674477033	3.2663244838	2.3921199541
H	-0.1736440123	1.9348310079	2.8041110858
H	-0.6154697431	2.2326800930	1.0897121830
C	-3.5115045314	2.7436103657	7.1363451436
H	-4.7050832698	4.0424658675	5.9668399339
C	-3.9450870254	3.2246858723	8.4290072147
H	-2.7333769295	1.9809126389	7.1246008187
C	-3.4426316262	2.7674745722	9.5906800174
H	-4.7213986824	3.9894386188	8.4400655273
H	-3.7923136934	3.1377715894	10.5496410177
H	-2.6657478906	2.0064955483	9.6103936760

22(1st)

C	0.2529943065	-0.7073137018	-1.4319294533
P	0.4017847798	-0.1763875613	0.3326481644
C	1.3811012538	1.3757128764	0.2116726127
H	0.9053778707	2.0644451728	-0.4958228165
Ru	1.2935554393	-1.9089527444	1.5930597883
C	2.0859132820	-2.6675991460	3.4456769169
C	1.2556438835	-3.8472370305	3.6441494249
C	0.3438870696	-3.9519710309	4.6352288842
Cl	1.3013754443	-3.6200106316	-0.0049247189
Cl	0.9750278287	0.0256054557	3.2172142135
C	3.3093808280	-1.6515956023	1.5214285056
C	3.3903201952	-2.7375305809	2.6267741954
H	2.1006422401	-1.9583635005	4.2654475565
H	3.5311227785	-3.7295472492	2.1889642901
H	3.6405032820	-0.6689935633	1.8650731296
H	3.7792135539	-1.9451455329	0.5802316344
H	4.2248640518	-2.5254317173	3.3132072362
H	1.3827039709	-4.6713912049	2.9432352099
H	-0.2616519001	-4.8456287177	4.7537590526
H	0.1833540202	-3.1442953753	5.3449791703
H	1.4542293776	1.8353982457	1.1984242425
H	2.3872223987	1.1342279354	-0.1436015717
H	1.2333390849	-1.0027965692	-1.8124624309
H	-0.4082230777	-1.5737886119	-1.5029818554
H	-0.1456243552	0.1177499583	-2.0345164124
C	-1.3096901432	0.3552533469	0.7449746180
H	-1.3229597114	0.7542736993	1.7602917547
H	-1.6529190571	1.1162266693	0.0343463575
H	-1.9784953894	-0.5096131061	0.6930900323

23(1st)

C	-1.0139443684	0.0407984554	-0.5107889758
P	0.4507819065	-0.3562550158	0.5326467686
C	1.7374299708	-0.8945582227	-0.6682863754
H	1.3602144018	-1.7040608480	-1.3030800966
Ru	1.0049775991	1.5218271701	1.9376707697
C	0.7864298026	3.6054974734	2.9116581019
C	1.8243846571	2.8892245236	3.4981011517
C	2.8757353694	2.4305563346	2.6448075511
C	3.5965730213	1.1553273431	3.0064648915
C	2.4166271199	0.1905248928	2.8825244152
Cl	-0.6287842575	0.7421057988	3.5366589793
Cl	1.6869267549	2.5362180418	-0.1730424111
H	3.2605763407	3.0821925935	1.8656600413
H	4.0605721670	1.1779776960	4.0039515381
H	2.6234194775	-0.6764144676	2.2535282777
H	1.9681463294	-0.1218474535	3.8261410194
H	4.3799073303	0.9413201093	2.2737217342
H	1.6812759779	2.4449234782	4.4803711276
H	-0.1416359232	3.7498521859	3.4555008316
H	0.9470591189	4.1999674134	2.0164043767
H	-1.8623765558	0.2791624342	0.1379214330
H	-0.7820195187	0.9136516815	-1.1267432810
H	-1.2778336151	-0.8070844953	-1.1528198607
H	2.0254058702	-0.0376586946	-1.2814926756

H	2.6207780113	-1.2498172954	-0.1286285613
C	-0.0300252143	-1.9080323481	1.3978208273
H	0.8191874246	-2.2947456359	1.9689955186
H	-0.8362874240	-1.6853629788	2.1003929922
H	-0.3523794400	-2.6683932695	0.6779580465

24(1st)

P	-0.0881869670	-0.3944758188	0.0890113848
C	0.7526356128	-1.6783589621	-0.9364251385
H	0.3661928816	-1.6771743765	-1.9624122912
Ru	0.7343181138	-0.4117265969	2.1574712169
Cl	-0.4934480746	-2.4537862758	2.7249982521
Cl	2.4108781181	1.2939876113	1.9016764757
C	-0.8251300932	0.3670494801	4.2383588762
C	-0.7821938927	1.5415422239	4.6709420962
C	-0.6268963326	1.0516709144	2.7920233833
H	-1.6098627648	1.1903901688	2.3378241773
H	-0.6342218936	2.5539972229	4.9820124433
H	-1.0615830811	-0.6798133281	4.3799960643
H	0.0067447132	1.9395707594	2.6989892103
H	1.8292595491	-1.4827161763	-0.9602543278
H	0.5813439478	-2.6594558396	-0.4837086676
C	-1.8768025097	-0.7896054658	-0.1195742591
C	0.1341728262	1.1592245963	-0.8776079857
H	-0.4428978875	1.9665502032	-0.4158211104
H	1.1886390602	1.4448287135	-0.8525978818
H	-0.2000674956	1.0278105508	-1.9132793023
H	-2.4882083317	-0.0141429845	0.3527508795
H	-2.1418307689	-0.8503274918	-1.1813329796
H	-2.0823760594	-1.7408754215	0.3776793490

25(1st)

C	-1.3759583425	0.8048715572	1.8434039335
P	0.1009369324	0.5567911471	2.9071070085
C	1.3764963647	1.6894596352	2.2155391252
Ru	-0.3163840694	0.7853175304	5.1373597358
C	-2.0337598254	1.7024219114	5.7509271450
C	-1.6170216983	2.9671613037	5.7189821043
C	-0.4467488379	2.9359627355	4.8050821304
Cl	-1.8571211554	-1.0285808876	4.8751322817
Cl	1.9158160370	1.2159695401	5.7203235485
H	-0.7076964879	3.1616178443	3.7689358087
H	-2.0001638913	3.8328648711	6.2658173951
H	-2.8970871196	1.1880056682	6.1573997481
H	0.4652804612	3.4543948487	5.1060394378
H	1.5427316883	1.4668578747	1.1555580305
H	1.0608029707	2.7307105204	2.3173191857
H	2.3063945550	1.5574459001	2.7742997044
H	-1.7726430252	1.8134625218	1.9914765092
H	-2.1421201007	0.0830561441	2.1357920875
H	-1.1166100599	0.6708195791	0.7870412858
C	0.7295873990	-1.1141418729	2.4625346980
H	-0.0010444777	-1.8630531093	2.7763692761
H	0.9022064574	-1.1858728598	1.3824608836
H	1.6698434399	-1.2949886177	2.9920088689

26(1st)

H	-0.4877171065	-0.4267001737	-2.4874275077
C	-0.6811460169	-0.0792865111	-1.4659941499
P	0.8765336262	0.4764243313	-0.6564545128
C	1.5734859512	1.7389304423	-1.7998327994
Ru	0.5744254582	0.9656335843	1.6004981515
Cl	2.6719264348	1.0582739834	2.5907410536
Cl	-0.2528293984	-1.2244880253	2.1548322218
C	0.8984443631	3.1449985638	1.2475576588
C	-0.0285938315	3.1902095896	2.3672733644
C	-0.8384663365	2.0937735679	2.2930202219
H	-1.6954224943	1.7102463797	2.8366565684
H	0.0784514787	3.8366388741	3.2447058180
H	1.8937125388	3.5659382487	1.3797168495
H	0.4558001394	3.3601902293	0.2790375575
H	0.9031623560	2.5999621112	-1.8710453150
H	2.5381951633	2.0821152087	-1.4154238091
H	1.7112484855	1.3130451098	-2.8000081611
H	-1.4003892753	0.7447625207	-1.4957844903
H	-1.1053986010	-0.8921094041	-0.8698056582
C	2.0153170382	-0.9612848852	-0.8143742860
H	2.9886051536	-0.7028025229	-0.3876303152
H	1.5976445077	-1.7938740505	-0.2417269654
H	2.1367010061	-1.2481543342	-1.8654042933

27(1st)

H	-0.8684137610	0.0634937603	-2.5804379847
C	-1.0336718425	0.2373659529	-1.5112184712
P	0.5652887208	0.4999637583	-0.6421240004
C	1.2720934661	1.9565250482	-1.5371739020
Ru	0.4101373484	0.4939101290	1.7487653189
Cl	1.0307038637	-0.2801889991	3.8898446701
Cl	-0.6320839829	-1.6336832347	1.3326339884
C	1.5885939498	2.5339800182	1.8770383083
C	0.3533062777	2.5741668709	2.5235305687
C	-0.7529867994	1.9026177066	1.9067399064
H	-1.8310460117	2.0211607541	2.0016485882
H	0.3236989732	2.7103096553	3.6080620403
H	2.4920333053	2.6145686977	2.4746577713
H	1.6843231346	2.7720367656	0.8279035856
H	2.3091429671	2.1286119747	-1.2340047703
H	1.2520951939	1.7709860933	-2.6168897279
H	0.6883363823	2.8582006958	-1.3272914288
H	-1.6634154213	1.1233758775	-1.3831670309
H	-1.5340115113	-0.6227247793	-1.0614486324
C	1.6473848520	-0.8791861146	-1.2046435143
H	1.2383097817	-1.8181608176	-0.8252093598
H	1.6987702283	-0.9039627954	-2.2991457572
H	2.6558563183	-0.7465551527	-0.8003070013

28(1st)

P	0.1431318845	0.1952356944	-0.2598461814
C	1.4546543769	0.8630019409	-1.3584412153
H	1.0331201275	1.1949103489	-2.3148080248
Ru	0.7614334784	-0.1287168130	2.0081649362
Cl	0.2920235995	0.1250895473	4.2997284835
Cl	1.5623543214	2.0982212112	1.8821230987
C	2.2497710547	-1.1465744175	1.7672336245
C	1.6977858574	-2.3916094551	2.2680751101
C	0.5682290065	-2.9530946025	1.7633374810
H	3.3027443780	-0.8700651685	1.6919879871
H	2.0719108113	-2.7419691505	3.2331979783
H	0.0320865141	-3.7172351801	2.3188425366
H	0.2133215400	-2.7243332125	0.7669818032
H	1.9306228651	1.7028820900	-0.8465007814
H	2.2063345909	0.0861082382	-1.5404322396
C	-1.1960880178	1.4592837367	-0.2991714645
C	-0.5651798530	-1.1918666043	-1.2544671104
H	-1.4112778415	-1.6400346591	-0.7256687018
H	-0.9085334620	-0.8206887332	-2.2287763148
H	0.1902464427	-1.9648764193	-1.4248726569
H	-2.0621710910	1.1021227803	0.2668601478
H	-0.8234295875	2.3720693568	0.1727735610
H	-1.5029803968	1.6667369069	-1.3304044945

29(1st)

C	-3.9370902520	1.2178784771	1.0907631341
P	-2.5567567622	0.8822004039	2.2563591017
Ru	-3.0882952248	0.9970568324	4.4451623260
C	-3.9659988923	2.5956617866	4.5505608903
C	-1.1587165539	1.9040835117	1.6330785779
C	-2.0229487581	-0.8360881867	1.8573091661
Cl	-0.8887396009	1.4590293826	5.1670494010
Cl	-4.7947665418	-0.6267346363	4.1624216273
H	-4.5329999783	2.6157038906	5.5018966414
C	-4.1072510554	3.7907251872	3.7341429568
H	-4.2659377140	2.2538221028	1.2087134680
H	-4.7690785377	0.5520217266	1.3335154243
H	-3.6153633913	1.0547072444	0.0558240017
H	-1.1342185043	-1.0841960701	2.4459721388
H	-2.8249380688	-1.5310679263	2.1176448899
H	-1.7833523081	-0.9246705420	0.7913567366
H	-1.4402109631	2.9589210881	1.6149747271
H	-0.2999248332	1.7796468983	2.2971280680
H	-0.8971553901	1.5885112701	0.6164805338
C	-3.0838134413	4.4916427996	3.2164621886
H	-5.1255845233	4.1754411184	3.6293694305
H	-3.2513293959	5.4179247870	2.6735680207
H	-2.0560297836	4.1831214414	3.3818433703

32(1st)

C	-1.5030290056	-0.0306051995	-1.1795297517
P	-0.2164210455	-0.0147168286	0.1378013972
C	1.3505046190	0.2327728373	-0.8033755783

Ru	-0.2695268841	-1.9913716798	1.6326907799
C	-0.8166784265	-4.1350911279	1.7787725109
C	-1.0530322757	-3.2628174066	2.8218911236
C	-0.4613925592	1.6033010995	0.9861167576
Cl	2.0180451858	-2.3959369406	1.2591405584
C	-1.0631783471	-3.5536316005	0.4668850210
Cl	-2.5729773327	-1.0827826246	1.9597461108
H	1.2764201805	1.1146058496	-1.4501824234
H	-0.4662660359	-3.9382883261	-0.3585850763
H	-2.0873850389	-3.2858017823	0.2156020870
H	-1.3331180088	-3.3177496016	3.8673252291
H	-0.1870345763	-5.0211099304	1.9156173052
H	-1.4520372697	0.8837346348	-1.7816746165
H	-1.3439310747	-0.8963727885	-1.8295833275
H	-2.4869444829	-0.1161358697	-0.7133409185
H	2.1815705127	0.3543188969	-0.1042302918
H	1.5569192549	-0.6530390829	-1.4097022534
H	-1.4130935458	1.5812720737	1.5224983336
H	0.3455577573	1.7627273516	1.7086441487
H	-0.4603262742	2.4275941302	0.2638252532

33(1st)

C	-1.0366706550	-3.1971091527	0.5223204116
C	-0.7502314178	-3.9606837289	1.7180775258
C	-0.8125903118	-3.2471767771	2.9057524846
Ru	-0.1024076607	-1.8476495160	1.8691378831
Cl	2.1602002008	-2.3222292138	1.4071908048
Cl	-2.3732692753	-0.8486036482	2.0271262762
P	0.3848936574	0.6209710733	1.6036743297
C	-0.1221791057	1.6158721074	3.0690208205
C	2.1563722643	1.0728750341	1.3661625798
C	-0.4579098437	1.4200773330	0.1753858274
H	-0.4893451682	-3.4806152846	-0.3750858437
H	-2.0385202496	-2.8101337101	0.3634662691
H	-0.1103396689	-4.8486363273	1.6714297951
H	-0.8106695833	-3.5210854364	3.9562975246
H	2.7398387332	0.7379277741	2.2280263354
H	2.2649512659	2.1575111774	1.2509069608
H	2.5494790208	0.5652652014	0.4819440374
H	-0.0758101521	0.9893223316	-0.7553436432
H	-0.2706112095	2.5001936686	0.1725780196
H	-1.5297891037	1.2240260871	0.2428742990
H	-1.1828698758	1.4407504944	3.2620254205
H	0.0576610033	2.6825249802	2.8924175744
H	0.4527729890	1.2987317994	3.9449940797

Intramolecular Enyne Metathesis

1-vinyl cyclopentene

C	1.5249533548	1.2448281916	-1.3825725373
C	1.3921091879	-0.0415343182	-0.5244666591
C	-0.0149666564	0.0388115908	0.1215143083
C	-0.7640146829	1.0132857212	-0.7737396299
C	0.0907159853	1.6627746253	-1.5878054566
C	-2.2015137307	1.2378036437	-0.7098057495
C	-3.0460164672	0.6239655187	0.1335142569
H	0.0274927671	0.4257539960	1.1507192264
H	-0.5027766341	-0.9422327508	0.1788184000
H	-0.2037257872	2.4355548130	-2.2938809317
H	2.0612564205	1.0695276273	-2.3243177449
H	2.0853689797	2.0321454751	-0.8531033953
H	1.4406000614	-0.9188449198	-1.1797739307
H	2.1929723862	-0.1439442455	0.2147340024
H	-2.5971658241	1.9717564782	-1.4123250689
H	-4.1097284098	0.8428010544	0.1286599060
H	-2.7045998157	-0.1135842112	0.8552055980

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C	-0.0809126061	-0.3806654749	0.2297448881
C	0.1823084200	0.4542117328	1.2361015452
H	0.6478793749	-1.1526106640	-0.0244150517
H	1.1006708630	0.3856130007	1.8133716338
H	-0.5142302600	1.2406427411	1.5216321429
C	-1.3206424869	-0.3446907549	-0.6231911003
C	-1.0097323917	-0.0834336328	-2.1087404821
H	-1.8516522156	-1.3060029460	-0.5392309688
H	-2.0059158910	0.4268203356	-0.2467356073
C	-2.2822844266	-0.1006915940	-2.9823706449
H	-0.5088916876	0.8859949488	-2.2157690808
H	-0.3091851643	-0.8406211377	-2.4833488479
C	-2.0039748668	0.1390201926	-4.4002481256
H	-2.7900468952	-1.0692479502	-2.8691433992
H	-2.9879571090	0.6583797186	-2.6158553847
C	-1.7437296980	0.3379002435	-5.5631168835
H	-1.5235810813	0.5132406298	-6.5910107029

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N	1.2834890000	0.2335070000	-0.8602190000
C	1.0461500000	-0.0227120000	-2.2891900000
C	-0.4828420000	-0.0824530000	-2.3679600000
N	-0.8597380000	-0.2087900000	-0.9557200000
C	0.1579750000	0.0732860000	-0.1140660000
C	-2.2481990000	-0.4931840000	-0.6337520000
Ru	0.0080690000	0.2017430000	1.9046270000
C	1.2172640000	1.5641190000	1.9540610000
C	2.6657320000	0.1473590000	-0.4050390000
Cl	1.1844840000	-1.8852780000	2.0417070000
Cl	-1.9598940000	1.5907380000	1.8389470000
C	0.0910520000	0.4869460000	4.4961230000
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C	-2.2581870000	-0.4744760000	4.5286980000
C	-2.7244270000	-1.0651120000	5.8758890000
C	-4.2636880000	-1.0470050000	6.0009720000
C	-4.7381840000	-1.6038410000	7.2699640000
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H	3.1423040000	-0.7275250000	-0.8663180000
H	-2.5735750000	-1.3498290000	-1.2368890000
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H	-2.8930970000	0.3667040000	-0.8450880000
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H	1.5555170000	2.1016580000	1.0622180000
H	-0.2724850000	1.5025490000	4.6319840000
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H	-2.5878590000	0.5641650000	4.4280460000
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C	-1.4873536837	-0.3483001337	-1.9137674118
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C	-0.2834912050	0.1617836622	0.0259125166
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C	-0.0289450612	-0.7803085794	-2.0948302917
C	-2.7733941506	0.4782933510	0.0817921643
Ru	0.0322157456	0.7011547289	1.9936623486
Cl	-0.8827353598	2.9248851038	1.4661871934
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C	0.0729141683	1.6470202183	4.2947916058
C	-0.5857005566	0.4500054748	4.2814009372
C	-2.0787874250	0.3050295059	4.0989251898
C	-2.7526235194	-0.2078496258	5.3882662498
C	-4.2623463683	-0.4545187826	5.1848900374
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C	-5.4248285380	-1.3993877174	7.3973783995
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H	-2.2064294101	-1.1430249876	-2.1354120743
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H	-2.5182990730	1.2623751575	3.7932076658
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H	-2.2763249445	-1.1426561776	5.7068421471
H	-2.6054272871	0.5180100745	6.1965227152
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H	-4.4051095976	-1.1674311125	4.3601727768
H	-5.8812789353	-1.7790810421	8.2824788898

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N	-1.3221096096	-0.1563232372	-0.7082645705
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C	-1.1746114162	-0.2771425828	-2.1660253987
Ru	-0.0501061253	0.5089616997	1.9208745346
C	0.1071670000	1.0356400000	4.3098610000
C	-0.7784629000	0.0030565799	4.0682718496
C	-2.2819608987	0.1734115917	4.0422299193
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C	-5.0614353256	-0.3500308573	6.6717333850
C	-5.5454510556	-0.5968276963	7.7507550725
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H	0.7049011459	-1.3812139746	-2.4279335740
H	-1.6901468857	-1.1666556659	-2.5410385389
H	-1.6032369847	0.6091099013	-2.6561225204
H	2.7596542315	0.5981068126	-1.6528074071
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H	2.6097891715	-0.7893483868	-0.5249223448
H	-3.2427838752	-0.9260908251	-0.4114758135
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H	-3.1597683598	0.8614356704	-0.5080490411
H	1.4643863688	2.5571618479	2.2596148757
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H	-2.5029255858	0.5038166441	6.1770320949
H	-4.7214586849	0.9604832635	5.0619403397
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C	-0.0079881762	0.0736457942	-1.3666293507
N	0.5141038432	1.0730322834	-2.0918290955
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Ru	0.0259574425	-0.0270014999	0.6574955731
Cl	-2.2816832864	0.7797626984	0.6221719366
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C	-1.4415198293	-1.9114827363	-1.7610073232
C	0.4543086355	1.2132375390	2.1395659750
C	0.0649185399	-0.0914461980	2.9307808147
C	-0.5187824796	-1.3115967268	2.0778685918
Cl	2.3714522145	-0.7016431590	0.5108585677
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H	-1.2193841082	-2.1933481808	-0.7310513389
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C	-0.1977959365	-3.3206613727	3.6010649492
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C	0.4760279930	-4.7030112573	3.7436737082
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H	-1.2855140674	-3.4378243953	3.6879515006
C	0.1692737483	-5.3579658637	5.0172365661
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C	-0.0984158665	-5.8735473217	6.0766120915
H	-0.3286497943	-6.3362422921	7.0086398492

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C	-0.5762335874	-0.4566827586	-3.5328230417
N	-0.6034047956	-0.8689377180	-2.1194625842
C	-0.0206012708	0.0532533262	-1.3377890484
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C	0.5134410618	0.6259189702	-3.5208796364
C	-1.5629520811	-1.8592868418	-1.6542101894
Ru	-0.0193600063	0.0245885663	0.6903893834
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H	-0.3387142625	-1.3034182277	-4.1832406492
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H	-2.5794576919	-1.4484508820	-1.6290619608
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H	0.5210297796	-2.0200079238	2.1821064074
H	0.8909267981	-0.2770594102	3.6010024995
H	-1.8765238893	-2.6645687848	1.6339612802
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H	-3.0093012233	-5.3003216892	7.2574010820

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C	0.072628	0.772134	-2.341415
C	-1.048478	-0.272148	-2.244688
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Ru	-0.104756	-0.035910	1.935157
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H	2.349372	1.642623	-0.989406
H	-1.902548	-2.536790	-0.972967
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C	2.9662228156	4.0207283104	4.3078152217
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C	3.9032801156	5.1044271882	4.0023699951
H	2.1194566743	4.4230798680	4.8820186998
H	3.4568855845	3.2843137265	4.9595524888
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H	5.3433208693	6.7863830920	3.4839740049

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C	1.1116314337	0.5797167402	-2.2186126895
C	-0.3948830810	0.4558055092	-2.4756235397
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C	0.0090858330	0.2655115645	-0.1682899028
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C	-2.3699801115	0.2131092075	-0.9574735432
Ru	-0.2339730039	0.0182476497	1.9155782719
Cl	-1.1689506302	-2.2078858261	1.4946210081
C	2.5143436896	0.1508249521	-0.1726525411
P	-0.1115184877	-0.6112419726	4.2565074090
C	0.3068993998	0.6820537943	5.5022018209
C	-1.7832242968	0.9543873413	2.1630636976
Cl	1.2609213801	1.9383538739	2.3379464491
C	-1.6090214747	-1.4274692740	4.9570556289
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H	-2.6731797739	-0.6419274229	-1.5761689948
H	-2.5884221426	-0.0281120947	0.0799094090
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C	-2.0525772821	2.3936333732	1.8363443382
H	-1.4192325101	-1.8255972646	5.9602361625
H	-2.4272161798	-0.7017213713	5.0131383050
H	-1.9072741715	-2.2347755117	4.2822349799
H	1.2550056162	-2.2170396190	5.5409550452
H	0.9905507648	-2.7351580300	3.8490688153
H	2.1765262712	-1.4593279879	4.2160971414
H	0.4860530894	0.2449120217	6.4911452083
H	1.1923265339	1.2251997784	5.1611702999
H	-0.5169629676	1.3995844710	5.5711538565
C	-2.2148463035	3.2269182129	3.1284988535
H	-1.2456349279	2.8103695182	1.2284042094
H	-2.9916616965	2.4510434710	1.2589021822
C	-2.5438387303	4.7033604632	2.8179198098
H	-3.0105185127	2.8051254923	3.7560337766
H	-1.2808258049	3.1798120283	3.6968844333
C	-2.7271014948	5.5064386475	4.0292383549
H	-1.7333502498	5.1329067790	2.2134062867
H	-3.4539782477	4.7582017023	2.2034891687
C	-2.8755177686	6.1430257876	5.0452784749
H	-3.0031437156	6.7143064742	5.9359092196

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C	0.8524286260	0.0302165089	-2.0383419637
C	-0.6753317507	-0.0322927896	-2.1115483551
N	-1.0596758611	0.1910420727	-0.7135911535
C	-0.0236851513	0.0084358370	0.1387906841
N	1.1088242947	-0.1505802267	-0.6021519193
C	-2.4745679885	0.3171536837	-0.4014190170

Ru	-0.1265015363	-0.0275198033	2.1074099557
Cl	-2.1793096388	-1.1493023931	2.5330490412
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C	1.0051725561	-1.4494519901	2.2672191446
C	1.4584418890	-1.9956859222	3.5880391456
C	1.0429894009	-1.1955842364	4.8317670994
C	1.5749697616	-1.8418181108	6.1297434103
C	1.2173351018	-1.0858828940	7.3316722864
C	0.9133488303	-0.4452517083	8.3095063485
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H	1.3458879156	-0.7509351711	-2.6256030983
H	-1.0385786989	-1.0149472493	-2.4459778564
H	-1.1099856699	0.7336687936	-2.7615283301
H	2.9126818085	0.9215548422	-0.5946520766
H	2.5381990563	0.0851291930	0.9171017128
H	3.0888973776	-0.8502027234	-0.5077230094
H	-2.9107048286	1.0659099465	-1.0724338563
H	-2.9979748866	-0.6370605692	-0.5360349720
H	-2.6091190643	0.6326443703	0.6300694279
H	1.3615680919	-2.0049297418	1.3899179823
H	2.6695064289	-1.9310562723	6.0702595424
H	1.0728148714	-3.0287338419	3.6573748442
H	2.5576365590	-2.0965667046	3.5533686549
H	-0.0513025075	-1.1364260179	4.8864902730
H	1.4237070877	-0.1699430287	4.7570327409
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C	-0.6067508353	0.0484229452	-2.1020638810
N	-0.9929391966	0.3064243691	-0.7106077693
C	2.4881495940	-0.2080356309	-0.0527798501
C	-2.3839958079	0.5938374722	-0.4062699543
Ru	-0.2543254951	0.0497877236	2.1862682474
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Cl	0.8875341568	2.1816989652	2.2234660195
C	1.0054324435	-1.2483753793	2.4707013554
C	-1.3744650823	0.3200142863	4.2757586105
C	-0.2380270534	0.2688690714	4.7219082525
H	1.4164141828	0.8817251548	-2.3214101934
H	1.3413016962	-0.8792004685	-2.5623759378
H	-1.0584438497	-0.8922920717	-2.4477359829
H	-0.9468502831	0.8562701571	-2.7582660376
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H	2.4909320547	0.0682894638	0.9993256315
H	2.9742233533	-1.1819342142	-0.1928579182
H	-2.7287431707	1.3932343884	-1.0730990602
H	-3.0140141081	-0.2929221110	-0.5325897570
H	-2.4780359075	0.9300312168	0.6253282598
C	1.9902666564	-1.4007723634	3.5958452612
H	1.0475649627	-2.0812605115	1.7539183132
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H	2.9466947897	-1.7026801174	3.1371426183
H	2.4727409663	0.6793057748	3.8835074037
H	3.1038161768	-0.3928856917	5.1437100858

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C	-2.4117625617	0.9245250847	-1.4112889720
N	-2.2305032260	0.8662248581	0.0463679436
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N	-0.1828564922	0.7638575269	-0.7245366002
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C	-3.3552677054	0.5962771332	0.9291065448
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H	1.6849724262	0.4176267292	0.1233935948
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H	-3.6137229452	-0.4685288473	0.9401999732
H	-3.1027502313	0.9090455038	1.9465609869
C	2.6065492560	0.4352436569	3.0263785999
H	1.4447318112	-1.4067779705	2.5900405110
H	-1.8884861607	0.1154524817	4.7717261629
C	1.6137802628	-0.0121055627	5.2829981109
H	3.4593000297	-0.2479288042	2.9142347323
H	2.7525465332	1.2857224043	2.3541269727
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N	1.1852455682	0.2750009481	-0.7826331062
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H	2.8371464807	1.5536698727	-0.4350912313
H	2.5960712645	0.2353872633	0.7580824887
H	-2.9959679781	-0.2869984610	-1.3944703740
H	-2.2785707499	-1.7949067314	-0.7692931569
H	-2.5856934818	-0.4068137146	0.3246875386
H	1.2622745184	2.2028301135	1.2871127865
C	2.2787483473	3.0510636809	3.7798095726
C	0.8138233229	2.7789388607	5.7408241986
H	-0.7013272439	1.5566628201	4.5357549380
C	1.9219014048	3.6877245323	5.1464348591
H	0.0571753888	3.3384501689	6.3045266979
H	1.2276196323	2.0328834011	6.4387759509
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H	3.1588714595	2.3964595527	3.8547969991
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C	2.1972162839	3.6086940705	5.0212945792
C	2.4049418621	2.8721826270	3.6739187472
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C	0.2588252475	2.2973983581	4.5070507658
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N	0.1361964233	-0.9064362128	-0.9183739140
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C	1.0650209045	0.1578907194	-2.1854600742
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N	-0.8722460679	-0.3607875553	-0.9926407845
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Ru	-0.2604581923	0.1854250363	1.8605475544
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C	0.9151882285	2.3512149385	3.3275398829
C	1.5625067859	3.5257280092	3.5357809741
C	2.5119219526	0.6410807824	-0.1878446364
Cl	1.2976060952	-1.5359931862	2.3443803304
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H	-0.9123867631	-0.1813481730	-3.1036760129
H	3.2854642119	0.0344736379	-0.6728054688
H	2.7338211382	1.7002008173	-0.3798320264
H	2.5357233485	0.4416524882	0.8812165223
H	-2.8518741481	-0.7490983625	-1.5159282017
H	-2.0388937758	-2.0933586778	-0.6721902639
H	-2.5535790735	-0.6276326269	0.2262148160
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C	0.5771975944	1.6829889872	4.6545863447
C	1.7514021861	3.8261218332	4.9975383691
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H	2.8051106693	3.6685755450	5.2802402162
H	1.5212331521	4.8692533184	5.2504918179
H	-0.1473022770	3.2999508650	5.9184852490
H	1.2127691181	2.4361828711	6.6395397984

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N	-0.8089829515	-1.1308951021	-0.6964022840
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N	0.7027343326	0.3275841296	-1.2897274528
C	0.1973730302	-0.2004479752	-2.5685257643
C	-0.5773197875	-1.4425428035	-2.1123031449
Ru	0.1089571067	0.1596286715	1.8161394553
P	-0.3389268728	-0.0263109453	4.1793644805
C	0.9905492575	-0.6981056716	5.2650504836
C	1.5124077458	1.5290683154	-1.3008683855
C	-1.5454522299	-2.0445191104	0.1615523189
C	1.1728109081	1.6564623029	2.0477853110
C	2.5846781162	1.8226707330	2.3267418955
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Cl	-1.8857880971	1.6042140149	1.6140301163
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H	-0.4572757111	0.5428697350	-3.0474527322
H	1.0225096656	-0.4295445167	-3.2499801260
H	0.0223811325	-2.3597691159	-2.2072121091
H	-1.5228867785	-1.5840315649	-2.6447985472
H	0.9322337693	2.3958718781	-1.6491101423
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H	2.3682006988	1.3862713564	-1.9707656310
H	-2.4120306898	-2.4270861227	-0.3874212744
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H	-1.9212585672	-1.4922633500	1.0289338678
H	-1.2559496902	1.2924879337	6.0519655172
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H	-1.9840845836	-1.2924978035	5.5129217982
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H	-1.4791506127	-2.1783338915	4.0484981866
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H	1.3842379122	-1.6099956906	4.8076967554
H	1.8056486513	0.0300051830	5.3286837817
C	3.6510168167	0.7530240657	2.5140972842
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C	4.8650203576	1.5431434886	3.0654414322
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C	3.2860890000	-0.6236320000	3.0351900000
C	2.5431440000	0.7039340000	3.0310720000
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C	1.1939190000	0.9991910000	2.6051670000
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C	-1.4828620000	-0.6503850000	3.7706480000
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H	2.8050770000	1.5381130000	-1.2060350000
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H	5.4370230000	-0.8843970000	3.5103660000

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C	4.8483656483	0.0513967087	2.9407860403
C	3.3945992981	-0.4460298422	2.7322860646
C	2.5921430728	0.8409713373	2.6265043164
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C	4.8688425116	1.5073742081	2.4056070842
C	1.1514947146	1.0241587242	2.5984085501
Ru	-0.2808115076	-0.1598163832	2.2676921613
C	0.3179791028	0.3820571363	4.4783824288
C	-0.8623708356	-0.3904234130	4.3367122668
C	-0.7343521277	-0.5309116048	0.2955206936
N	-1.7593031509	-1.3283667687	-0.0494167871
C	-1.7947568974	-1.5815394653	-1.4967695647
C	-0.9171341585	-0.4408883054	-2.0244206870
N	-0.1442428884	-0.0733344385	-0.8249239855
C	-2.4824744056	-2.1797221747	0.8800726493
C	0.7922276682	1.0361079396	-0.8976594204
Cl	0.7502328370	-2.3849029690	2.3563040447
Cl	-1.7575130021	1.8009346512	2.1389732528
H	-1.5159890377	0.4176789878	-2.3598672263
H	-0.2536404846	-0.7459295174	-2.8385216975
H	-1.3647747454	-2.5679253509	-1.7197936291
H	-2.8202072361	-1.5505244129	-1.8764821544
H	0.2675473960	1.9952512953	-1.0199033762
H	1.3850046265	1.0707980685	0.0142534154
H	1.4635293664	0.8820340064	-1.7506337420
H	-3.4917391680	-2.3513033540	0.4933189986
H	-1.9705081936	-3.1342180264	1.0327806365
H	-2.5734659887	-1.6687681290	1.8405085066
H	0.8555671379	2.0794248703	2.6176860656
H	3.0777392537	2.9274359558	2.3302483196
H	0.2144548743	1.4312562178	4.7405772815
H	-0.8089670058	-1.4566427807	4.5391566794
H	-1.8246464318	0.1033356099	4.4455438394
H	1.2279978488	-0.1148819647	4.7977036897
H	5.2384710714	1.5609442993	1.3688530921
H	5.5119659853	2.1764820912	2.9916035405
H	3.0433127403	-1.0957053266	3.5380573432

H	3.2777190072	-1.0361165596	1.8162082939
H	5.0851699538	0.0574634354	4.0112307198
H	5.5866369604	-0.5897691425	2.4500556831

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N	-1.0567358583	-0.8527432831	-0.5410125933
C	-0.1080299586	-0.1629254566	0.1144318077
N	0.6845975199	0.4674931996	-0.7627448616
C	0.3680788578	0.0676108413	-2.1432825164
C	-1.0355493133	-0.5353564882	-1.9786099319
Ru	0.0869334094	-0.1206799971	2.1255777068
Cl	-1.5961188591	1.6723899716	2.0418224889
C	1.9599790199	1.0871463751	-0.4345223931
C	-2.2532828064	-1.4015981500	0.0811230273
C	1.1429166822	0.9428446676	3.4166742113
C	0.3011850137	0.0310761770	4.3965816611
C	-0.9085537164	-0.7772365406	3.7602463872
C	-1.0679843873	-2.2089541621	4.0423631169
C	-2.2750356391	-2.8166978629	3.9845522936
Cl	1.8983490870	-1.7365044510	1.9155694014
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H	1.0979233274	-0.6761695932	-2.4937778519
H	-1.1936436135	-1.4350588640	-2.5802568287
H	-1.8260212584	0.1923838100	-2.2117795172
H	1.9080948173	1.4940105368	0.5765141014
H	2.7793574416	0.3599114490	-0.4818004467
H	2.1479894816	1.9067736665	-1.1353471768
H	-2.6146793515	-2.2385302453	-0.5248171359
H	-2.0092094083	-1.7777878935	1.0767691390
H	-3.0377518442	-0.6403554400	0.1724587864
H	2.2089874504	0.7170001556	3.4415849416
H	0.8875444695	1.9998555814	3.4812930284
H	-0.1816882491	0.7223611161	5.0915953048
H	-1.8435668543	-0.2246789203	3.8509483891
H	0.9722914454	-0.6686315266	4.8920471883
C	0.0160182968	-3.2185073576	4.3901370514
C	-2.1962592064	-4.2953332912	4.2611551354
H	-3.2029320742	-2.3078741913	3.7328553581
H	-2.9968062445	-4.6525632260	4.9215245570
H	-2.2917742604	-4.8675358182	3.3238448621
C	-0.7843862812	-4.4502417852	4.8839290017
H	0.6220817920	-3.4358384932	3.5031384315
H	0.7145561270	-2.8492515860	5.1504085309
H	-0.3048774354	-5.3973410569	4.6177652842
H	-0.8698727105	-4.4222319906	5.9768385928

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C	-1.2748159317	-4.4702479192	5.0307497522
C	-0.2634534318	-3.3105417918	4.8351578589
C	-1.1431863390	-2.1448379695	4.4129282638
C	-2.3834744031	-2.5720191836	4.0851780639
C	-2.5290590612	-4.0665693008	4.2104710108
C	-0.7576817281	-0.7301365006	4.3874627243
C	0.5181274586	-0.2288026028	4.7013099759
Ru	0.1463477746	-0.4012980387	2.3512302238

Cl	1.8125827251	-2.2062902324	2.2692108862
C	-0.0097569798	-0.5888745452	0.3071054318
N	-1.0755208401	-1.1535013602	-0.2960675547
C	-0.9998633916	-1.0296926197	-1.7596991949
C	0.4873634187	-0.7244444626	-1.9656260522
N	0.8830757607	-0.2332688521	-0.6348101080
C	-2.3612060693	-1.4161073642	0.3328103987
C	2.2723346530	0.1288187646	-0.4043201646
Cl	-1.5144813700	1.4128719928	2.1972601261
C	1.4405225470	0.7991952021	2.8742091800
H	0.6736149322	0.0325643836	-2.7331805990
H	1.0630553005	-1.6277475962	-2.2144986875
H	-1.3259179420	-1.9524827360	-2.2490560855
H	-1.6430974176	-0.2045095142	-2.0987132785
H	2.3456038471	0.7055718142	0.5164723005
H	2.9054014166	-0.7616664879	-0.3129456819
H	2.6154390592	0.7463987047	-1.2406889469
H	-2.8416509296	-2.2511901233	-0.1884045663
H	-2.2138327027	-1.7018922710	1.3752818198
H	-3.0095429494	-0.5328325452	0.3023040174
H	2.4794731628	0.4899217879	3.0315195552
H	1.2045473068	1.8560702629	3.0373513741
H	0.5858136173	0.7787867347	5.1004113390
H	-1.5830533638	-0.0228059598	4.3981789928
H	1.3375362621	-0.9051769086	4.9212112972
H	-3.1857777759	-1.9195569759	3.7485848204
H	0.4765775329	-3.5259838303	4.0561302529
H	0.2986452059	-3.0898841594	5.7514964358
H	-3.4695599093	-4.3663004537	4.6904484257
H	-2.5300171712	-4.5354735408	3.2131695974
H	-0.8652360713	-5.4379679049	4.7251921063
H	-1.5479577547	-4.5496839159	6.0895228087

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N	-0.9998932080	-0.8333169611	-0.5206328166
C	-0.0523346445	-0.1236626311	0.1285384330
N	0.7656128480	0.4344449633	-0.7872109587
C	0.4697306809	-0.0512476773	-2.1459562350
C	-0.9372485704	-0.6276943021	-1.9748993889
Ru	0.0720662554	-0.0584909184	2.1827254246
Cl	-2.0338689841	1.2277350365	2.2037798761
C	2.0767422176	1.0132614383	-0.5314486778
C	-2.2186204354	-1.3831205691	0.0516478084
C	0.9935835919	1.4944439059	2.4090366881
C	0.5012943172	-0.2303764739	4.6263684031
C	-0.7063808922	-0.8076808237	4.3195104276
C	-0.8995011676	-2.2250363363	4.0031753084
C	-2.0645583531	-2.7308861184	3.5400141645
Cl	2.1199155541	-1.4126263606	1.9748704698
H	0.5196325860	0.7652058325	-2.8723450101
H	1.1992721609	-0.8225429337	-2.4321810041
H	-1.0904530997	-1.5693238879	-2.5108231871
H	-1.7179359038	0.0832113179	-2.2831502935
H	2.0120194675	1.7287140677	0.2895468377
H	2.8094749640	0.2431444121	-0.2690700816
H	2.3929507982	1.5490613498	-1.4313018631
H	-2.4747564938	-2.3008985610	-0.4900104572

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H	2.0704664401	1.4891490325	2.6195441529
H	0.4884928886	2.4678470563	2.4091553476
H	0.5303579569	0.7769214731	5.0283246374
H	-1.6100281753	-0.2134099017	4.4220036965
H	1.4268371576	-0.7959675515	4.6238444794
C	0.1415495517	-3.3211562936	4.1729076405
C	-1.9934502825	-4.2178635357	3.3068228084
H	-2.9500621557	-2.1331030102	3.3387129308
C	-0.6859030043	-4.6269416052	4.0382021217
H	0.9169884720	-3.2333370081	3.4031884874
H	0.6519590182	-3.2497650897	5.1415800202
H	-2.8779805505	-4.7496856355	3.6801787905
H	-1.9407062265	-4.4325352530	2.2272843470
H	-0.1393745971	-5.4147600763	3.5107961340
H	-0.9352813079	-5.0126870268	5.0334407433

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N	-0.2240179620	-1.1545927058	-0.3256592168
C	0.1791389438	-0.1102764264	0.4306635915
N	0.8214667445	0.7639688987	-0.3869378698
C	0.7632163689	0.3632722484	-1.7998421963
C	0.2458701996	-1.0760995966	-1.7140836726
Ru	-0.2530950699	0.1415280826	2.4213788941
Cl	-1.6552491737	1.9879104025	1.6978160485
C	1.1653613765	2.1502273890	-0.1165551285
C	-0.9669735708	-2.3354952363	0.0770713767
C	1.3857152391	0.9152922758	2.8362532973
C	2.7431947127	0.5760960341	2.4886808542
C	3.7946679927	1.2743473297	2.9974896595
C	5.1227012303	0.7333806472	2.5462638519
C	4.7474248465	-0.6582619035	1.9746639410
C	3.2490156244	-0.5490990617	1.5955079845
Cl	0.4854110924	-2.1245614539	3.0183243554
C	-0.8941661043	0.9574067000	4.7160255202
C	-1.5600771159	-0.2146865294	4.5501878225
C	-2.9704427818	-0.3423390295	4.0385803864
H	0.0739509618	1.0252692042	-2.3433198986
H	1.7503434901	0.4393603640	-2.2689308326
H	1.0369942007	-1.8202867692	-1.8832288234
H	-0.5721947138	-1.2837437892	-2.4123876033
H	0.5328611489	2.8129404839	-0.7206229054
H	0.9929979448	2.3815072073	0.9294867639
H	2.2173058549	2.3309218047	-0.3731519572
H	-1.8471693179	-2.4435963316	-0.5698351506
H	-0.3444521461	-3.2340169452	-0.0131669057
H	-1.2746833946	-2.2499590799	1.1154840610
H	1.3343435479	1.7675596447	3.5285826773
H	3.6943252052	2.1412016117	3.6465463633
H	-1.3358510488	1.9116785169	4.4463639843
H	-1.0990037124	-1.1274561089	4.9179327790
H	0.0518541614	0.9728967744	5.2484385015
H	5.5543678978	1.3933612675	1.7747943510
H	5.8626640691	0.6871793419	3.3554905704
H	2.6939852158	-1.4752153205	1.7549051542
H	3.1253520764	-0.2654243822	0.5411431172

H	4.8664932658	-1.4121966714	2.7614799470
H	5.3815947712	-0.9573743942	1.1339340251
H	-3.0518752915	-1.1376614338	3.2856693720
H	-3.6316570437	-0.6328931495	4.8674044624
H	-3.3319739058	0.5919447011	3.6031388327

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C	3.4860175370	1.8034550735	2.4006897687
C	2.6266832150	0.7759615588	2.6151177417
C	3.3944212030	-0.5218987562	2.8127362888
C	4.8512454902	-0.0463043414	3.0405270112
C	4.9250347413	1.3634309386	2.3990024294
C	1.1916338300	0.9968949979	2.5570875012
Ru	-0.2867898544	-0.1459308214	2.2588355030
Cl	0.7498799058	-2.3794465819	2.3256259007
C	-0.7632534771	-0.5488879310	0.2962347021
N	-0.2506904516	0.0144647009	-0.8148967099
C	-1.0424137184	-0.3410511327	-2.0054467723
C	-1.7958270935	-1.5850007023	-1.5204347272
N	-1.7281245535	-1.4161379685	-0.0615278913
C	0.5657956872	1.2191260622	-0.8401330553
C	-2.3415629950	-2.4002742470	0.8165438352
Cl	-1.6682647173	1.8856509765	2.0093823185
C	0.2877774350	0.4958334287	4.4366353054
C	-0.7584727150	-0.4633792789	4.3712136411
C	-2.1912826319	-0.1265680102	4.7160717202
H	-1.7275669254	0.4818755703	-2.2563009550
H	-0.3932689016	-0.5336408148	-2.8646674342
H	-1.2899056555	-2.5165001126	-1.8139070490
H	-2.8340269105	-1.6252689869	-1.8635867461
H	-0.0500954070	2.1193716597	-0.7237506803
H	1.2921245734	1.1810246944	-0.0289095545
H	1.1032340355	1.2566376736	-1.7931347209
H	-3.3799457476	-2.5569919716	0.5045996400
H	-1.7961355648	-3.3507337399	0.7955384183
H	-2.3408808462	-2.0315240041	1.8433775919
H	0.9303376163	2.0607063859	2.5214711806
H	3.1762755210	2.8280848234	2.2082684382
H	0.0249549779	1.5297914445	4.6449082151
H	-0.4619682362	-1.4964693867	4.5462647966
H	1.2586629425	0.1601320833	4.7866539776
H	5.3063606010	1.3238798620	1.3656549753
H	5.5826205702	2.0546931044	2.9414913182
H	3.0043332628	-1.1229225640	3.6388112419
H	3.2913608984	-1.1548028168	1.9239440188
H	5.0467572178	0.0386119562	4.1163872064
H	5.5909536536	-0.7399471437	2.6292698887
H	-2.8945357185	-0.7814219696	4.1878497947
H	-2.3477648275	-0.2924357540	5.7928804501
H	-2.4372912315	0.9075275774	4.4698057596

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C	3.3352820000	-0.4398050000	3.6313460000
C	2.5121730000	0.7698260000	3.2152220000
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C	4.7384190000	1.2520690000	2.5203740000
C	4.7964900000	0.0636350000	3.5143200000
C	1.0684150000	0.9739220000	3.3770050000
C	0.2889490000	0.2658290000	4.5528120000
C	-1.0340710000	-0.5580540000	4.1925180000
C	-2.3405660000	0.0030690000	4.7120310000
Ru	-0.2908520000	-0.1596860000	2.3897350000
Cl	0.7730390000	-2.3616050000	2.4079780000
C	-0.8390200000	-0.5517640000	0.4794460000
N	-1.8444680000	-1.3530810000	0.0969140000
C	-1.8260950000	-1.5653420000	-1.3597860000
C	-0.9487960000	-0.3968370000	-1.8335380000
N	-0.2163520000	-0.0568760000	-0.6025360000
C	-2.5515800000	-2.2764080000	0.9713770000
C	0.7161580000	1.0617280000	-0.5807610000
Cl	-1.5401970000	1.9499950000	2.0708460000
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H	0.1842570000	2.0203140000	-0.6001450000
H	1.3222050000	1.0153450000	0.3260380000
H	1.3814340000	0.9832740000	-1.4466090000
H	-3.5682030000	-2.4188670000	0.5908900000
H	-2.0345390000	-3.2417180000	1.0299480000
H	-2.6063130000	-1.8487650000	1.9732880000
H	0.7808190000	2.0206370000	3.2790260000
H	2.9380780000	2.6325710000	2.2085980000
H	-0.0512510000	1.0800360000	5.1967710000
H	-0.8889010000	-1.6127260000	4.4378780000
H	0.9710910000	-0.4162090000	5.0590800000
H	4.9784570000	0.9341720000	1.4924610000
H	5.4477940000	2.0526280000	2.7669760000
H	3.0994450000	-0.7900790000	4.6433620000
H	3.1244700000	-1.2826920000	2.9634380000
H	5.1404490000	0.4284520000	4.4896520000
H	5.4878980000	-0.7233020000	3.1969600000
H	-3.1870460000	-0.5362620000	4.2701970000
H	-2.4003930000	-0.1399580000	5.8024160000
H	-2.4578790000	1.0620430000	4.4762880000

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C	-0.5529005063	-3.1524616445	5.0435254526
C	-1.3692177149	-1.9985831030	4.4822569218
C	-2.5988796293	-2.4177088894	4.1058046912
C	-2.7906836682	-3.8969014888	4.3150260523
C	-1.6077900513	-4.2705042254	5.2478475442
C	-0.9395041010	-0.6005390483	4.3837838147
C	0.3287683058	-0.1122731405	4.7783714310
Ru	0.1277294590	-0.3549984436	2.4485540088
C	1.4707401889	0.7769542546	3.0833108586
C	1.4869480234	2.2674689569	3.2319677917
C	0.1073746283	-0.6310862023	0.4026811169
N	-0.9180184127	-1.2157518241	-0.2490340983
C	-0.7307796266	-1.1689403067	-1.7070672564
C	0.7748246632	-0.9120380993	-1.8124094414
N	1.0747096100	-0.3419602525	-0.4885977857

C	-2.2505704205	-1.4348534565	0.2923993976
C	2.4519901158	-0.0115323650	-0.1628842415
Cl	1.7198037326	-2.2297544243	2.5358197944
Cl	-1.5421204118	1.4370370932	2.0463372176
H	1.0434043767	-0.2144849564	-2.6110632915
H	1.3414185258	-1.8444628317	-1.9525063124
H	-1.0458472219	-2.1067255105	-2.1745199671
H	-1.3218575134	-0.3448628569	-2.1333319663
H	2.4716394781	0.5944662133	0.7414333340
H	3.0490095917	-0.9156919555	0.0080056500
H	2.8792185219	0.5652239552	-0.9895200047
H	-2.6964545278	-2.2955972890	-0.2157013563
H	-2.1879255297	-1.6589712258	1.3570024845
H	-2.8865837773	-0.5528775194	0.1598748332
H	2.4283172343	0.2875880251	3.3081329385
H	0.3729099349	0.8952975633	5.1806682566
H	-1.7465610556	0.1247066686	4.3139169515
H	1.0907943395	-0.8058929117	5.1222291040
H	-3.3603978871	-1.7723283770	3.6740506832
H	0.2325773557	-3.4386082911	4.3348726920
H	-0.0476328012	-2.8822856908	5.9796960812
H	-3.7710768567	-4.1476543446	4.7407212879
H	-2.7292530651	-4.4280147767	3.3514636994
H	-1.2057950498	-5.2671888628	5.0412229657
H	-1.9561382497	-4.2669386770	6.2878105447
H	2.0363815982	2.5673187535	4.1327895660
H	2.0467168579	2.6814355162	2.3798577449
H	0.4941494388	2.7037189238	3.2179511103

48-OMe

C	3.6649922949	1.4583325615	2.9572959650
C	2.6686877053	0.6867173336	2.4462042379
C	3.2562450564	-0.4270933636	1.5891836149
C	4.7535695957	-0.4308430022	1.9884472065
C	5.0312947151	0.9937412865	2.5349248663
C	1.2835594607	0.9253466052	2.7654129688
Ru	-0.2690749396	0.0224161991	2.3068545690
Cl	0.4919497631	-2.1983434546	3.0086782044
C	0.2020707122	-0.1769986911	0.3319586287
N	0.7725704204	0.7618242852	-0.4675546240
C	0.8023000947	0.3671095383	-1.8821998449
C	0.3714577983	-1.1035883460	-1.8288714180
N	-0.0895708401	-1.2470850313	-0.4432636320
C	1.0246367364	2.1622385134	-0.1706036168
C	-0.7403995560	-2.4896320160	-0.0688641784
Cl	-1.8112928258	1.7577353017	1.6562409900
C	-0.7372135874	0.3125611164	4.8248981781
C	-1.9190245616	-0.2527416840	4.4755283765
O	-3.0595920547	0.4497061323	4.4498455784
C	-4.1204452317	-0.0800698937	3.6541348062
H	0.1018705849	0.9910407689	-2.4549483059
H	1.8037588211	0.5059058998	-2.3054246868
H	1.2036414816	-1.7960014247	-2.0183365507
H	-0.4346227818	-1.3423945099	-2.5318884398
H	0.4284447682	2.7906802609	-0.8442737077
H	0.7295276759	2.3854592583	0.8497600367
H	2.0872401377	2.3974228994	-0.3162876035

H	-1.6629599051	-2.6128056710	-0.6519059130
H	-0.0786304759	-3.3406885982	-0.2737769086
H	-0.9602901795	-2.4905091557	0.9954972531
H	1.1425229455	1.7555580456	3.4731078850
H	3.5002497562	2.3278426340	3.5892829956
H	-0.6926634046	1.3702847512	5.0635886857
H	-1.9994410142	-1.3239419387	4.2782179109
H	0.1014836191	-0.3274907162	5.0644645633
H	5.4330997205	1.6627610013	1.7553043838
H	5.7606034305	1.0101731299	3.3549187058
H	2.7584198545	-1.3825663102	1.7694545513
H	3.1278611838	-0.1839674335	0.5252445574
H	4.9103154098	-1.1590128619	2.7927330146
H	5.4170609611	-0.7061205817	1.1623073608
H	-4.1871681151	-1.1705031755	3.7696646841
H	-5.0405579222	0.3822120305	4.0159453275
H	-3.9584547379	0.1847799477	2.6048109583

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N	-0.1640856004	0.0080866844	-0.8026681387
C	-0.7023118510	-0.5782817387	0.2843677427
N	-1.6302002203	-1.4667321610	-0.1194949173
C	-1.6444547419	-1.6209279205	-1.5812142555
C	-0.8956496991	-0.3597510344	-2.0273969131
Ru	-0.2910115436	-0.1933065527	2.2675805822
Cl	-1.7337835647	1.7826091792	1.9178098655
C	-2.2606588597	-2.4685137393	0.7249585163
C	0.6111292703	1.2396125320	-0.7914303908
C	1.1158547250	1.0067437019	2.6417436238
C	2.5594288748	0.8443829410	2.6313915349
C	3.3757086822	-0.4383599312	2.5781975504
C	4.8317186661	0.0508413600	2.7886182365
C	4.8230526919	1.5519652499	2.3991575723
C	3.3728567076	1.9262208402	2.5411929880
C	0.3358181085	0.1897641803	4.4938868252
C	-0.9578702398	-0.3705648131	4.3980910714
Cl	0.7183715714	-2.4288902901	2.4778455362
H	-1.5852345497	0.4508332856	-2.3048930718
H	-0.2064009529	-0.5347689184	-2.8588266431
H	-1.1146296805	-2.5413768961	-1.8674958715
H	-2.6694837824	-1.6742865502	-1.9609102792
H	-0.0441627450	2.1173748961	-0.7346834569
H	1.2757728287	1.2425478069	0.0710209672
H	1.2133392417	1.2823348604	-1.7050248968
H	-3.2786530878	-2.6493206049	0.3623317211
H	-1.6934726244	-3.4064872520	0.7291003901
H	-2.3197024232	-2.1022906120	1.7507855685
H	0.8037218029	2.0533175295	2.7340881187
H	3.0196838366	2.9546126536	2.5242843494
H	0.3952318107	1.1907890475	4.9111342379
H	-1.0785623690	-1.4565823494	4.4282613433
O	-2.0093659927	0.3627287405	4.8286770364
H	1.1613720775	-0.4864173126	4.6816483297
H	5.1523453751	1.7098970998	1.3591303079
H	5.4842591091	2.1659396598	3.0241657209
H	3.0585936914	-1.1747127313	3.3200404343
H	3.2343508668	-0.9286628219	1.6066390925

H	5.1009644316	-0.0445818467	3.8472783755
H	5.5595415022	-0.5316654187	2.2154152729
C	-3.2983627513	-0.0884866042	4.4179777662
H	-4.0202905457	0.4041986597	5.0719159162
H	-3.4752419368	0.2076090658	3.3794497867
H	-3.3858229556	-1.1787657451	4.5331590660

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N	-1.8000410000	-1.3719650000	0.0483260000
C	-0.8130150000	-0.5622400000	0.4665450000
N	-0.1794440000	-0.0393850000	-0.5963900000
C	-0.8862860000	-0.3632010000	-1.8459780000
C	-1.7606220000	-1.5478100000	-1.4122680000
Ru	-0.3169200000	-0.1735300000	2.3926050000
Cl	-1.5781450000	1.9120410000	2.0120460000
C	0.7340920000	1.0940790000	-0.5429590000
C	-2.5046310000	-2.3342620000	0.8801180000
C	1.0423130000	0.9579370000	3.3691410000
C	0.2914190000	0.2253710000	4.5555180000
C	-1.0723730000	-0.4940370000	4.2175480000
O	-2.1306080000	0.1975340000	4.7357390000
C	-3.4097850000	-0.3330630000	4.4210730000
C	2.4901620000	0.7836000000	3.2076390000
C	3.2663400000	1.7425880000	2.6533840000
C	4.7102890000	1.3280450000	2.5392390000
C	4.7827890000	0.0895570000	3.4690640000
C	3.3278100000	-0.4365240000	3.5595170000
Cl	0.7175430000	-2.3951810000	2.5020110000
H	-1.4890800000	0.4987140000	-2.1660940000
H	-0.1795200000	-0.6153840000	-2.6419320000
H	-1.2985690000	-2.5148400000	-1.6581420000
H	-2.7682920000	-1.5206360000	-1.8375110000
H	0.1866270000	2.0433610000	-0.5761280000
H	1.3120250000	1.0547630000	0.3814820000
H	1.4246990000	1.0288130000	-1.3902640000
H	-3.5465180000	-2.4030670000	0.5490760000
H	-2.0336490000	-3.3233360000	0.8256310000
H	-2.4808790000	-1.9980870000	1.9165950000
H	0.7395300000	2.0030200000	3.2946370000
H	2.8926570000	2.6996430000	2.2963440000
H	-0.0086140000	1.0229070000	5.2388250000
H	-1.0853410000	-1.5628010000	4.4640790000
H	0.9586010000	-0.5048410000	5.0117700000
H	4.9553610000	1.0688010000	1.4961320000
H	5.4093500000	2.1231740000	2.8291500000
H	3.0969360000	-0.8457270000	4.5499650000
H	3.1261270000	-1.2459690000	2.8484530000
H	5.1225190000	0.4067240000	4.4623880000
H	5.4837850000	-0.6712940000	3.1115300000
H	-4.1276300000	0.1864060000	5.0584500000
H	-3.6471150000	-0.1385500000	3.3689210000
H	-3.4540400000	-1.4134130000	4.6262400000

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N	-0.9614053619	-1.2226833239	-0.2203761550
C	0.0001540374	-0.5450925595	0.4336515956
N	0.8785984717	-0.0589876925	-0.4558007499
C	0.6076442354	-0.5657028966	-1.8103965998
C	-0.8420437243	-1.0513631590	-1.6766110557
Ru	0.0832244952	-0.3467692868	2.4753542679
Cl	1.6931670729	-2.2102693306	2.4682739718
C	2.1730294597	0.5155912394	-0.1199911247
C	-2.2259571294	-1.6338343096	0.3692622161
C	-0.9747127374	-0.7240389213	4.2849428143
C	0.2772929929	-0.1059822763	4.7332462009
C	-1.3199938581	-2.1300081384	4.4988449894
C	-2.5511558607	-2.6245938045	4.2418401759
C	-2.6543261506	-4.0981520224	4.5264722026
C	-1.3780549175	-4.3770059498	5.3614701266
C	-0.4026466271	-3.2216799874	5.0232964621
Cl	-1.5581315544	1.4580631604	2.1427926122
C	1.3871032790	0.6731368044	3.4012148189
O	1.4166473372	2.0159304322	3.4791067384
C	2.5480546200	2.5866142532	4.1488229199
H	0.7321241153	0.2243164192	-2.5561487670
H	1.2958401996	-1.3892266369	-2.0482360364
H	-1.0332199940	-1.9931613423	-2.1993253347
H	-1.5618319604	-0.2984488139	-2.0275051107
H	2.0693221229	1.1147710679	0.7850338551
H	2.9295208193	-0.2644301420	0.0463600497
H	2.4911186339	1.1690405649	-0.9401886945
H	-2.6212093749	-2.4820505562	-0.1986201243
H	-2.0635473561	-1.9574661955	1.3993242223
H	-2.9507625238	-0.8118210926	0.3673549229
H	2.3583174955	0.2019495668	3.6087979318
H	0.1228852090	0.8471969006	5.2384940371
H	-1.8313942213	-0.0544964568	4.2498614727
H	0.9866673785	-0.7796408532	5.2069395383
H	-3.3750983968	-2.0361181785	3.8463128948
H	0.3279240128	-3.4970508700	4.2543082884
H	0.1740839409	-2.8983668720	5.8979817773
H	-3.5789051193	-4.3702183874	5.0519594756
H	-2.6553034737	-4.6701295742	3.5856149925
H	-0.9460113794	-5.3599424856	5.1568506238
H	-1.6338744717	-4.3466893358	6.4259669431
H	2.5131995495	3.6583389439	3.9497782905
H	2.4854617902	2.4130092988	5.2304347173
H	3.4844586935	2.1669073348	3.7640372274

Disfavored Intramolecular Pathway

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N	-1.2214345540	0.2132602082	-0.5904360459
C	-0.1042611604	-0.0751324478	0.1023479549
N	0.8629910203	-0.4372678305	-0.7539270493
C	0.4391584609	-0.2434098114	-2.1526019923
C	-1.0830598208	-0.1326679574	-2.0126115450
Ru	-0.1222895088	0.1758957725	2.1728934878
C	-0.7799624341	1.4936684503	3.8209246605
C	-1.4259707096	0.4216793995	3.8508117573
C	2.2832043914	-0.5401205013	-0.4695487195
C	-2.5461065095	0.4070429880	-0.0194080122
Cl	-1.3183263473	-2.0023067400	2.1182204300
Cl	1.2503660184	2.1484788372	1.5562803538
C	1.3865937475	-0.7041942618	2.6737947071
H	0.8862150158	0.6803505049	-2.5467254243
H	0.7590268834	-1.0831175627	-2.7762119103
H	-1.5892207492	-1.0874987903	-2.2149855634
H	-1.5230733145	0.6411652416	-2.6486505521
H	2.7776406038	0.4320104813	-0.5830502147
H	2.4201026791	-0.8858344423	0.5539160277
H	2.7273802679	-1.2670661082	-1.1572137015
H	-3.1180800527	1.0687103283	-0.6781256107
H	-3.0701717554	-0.5472601843	0.1048561550
H	-2.4664160735	0.8861845903	0.9587599734
H	2.3294512510	-0.1635708937	2.8020908952
H	1.3463972720	-1.7610443167	2.9525784468
H	-2.1029676984	-0.3429654049	4.1804627303
C	-0.3249523245	2.8339055450	4.2326956905
C	-1.1422336726	3.4041968443	5.4074731646
H	0.7389546836	2.7741309222	4.4948214337
H	-0.3635911959	3.5061199112	3.3682478773
C	-0.6558499674	4.8139435078	5.7966184968
H	-2.2038155685	3.4423467250	5.1287340717
H	-1.0680340024	2.7360104815	6.2741866499
C	-1.4727285493	5.4288831805	6.9007529696
H	0.3996629878	4.7710223077	6.0965584644
H	-0.7023937441	5.4570948822	4.9039485512
C	-0.9967230772	5.8021901484	8.0897583320
H	-2.5358838258	5.5591281668	6.6893921783
H	-1.6362879836	6.2385491320	8.8526146034
H	0.0559443132	5.6887707165	8.3430657594

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C	-0.0360025643	2.1545238261	-1.6133842775
C	-1.4413704818	1.5428254593	-1.6352508604
N	-1.5574061914	1.0262256389	-0.2637663806
C	-0.3515821433	0.9085693857	0.3276198905
N	0.5822804715	1.4580852364	-0.4716061795
C	-2.7609358002	0.3166845087	0.1430407918
Ru	-0.1333636737	0.0751502240	2.1780094719
Cl	-0.0017877240	2.3502732348	3.0784434010
C	1.9261902306	1.8364623433	-0.0621294252
C	1.6126578763	-0.3073331286	2.6073184618
C	0.2205807866	-0.8889762474	4.3548609934

C	-0.9616525266	-0.5745739475	4.1342112995
C	-2.4047815487	-0.3635354394	4.3597765021
C	-2.8530341655	-0.7448573433	5.7858736087
C	-4.3565741764	-0.4785530194	5.9924432717
C	-4.8311104634	-0.8783284018	7.3639268857
C	-5.3337713250	-0.0404614936	8.2721051025
Cl	-0.5163839569	-2.1443182263	1.2297687377
H	-0.0616938312	3.2363450653	-1.4178799948
H	0.5291768882	1.9769234803	-2.5330200233
H	-1.5217441281	0.7156766326	-2.3556242349
H	-2.2286868608	2.2721864398	-1.8485787590
H	1.9225737745	2.7903593604	0.4792969244
H	2.3360834505	1.0651869929	0.5890229637
H	2.5541115327	1.9170969913	-0.9549560600
H	-3.6347743187	0.9063724351	-0.1535330953
H	-2.8104060059	-0.6823701792	-0.3046602271
H	-2.7790900842	0.2058466509	1.2288403100
H	2.2529197861	0.4247266259	3.1123198696
H	2.0494763518	-1.2838551905	2.3706319960
H	1.0795477261	-1.2821913682	4.8559482379
H	-2.6274884394	0.6950070694	4.1714625925
H	-2.9655730301	-0.9526269235	3.6213083754
H	-2.6300904689	-1.8044132728	5.9638736592
H	-2.2734227743	-0.1664461203	6.5144861086
H	-4.5671421917	0.5861355836	5.8248392790
H	-4.9212022412	-1.0380105649	5.2301839070
H	-4.7335439179	-1.9368501726	7.6116280170
H	-5.6550186439	-0.3826562703	9.2523890304
H	-5.4453653486	1.0227420195	8.0666518383

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N	1.1531040983	-0.0699782397	-0.8150597152
C	0.9387406725	-0.4121544868	-2.2257882969
C	-0.4367045591	-1.0883514489	-2.1903127205
N	-0.9466560143	-0.7006646453	-0.8686493247
C	0.0224467956	-0.1814443477	-0.0721826512
C	-2.2029590925	-1.2987367239	-0.4404613452
Ru	-0.1713771210	0.2523406744	1.8603366323
C	0.7021112876	1.8524625249	2.0189144258
C	0.8946966622	2.0049252905	3.4714992125
C	-0.1120416042	2.0104619773	4.3679414422
C	2.4880678760	0.2992653644	-0.3834368589
Cl	1.3222321813	-1.5145468285	2.4139414780
Cl	-2.3636345045	1.2358351175	1.7596459746
H	0.9433229239	0.4971523806	-2.8435051161
H	1.7342357984	-1.0731445111	-2.5859690927
H	-0.3653640440	-2.1837781134	-2.2565582065
H	-1.1091874807	-0.7401179676	-2.9810706534
H	3.1952719532	-0.4781315331	-0.6967050419
H	2.8006312547	1.2521953743	-0.8321190369
H	2.5125397066	0.3687896488	0.7012733414
H	-2.9825508149	-1.0624888296	-1.1728717040
H	-2.1007445895	-2.3915272487	-0.3725704230
H	-2.5052140242	-0.8887557649	0.5200389301
C	1.0742248845	2.9332841811	1.0519371597
H	1.9284432222	2.0137497453	3.8259918368
H	0.0984139244	2.0237625301	5.4341938194

H	-1.1519720992	2.0290263779	4.0557620844
C	2.4310936448	3.6175325381	1.3223983603
H	1.0219122415	2.5636795604	0.0237917709
H	0.2718206802	3.6862142629	1.1447845623
C	2.7257652543	4.7431594888	0.3117843516
H	2.4416496743	4.0351381429	2.3362459003
H	3.2362252489	2.8711247547	1.2821618723
C	4.0767978483	5.3721849572	0.5267133369
H	2.6725655323	4.3251091282	-0.7059950249
H	1.9432418104	5.5106753391	0.3766527863
C	4.2862572767	6.6510982803	0.8428360601
H	4.9337056293	4.7035853598	0.4233970770
H	5.2868722472	7.0475124544	0.9944989684
H	3.4620025886	7.3525447935	0.9590872596

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C	0.2423368725	-0.4041595103	0.0443975111
N	1.4577867617	-0.4408922888	-0.5571605525
C	1.3741017482	-0.8717422390	-1.9575037895
C	-0.0240946823	-1.4932706455	-2.0145442531
N	-0.6668908554	-0.9179568372	-0.8256824885
C	2.7452919602	-0.0434733369	-0.0197735772
C	-2.0131854714	-1.3674589698	-0.4991014391
Ru	-0.1617987667	0.1826830120	1.8889846742
Cl	-2.2358990603	1.3424397705	1.5251714569
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C	0.3828306047	2.9619384840	4.1238154647
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H	-0.5778326859	-1.2303078657	-2.9211488931
H	3.4826390837	-0.8212580381	-0.2511413320
H	3.0882330191	0.9013590644	-0.4630710444
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H	-2.6427015087	-1.2652015997	-1.3891895017
H	-2.0088815308	-2.4230041900	-0.1899308151
H	-2.4308694919	-0.7435041489	0.2891805591
C	1.1053512364	2.7498911637	0.9428482664
H	1.7846745493	1.3957216081	3.9457003126
H	0.5561493827	3.1089863517	5.1863131088
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C	2.5865815139	4.5983118922	-0.0147001656
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H	2.5718871548	4.1185730052	-1.0027115868
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C	-2.0561780635	-1.4699604156	-0.6701608849
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H	2.1559105466	-1.1205044943	-2.2779646225
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C	-0.5477341273	4.9264850675	-0.5130985093
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H	0.4470656418	5.3995531407	-0.4808019613
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Ru	0.1514898787	0.1531361450	1.9323866347
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H	-0.2135818319	1.2235077955	-2.9078110946
H	0.9401572388	-0.1091688278	-3.1505072585
H	-0.6467869371	-1.7530708466	-2.4013649997
H	-1.8772274770	-0.5053068146	-2.7198115755
H	1.8232230199	2.3397242617	-1.1658397212
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C	0.3643955362	-0.5421308826	2.1076459456
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Cl	1.0592065421	-2.2609342365	-2.3100584583
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H	0.7371972725	-1.5190662483	2.4448555761
H	-1.6557101817	-1.3897326631	2.3968089469
H	-1.6164930385	0.3865621204	2.3768033621
H	2.4196970617	-0.6604939895	-0.5644555906
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H	-0.4803870913	-1.6218224761	-4.5914069047
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C	1.1089950022	0.8117744624	-3.2959266848
C	1.0899509886	2.2913641862	-3.2675953557
C	2.1742249105	3.0799315787	-3.1699133535
C	2.3442045235	0.1549363396	-3.8991680056
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C	0.1362632667	-0.1522140736	0.1029453740
N	-0.8217954722	-0.7189554159	-0.6565069512
C	-0.5644031998	-0.5131430854	-2.0902728917
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H	-0.7938836135	-1.4161262970	-2.6638624568
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H	-2.8348862494	-0.1774500704	-0.2942371054
H	2.2104352524	0.8965241350	3.2211352045
H	0.8665469521	2.1891335746	3.1772637177
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H	-3.3094411003	-2.0001692744	3.4484683585
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N	-0.9342194070	-0.8647623445	-0.6020192660
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N	0.9289731922	0.2751143515	-0.7483270114
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H	0.8559593399	0.5967995371	-2.8500907841
H	1.3912945051	-1.0262748417	-2.3504622747
H	-0.9238967578	-1.6227593105	-2.5864135173
H	-1.4571754017	0.0690883847	-2.4248431850
H	2.3311751187	1.1822858170	0.5240662484
H	2.9508469756	-0.2110345711	-0.3771011398
H	2.6501850578	1.3422449600	-1.2228501469
H	-2.3895000068	-2.3511215788	-0.6829973625
H	-2.1684735533	-1.6062752322	0.9165181397
H	-3.0238927540	-0.7095904641	-0.3439723413
H	1.6992083457	1.7746163175	2.8162779236
H	0.4495627463	2.4380309002	1.6157678705
C	0.3174722575	1.1994952374	5.5459631989
C	-1.8687026481	0.1694713367	5.1173690046
H	1.4161439281	-0.5707028205	4.5680939888
H	-0.0755850708	-2.6037815616	3.8091798124
H	-2.2439056629	-3.4437803834	3.0770364391
H	-3.0579550227	-1.8486455445	3.5582354525
H	-2.2060473896	-0.3511193227	6.0268447152
H	-2.7339238992	0.2983622457	4.4635301146
H	0.6133645489	0.9885044207	6.5865022887
H	0.9595240841	2.0196383689	5.2001004397
C	-1.1936327861	1.5221441244	5.4409393762
H	-1.5895972914	1.9963189366	6.3452428394
H	-1.3652284903	2.1999651900	4.5992343135

Basis sets and ECP

Effective Core Potential

F Potential	Maximum angular term		3
	1/r^n	Exponent	Coefficient
	0	554.3796303	-0.0515270
	1	155.1066871	-20.1816536
	2	48.4976263	-105.9966915
	2	14.7701594	-42.2166788
	2	5.2077363	-3.7675024
S-F Potential	1/r^n		Exponent
			Coefficient
	0	66.7118060	2.9578344
	1	77.3503632	25.3748707
	2	18.3571445	536.1262372
	2	11.8404727	-651.2057221
	2	8.1179479	381.3816943
P-F Potential	1/r^n		Exponent
			Coefficient
	0	54.9937915	4.9651557
	1	13.9399212	23.8861501
	2	15.2118246	464.4631344
	2	10.5460691	-714.4451788
	2	7.5539486	377.5503594
D-F Potential	1/r^n		Exponent
			Coefficient
	0	60.3444595	3.0352988
	1	45.2100305	23.2901723
	2	19.1190074	146.0926620
	2	4.2712090	28.9129770

Basis Set for Geometry Optimization (LACVP*)

atom	s	t	f	z	rcoef	rmfac	rcoef*rmfac
-----	-----	-----	-----	-----	-----	-----	-----
C	1	S	1	3047.524880	0.536345	1.000000	0.536345
C	2	S	1	457.369518	0.989452	1.000000	0.989452
C	3	S	1	103.948685	1.597283	1.000000	1.597283
C	4	S	1	29.210155	2.079187	1.000000	2.079187
C	5	S	1	9.286663	1.774174	1.000000	1.774174
C	6	S	1	3.163927	0.612580	1.000000	0.612580
C	7	S	2	7.868272	-0.399556	1.000000	-0.399556
C	8	S	2	1.881289	-0.184155	1.000000	-0.184155
C	9	S	2	0.544249	0.516390	1.000000	0.516390
C	10	X	3	7.868272	1.296082	1.000000	1.296082
		Y	4			1.000000	1.296082
		Z	5			1.000000	1.296082
C	11	X	3	1.881289	0.993754	1.000000	0.993754
		Y	4			1.000000	0.993754
		Z	5			1.000000	0.993754

C	12	X	3	0.544249	0.495953	1.000000	0.495953
		Y	4			1.000000	0.495953
		Z	5			1.000000	0.495953
C	13	S	6	0.168714	0.187618	1.000000	0.187618
C	14	X	7	0.168714	0.154128	1.000000	0.154128
		Y	8			1.000000	0.154128
		Z	9			1.000000	0.154128
C	15	XX	10	0.800000	1.113825	1.000000	1.113825
		YY	11			1.000000	1.113825
		ZZ	12			1.000000	1.113825
		XY	13			1.732051	1.929201
		XZ	14			1.732051	1.929201
		YZ	15			1.732051	1.929201
N	1	S	16	4173.511460	0.678998	1.000000	0.678998
N	2	S	16	627.457911	1.250431	1.000000	1.250431
N	3	S	16	142.902093	2.020356	1.000000	2.020356
N	4	S	16	40.234329	2.644212	1.000000	2.644212
N	5	S	16	12.820213	2.265005	1.000000	2.265005
N	6	S	16	4.390437	0.779188	1.000000	0.779188
N	7	S	17	11.626362	-0.515875	1.000000	-0.515875
N	8	S	17	2.716280	-0.255023	1.000000	-0.255023
N	9	S	17	0.772218	0.672735	1.000000	0.672735
N	10	X	18	11.626362	2.068052	1.000000	2.068052
		Y	19			1.000000	2.068052
		Z	20			1.000000	2.068052
N	11	X	18	2.716280	1.610011	1.000000	1.610011
		Y	19			1.000000	1.610011
		Z	20			1.000000	1.610011
N	12	X	18	0.772218	0.764490	1.000000	0.764490
		Y	19			1.000000	0.764490
		Z	20			1.000000	0.764490
N	13	S	21	0.212031	0.222695	1.000000	0.222695
N	14	X	22	0.212031	0.205088	1.000000	0.205088
		Y	23			1.000000	0.205088
		Z	24			1.000000	0.205088
N	15	XX	25	0.800000	1.113825	1.000000	1.113825
		YY	26			1.000000	1.113825
		ZZ	27			1.000000	1.113825
		XY	28			1.732051	1.929201
		XZ	29			1.732051	1.929201
		YZ	30			1.732051	1.929201
Ru	1	S	76	2.565000	-1.504161	1.000000	-1.504161
Ru	2	S	76	1.508000	1.289616	1.000000	1.289616
Ru	3	S	76	0.512900	0.242621	1.000000	0.242621
Ru	4	S	77	1.508000	-0.284585	1.000000	-0.284585
Ru	5	S	77	0.512900	-0.322652	1.000000	-0.322652
Ru	6	S	77	0.136200	0.159788	1.000000	0.159788
Ru	7	S	78	0.041700	0.065768	1.000000	0.065768
Ru	8	X	79	4.859000	-0.972528	1.000000	-0.972528
		Y	80			1.000000	-0.972528
		Z	81			1.000000	-0.972528
Ru	9	X	79	1.219000	1.357419	1.000000	1.357419
		Y	80			1.000000	1.357419
		Z	81			1.000000	1.357419
Ru	10	X	79	0.441300	0.188063	1.000000	0.188063
		Y	80			1.000000	0.188063
		Z	81			1.000000	0.188063

Ru	11	X	82	0.083000	0.063502	1.000000	0.063502
		Y	83			1.000000	0.063502
		Z	84			1.000000	0.063502
Ru	12	X	85	0.025000	0.014170	1.000000	0.014170
		Y	86			1.000000	0.014170
		Z	87			1.000000	0.014170
Ru	13	XX	88	4.105000	0.946049	1.000000	0.946049
		YY	89			1.000000	0.946049
		ZZ	90			1.000000	0.946049
		XY	91			1.732051	1.638605
		XZ	92			1.732051	1.638605
		YZ	93			1.732051	1.638605
Ru	14	XX	88	1.377000	1.470180	1.000000	1.470180
		YY	89			1.000000	1.470180
		ZZ	90			1.000000	1.470180
		XY	91			1.732051	2.546426
		XZ	92			1.732051	2.546426
		YZ	93			1.732051	2.546426
Ru	15	XX	88	0.482800	0.263615	1.000000	0.263615
		YY	89			1.000000	0.263615
		ZZ	90			1.000000	0.263615
		XY	91			1.732051	0.456595
		XZ	92			1.732051	0.456595
		YZ	93			1.732051	0.456595
Ru	16	XX	94	0.150100	0.059577	1.000000	0.059577
		YY	95			1.000000	0.059577
		ZZ	96			1.000000	0.059577
		XY	97			1.732051	0.103190
		XZ	98			1.732051	0.103190
		YZ	99			1.732051	0.103190
P	1	S	100	19413.300000	2.170359	1.000000	2.170359
P	2	S	100	2909.420000	4.010907	1.000000	4.010907
P	3	S	100	661.364000	6.506317	1.000000	6.506317
P	4	S	100	185.759000	8.609470	1.000000	8.609470
P	5	S	100	59.194300	7.373069	1.000000	7.373069
P	6	S	100	20.031000	2.261991	1.000000	2.261991
P	7	S	101	339.478000	-0.156820	1.000000	-0.156820
P	8	S	101	81.010100	-0.693775	1.000000	-0.693775
P	9	S	101	25.878000	-0.953723	1.000000	-0.953723
P	10	S	101	9.452210	0.372034	1.000000	0.372034
P	11	S	101	3.665660	1.160081	1.000000	1.160081
P	12	S	101	1.467460	0.383706	1.000000	0.383706
P	13	X	102	339.478000	9.481104	1.000000	9.481104
		Y	103			1.000000	9.481104
		Z	104			1.000000	9.481104
P	14	X	102	81.010100	11.672425	1.000000	11.672425
		Y	103			1.000000	11.672425
		Z	104			1.000000	11.672425
P	15	X	102	25.878000	11.627075	1.000000	11.627075
		Y	103			1.000000	11.627075
		Z	104			1.000000	11.627075
P	16	X	102	9.452210	8.017143	1.000000	8.017143
		Y	103			1.000000	8.017143
		Z	104			1.000000	8.017143
P	17	X	102	3.665660	3.260096	1.000000	3.260096
		Y	103			1.000000	3.260096
		Z	104			1.000000	3.260096
P	18	X	102	1.467460	0.549278	1.000000	0.549278

		Y	103			1.000000	0.549278
		Z	104			1.000000	0.549278
P	19	S	105	2.156230	-1.414076	1.000000	-1.414076
P	20	S	105	0.748997	0.083106	1.000000	0.083106
P	21	X	106	2.156230	-0.252893	1.000000	-0.252893
		Y	107			1.000000	-0.252893
		Z	108			1.000000	-0.252893
P	22	X	106	0.748997	1.040371	1.000000	1.040371
		Y	107			1.000000	1.040371
		Z	108			1.000000	1.040371
P	23	S	105	0.283145	0.276641	1.000000	0.276641
P	24	X	106	0.283145	0.294409	1.000000	0.294409
		Y	107			1.000000	0.294409
		Z	108			1.000000	0.294409
P	25	S	109	0.099832	0.126579	1.000000	0.126579
P	26	X	110	0.099832	0.079988	1.000000	0.079988
		Y	111			1.000000	0.079988
		Z	112			1.000000	0.079988
P	27	XX	113	0.550000	0.578155	1.000000	0.578155
		YY	114			1.000000	0.578155
		ZZ	115			1.000000	0.578155
		XY	116			1.732051	1.001394
		XZ	117			1.732051	1.001394
		YZ	118			1.732051	1.001394
Cl	1	S	179	25180.100000	2.611296	1.000000	2.611296
Cl	2	S	179	3780.350000	4.822217	1.000000	4.822217
Cl	3	S	179	860.474000	7.823932	1.000000	7.823932
Cl	4	S	179	242.145000	10.388253	1.000000	10.388253
Cl	5	S	179	77.334900	8.977789	1.000000	8.977789
Cl	6	S	179	26.247000	2.808761	1.000000	2.808761
Cl	7	S	180	491.765000	-0.170987	1.000000	-0.170987
Cl	8	S	180	116.984000	-0.778641	1.000000	-0.778641
Cl	9	S	180	37.415300	-1.213271	1.000000	-1.213271
Cl	10	S	180	13.783400	0.229508	1.000000	0.229508
Cl	11	S	180	5.452150	1.498690	1.000000	1.498690
Cl	12	S	180	2.225880	0.604202	1.000000	0.604202
Cl	13	X	181	491.765000	13.168757	1.000000	13.168757
		Y	182			1.000000	13.168757
		Z	183			1.000000	13.168757
Cl	14	X	181	116.984000	16.626258	1.000000	16.626258
		Y	182			1.000000	16.626258
		Z	183			1.000000	16.626258
Cl	15	X	181	37.415300	17.131445	1.000000	17.131445
		Y	182			1.000000	17.131445
		Z	183			1.000000	17.131445
Cl	16	X	181	13.783400	12.414939	1.000000	12.414939
		Y	182			1.000000	12.414939
		Z	183			1.000000	12.414939
Cl	17	X	181	5.452150	5.385835	1.000000	5.385835
		Y	182			1.000000	5.385835
		Z	183			1.000000	5.385835
Cl	18	X	181	2.225880	0.977199	1.000000	0.977199
		Y	182			1.000000	0.977199
		Z	183			1.000000	0.977199
Cl	19	S	184	3.186490	-0.428054	1.000000	-0.428054
Cl	20	S	184	1.144270	0.048564	1.000000	0.048564
Cl	21	S	184	0.420377	0.394476	1.000000	0.394476
Cl	22	X	185	3.186490	-0.086775	1.000000	-0.086775

		Y	186			1.000000	-0.086775
		Z	187			1.000000	-0.086775
Cl	23	X	185	1.144270	0.545848	1.000000	0.545848
		Y	186			1.000000	0.545848
		Z	187			1.000000	0.545848
Cl	24	X	185	0.420377	0.358735	1.000000	0.358735
		Y	186			1.000000	0.358735
		Z	187			1.000000	0.358735
Cl	25	S	188	0.142657	0.165436	1.000000	0.165436
Cl	26	X	189	0.142657	0.124970	1.000000	0.124970
		Y	190			1.000000	0.124970
		Z	191			1.000000	0.124970
Cl	27	XX	192	0.750000	0.994871	1.000000	0.994871
		YY	193			1.000000	0.994871
		ZZ	194			1.000000	0.994871
		XY	195			1.732051	1.723167
		XZ	196			1.732051	1.723167
		YZ	197			1.732051	1.723167
H	1	S	287	18.731137	0.214935	1.000000	0.214935
H	2	S	287	2.825394	0.364571	1.000000	0.364571
H	3	S	287	0.640122	0.415051	1.000000	0.415051
H	4	S	288	0.161278	0.181381	1.000000	0.181381

Basis Set of Single Point Energy Calculations (LACV3P**+)

Gaussian Functions - Normalized coefficients

atom	s	t	f	z	rcoef	rmfac	rcoef*rmfac
-----	-----	-----	-----	-----	-----	-----	-----
C	1	S	1	4563.240000	0.778202	1.000000	0.778202
C	2	S	1	682.024000	1.448695	1.000000	1.448695
C	3	S	1	154.973000	2.383089	1.000000	2.383089
C	4	S	1	44.455300	3.200089	1.000000	3.200089
C	5	S	1	13.029000	3.013004	1.000000	3.013004
C	6	S	1	1.827730	0.247599	1.000000	0.247599
C	7	S	2	20.964200	0.800629	1.000000	0.800629
C	8	S	2	4.803310	2.127420	1.000000	2.127420
C	9	S	2	1.459330	-0.002868	1.000000	-0.002868
C	10	X	3	20.964200	2.573592	1.000000	2.573592
		Y	4			1.000000	2.573592
		Z	5			1.000000	2.573592
C	11	X	3	4.803310	2.408248	1.000000	2.408248
		Y	4			1.000000	2.408248
		Z	5			1.000000	2.408248
C	12	X	3	1.459330	1.865281	1.000000	1.865281
		Y	4			1.000000	1.865281
		Z	5			1.000000	1.865281
C	13	S	6	0.483456	0.413217	1.000000	0.413217
C	14	X	7	0.483456	0.574627	1.000000	0.574627
		Y	8			1.000000	0.574627
		Z	9			1.000000	0.574627

C	15	S	10	0.145585	0.167976	1.000000	0.167976
C	16	X	11	0.145585	0.128185	1.000000	0.128185
		Y	12			1.000000	0.128185
		Z	13			1.000000	0.128185
C	17	XX	14	0.626000	0.725128	1.000000	0.725128
		YY	15			1.000000	0.725128
		ZZ	16			1.000000	0.725128
		XY	17			1.732051	1.255958
		XZ	18			1.732051	1.255958
		YZ	19			1.732051	1.255958
C	18	S	20	0.043800	0.068236	1.000000	0.068236
C	19	X	21	0.043800	0.028562	1.000000	0.028562
		Y	22			1.000000	0.028562
		Z	23			1.000000	0.028562
N	1	S	24	6293.480000	0.991968	1.000000	0.991968
N	2	S	24	949.044000	1.823240	1.000000	1.823240
N	3	S	24	218.776000	2.979891	1.000000	2.979891
N	4	S	24	63.691600	4.000007	1.000000	4.000007
N	5	S	24	18.828200	3.881008	1.000000	3.881008
N	6	S	24	2.720230	0.386764	1.000000	0.386764
N	7	S	25	30.633100	1.038501	1.000000	1.038501
N	8	S	25	7.026140	2.834794	1.000000	2.834794
N	9	S	25	2.112050	-0.003208	1.000000	-0.003208
N	10	X	26	30.633100	3.935616	1.000000	3.935616
		Y	27			1.000000	3.935616
		Z	28			1.000000	3.935616
N	11	X	26	7.026140	3.870994	1.000000	3.870994
		Y	27			1.000000	3.870994
		Z	28			1.000000	3.870994
N	12	X	26	2.112050	2.967271	1.000000	2.967271
		Y	27			1.000000	2.967271
		Z	28			1.000000	2.967271
N	13	S	29	0.684009	0.536051	1.000000	0.536051
N	14	X	30	0.684009	0.886681	1.000000	0.886681
		Y	31			1.000000	0.886681
		Z	32			1.000000	0.886681
N	15	S	33	0.200878	0.213850	1.000000	0.213850
N	16	X	34	0.200878	0.191693	1.000000	0.191693
		Y	35			1.000000	0.191693
		Z	36			1.000000	0.191693
N	17	XX	37	0.913000	1.403568	1.000000	1.403568
		YY	38			1.000000	1.403568
		ZZ	39			1.000000	1.403568
		XY	40			1.732051	2.431050
		XZ	41			1.732051	2.431050
		YZ	42			1.732051	2.431050
N	18	S	43	0.063900	0.090581	1.000000	0.090581
N	19	X	44	0.063900	0.045795	1.000000	0.045795
		Y	45			1.000000	0.045795
		Z	46			1.000000	0.045795
Ru	1	S	116	2.565000	-1.504161	1.000000	-1.504161
Ru	2	S	116	1.508000	1.289616	1.000000	1.289616
Ru	3	S	116	0.512900	0.242621	1.000000	0.242621
Ru	4	S	117	1.508000	-0.284585	1.000000	-0.284585
Ru	5	S	117	0.512900	-0.322652	1.000000	-0.322652
Ru	6	S	118	0.136200	0.159788	1.000000	0.159788
Ru	7	S	119	0.041700	0.065768	1.000000	0.065768

Ru	8	X	120	4.859000	-1.402272	1.000000	-1.402272
		Y	121			1.000000	-1.402272
		Z	122			1.000000	-1.402272
Ru	9	X	120	1.219000	1.957239	1.000000	1.957239
		Y	121			1.000000	1.957239
		Z	122			1.000000	1.957239
Ru	10	X	123	0.441300	0.512693	1.000000	0.512693
		Y	124			1.000000	0.512693
		Z	125			1.000000	0.512693
Ru	11	X	126	0.083000	0.063502	1.000000	0.063502
		Y	127			1.000000	0.063502
		Z	128			1.000000	0.063502
Ru	12	X	129	0.025000	0.014170	1.000000	0.014170
		Y	130			1.000000	0.014170
		Z	131			1.000000	0.014170
Ru	13	XX	132	4.105000	1.748105	1.000000	1.748105
		YY	133			1.000000	1.748105
		ZZ	134			1.000000	1.748105
		XY	135			1.732051	3.027807
		XZ	136			1.732051	3.027807
		YZ	137			1.732051	3.027807
Ru	14	XX	132	1.377000	2.716591	1.000000	2.716591
		YY	133			1.000000	2.716591
		ZZ	134			1.000000	2.716591
		XY	135			1.732051	4.705274
		XZ	136			1.732051	4.705274
		YZ	137			1.732051	4.705274
Ru	15	XX	138	0.482800	0.460259	1.000000	0.460259
		YY	139			1.000000	0.460259
		ZZ	140			1.000000	0.460259
		XY	141			1.732051	0.797192
		XZ	142			1.732051	0.797192
		YZ	143			1.732051	0.797192
Ru	16	XX	144	0.150100	0.059577	1.000000	0.059577
		YY	145			1.000000	0.059577
		ZZ	146			1.000000	0.059577
		XY	147			1.732051	0.103190
		XZ	148			1.732051	0.103190
		YZ	149			1.732051	0.103190
Ru	17	XX	150	0.042000	0.006414	1.000000	0.006414
		YY	151			1.000000	0.006414
		ZZ	152			1.000000	0.006414
		XY	153			1.732051	0.011109
		XZ	154			1.732051	0.011109
		YZ	155			1.732051	0.011109
P	1	S	156	77492.400000	2.585268	1.000000	2.585268
P	2	S	156	11605.800000	4.835730	1.000000	4.835730
P	3	S	156	2645.960000	8.193040	1.000000	8.193040
P	4	S	156	754.976000	12.670224	1.000000	12.670224
P	5	S	156	248.755000	16.883827	1.000000	16.883827
P	6	S	156	91.156500	11.842990	1.000000	11.842990
P	7	S	157	91.156500	3.369477	1.000000	3.369477
P	8	S	157	36.225700	6.605233	1.000000	6.605233
P	9	S	157	15.211300	1.448406	1.000000	1.448406
P	10	S	158	4.794170	2.309113	1.000000	2.309113
P	11	S	159	1.807930	1.111210	1.000000	1.111210
P	12	S	160	0.356816	0.329036	1.000000	0.329036
P	13	S	161	0.114783	0.140546	1.000000	0.140546

P	14	X	162	384.843000	22.367400	1.000000	22.367400
		Y	163			1.000000	22.367400
		Z	164			1.000000	22.367400
P	15	X	162	90.552100	27.821388	1.000000	27.821388
		Y	163			1.000000	27.821388
		Z	164			1.000000	27.821388
P	16	X	162	29.133900	28.217572	1.000000	28.217572
		Y	163			1.000000	28.217572
		Z	164			1.000000	28.217572
P	17	X	162	10.886200	20.522404	1.000000	20.522404
		Y	163			1.000000	20.522404
		Z	164			1.000000	20.522404
P	18	X	165	4.352590	5.630872	1.000000	5.630872
		Y	166			1.000000	5.630872
		Z	167			1.000000	5.630872
P	19	X	165	1.777060	1.251861	1.000000	1.251861
		Y	166			1.000000	1.251861
		Z	167			1.000000	1.251861
P	20	X	168	0.697005	0.907789	1.000000	0.907789
		Y	169			1.000000	0.907789
		Z	170			1.000000	0.907789
P	21	X	171	0.253532	0.256437	1.000000	0.256437
		Y	172			1.000000	0.256437
		Z	173			1.000000	0.256437
P	22	X	174	0.068493	0.049946	1.000000	0.049946
		Y	175			1.000000	0.049946
		Z	176			1.000000	0.049946
P	23	XX	177	0.550000	0.578155	1.000000	0.578155
		YY	178			1.000000	0.578155
		ZZ	179			1.000000	0.578155
		XY	180			1.732051	1.001394
		XZ	181			1.732051	1.001394
		YZ	182			1.732051	1.001394
P	24	S	183	0.034800	0.057424	1.000000	0.057424
P	25	X	184	0.034800	0.021425	1.000000	0.021425
		Y	185			1.000000	0.021425
		Z	186			1.000000	0.021425
Cl	1	S	279	105819.000000	3.085953	1.000000	3.085953
Cl	2	S	279	15872.000000	5.762728	1.000000	5.762728
Cl	3	S	279	3619.650000	9.809764	1.000000	9.809764
Cl	4	S	279	1030.800000	15.206778	1.000000	15.206778
Cl	5	S	279	339.908000	20.477497	1.000000	20.477497
Cl	6	S	279	124.538000	15.520664	1.000000	15.520664
Cl	7	S	280	124.538000	3.565041	1.000000	3.565041
Cl	8	S	280	49.513500	8.304458	1.000000	8.304458
Cl	9	S	280	20.805600	2.025653	1.000000	2.025653
Cl	10	S	281	6.583460	2.929212	1.000000	2.929212
Cl	11	S	282	2.564680	1.444392	1.000000	1.444392
Cl	12	S	283	0.559763	0.461225	1.000000	0.461225
Cl	13	S	284	0.183273	0.199634	1.000000	0.199634
Cl	14	X	285	589.776000	9.905547	1.000000	9.905547
		Y	286			1.000000	9.905547
		Z	287			1.000000	9.905547
Cl	15	X	285	139.849000	12.684690	1.000000	12.684690
		Y	286			1.000000	12.684690
		Z	287			1.000000	12.684690
Cl	16	X	285	45.141300	13.572482	1.000000	13.572482
		Y	286			1.000000	13.572482

		Z	287			1.000000	13.572482
Cl	17	X	285	16.873300	10.799801	1.000000	10.799801
		Y	286			1.000000	10.799801
		Z	287			1.000000	10.799801
Cl	18	X	285	6.741100	11.961641	1.000000	11.961641
		Y	286			1.000000	11.961641
		Z	287			1.000000	11.961641
Cl	19	X	288	6.741100	-24.342963	1.000000	-24.342963
		Y	289			1.000000	-24.342963
		Z	290			1.000000	-24.342963
Cl	20	X	288	2.771520	5.058474	1.000000	5.058474
		Y	289			1.000000	5.058474
		Z	290			1.000000	5.058474
Cl	21	X	291	1.023870	1.468068	1.000000	1.468068
		Y	292			1.000000	1.468068
		Z	293			1.000000	1.468068
Cl	22	X	294	0.381368	0.427189	1.000000	0.427189
		Y	295			1.000000	0.427189
		Z	296			1.000000	0.427189
Cl	23	X	297	0.109437	0.089721	1.000000	0.089721
		Y	298			1.000000	0.089721
		Z	299			1.000000	0.089721
Cl	24	XX	300	0.750000	0.994871	1.000000	0.994871
		YY	301			1.000000	0.994871
		ZZ	302			1.000000	0.994871
		XY	303			1.732051	1.723167
		XZ	304			1.732051	1.723167
		YZ	305			1.732051	1.723167
Cl	25	S	306	0.048300	0.073429	1.000000	0.073429
Cl	26	X	307	0.048300	0.032276	1.000000	0.032276
		Y	308			1.000000	0.032276
		Z	309			1.000000	0.032276
H	1	S	507	33.865000	0.255069	1.000000	0.255069
H	2	S	507	5.094790	0.460109	1.000000	0.460109
H	3	S	507	1.158790	0.678321	1.000000	0.678321
H	4	S	508	0.325840	0.307371	1.000000	0.307371
H	5	S	509	0.102741	0.129336	1.000000	0.129336
H	6	X	510	0.750000	0.994871	1.000000	0.994871
		Y	511			1.000000	0.994871
		Z	512			1.000000	0.994871