Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

for

Comparison of different Ruthenium-alkylidene bonds in the activation step with N-heterocyclic carbene Ru-catalysts for olefins metathesis

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Complete reference 6:

6: Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1. xyz coordinate data sets for DFT optimized complexes.

Precat-1

Ru	0.360959	-0.139377	-0.021950
Cl	0.434955	-0.167342	2.410506
Cl	0.037995	-0.335945	-2.418408
P	-0.817911	2.052649	-0.010562
N	0.062631	-3.209838	0.038878
N	2.183187	-2.610438	0.024376
C	0.901348	-2.131106	0.012503
C	0.782078	-4.498720	0.161116
H	0.429907	-5.215153	-0.609661
H	0.584260	-4.951838	1.157714
C	2.249806	-4.087916	-0.021331
H	2.912793	-4.473798	0.780551
H	2.672318	-4.421339	-0.995298
C	-1.379371	-3.248616	0.035084
C	-2.083424	-3.272781	1.269532
C	-1.370078	-3.177020	2.595959
H	-2.094158	-3.211433	3.433497
H	-0.778107	-2.238714	2.680339
H	-0.659548	-4.020291	2.739422
C	-3.485152	-3.431134	1.230772
H	-4.036644	-3.451643	2.185972
C	-4.191742	-3.593419	0.023961
C	-5.696164	-3.749076	0.010569
H	-6.021016	-4.508886	-0.730085
H	-6.193858	-2.794366	-0.269124
H	-6.086948	-4.046225	1.004422
C	-3.454472	-3.609513	-1.176970
H	-3.980791	-3.770799	-2.132943
C	-2.053607	-3.459258	-1.200342
C	-1.301143	-3.555673	-2.504359
H	-1.993172	-3.763503	-3.343839
H	-0.545741	-4.371015	-2.483675
H	-0.756809	-2.609279	-2.717211
C	3.423260	-1.882703	-0.018370
C	4.004897	-1.565568	-1.275478
C	3.308731	-1.901742	-2.571732
H	3.914050	-1.575759	-3.440235
H	2.308025	-1.418749	-2.639696
H	3.141623	-2.995916	-2.676491
C	5.259841	-0.921924	-1.281683
H	5.714447	-0.665319	-2.253462
C	5.949832	-0.611670	-0.093833
C	7.280862	0.106260	-0.126503
H	7.775912	0.009533	-1.113677
H	7.974006	-0.282907	0.647641
H	7.152642	1.193173	0.072838
C	5.359120	-0.978354	1.132767
H	5.892419	-0.765253	2.074717
C	4.107559	-1.620596	1.200060
C	3.512007	-2.005661	2.531584
H	3.288405	-3.092984	2.586694
H	2.550950	-1.471486	2.706836
H	4.206755	-1.764470	3.359929
C	1.986870	0.652637	-0.171396
C	-2.669443	1.730022	-0.273008
C	-3.168877	1.713543	-1.735108
C	-3.068037	0.410679	0.429047
H	-3.178883	2.577996	0.244447
C	-4.693738	1.488331	-1.790507
H	-2.646596	0.902341	-2.289099
H	-2.924598	2.666108	-2.249248
C	-4.590578	0.190463	0.386776
H	-2.564103	-0.435446	-0.096168
H	-2.701452	0.383875	1.474415
C	-5.118765	0.205585	-1.056618
H	-5.026326	1.457972	-2.851030
H	-5.209278	2.362453	-1.328360
H	-4.841693	-0.768756	0.886754
H	-5.092612	0.993615	0.975742
H	-6.225990	0.101600	-1.070621
H	-4.710130	-0.678276	-1.597690
C	-0.446038	3.433312	-1.292177
C	0.633118	4.464154	-0.881825
C	-0.125011	2.907174	-2.707180
H	-1.420996	3.978637	-1.326679
C	0.747560	5.606955	-1.912471
H	1.617501	3.949256	-0.794270
H	0.414227	4.908179	0.108874
C	-0.027663	4.046687	-3.737543
H	0.839688	2.357067	-2.667101
H	-0.861375	2.152697	-3.037190
C	1.022697	5.090848	-3.332051
H	1.541622	6.315251	-1.589530
H	-0.204112	6.187768	-1.911807
H	0.207625	3.621524	-4.737200
H	-1.021289	4.543609	-3.838207
H	1.045715	5.934822	-4.055637
H	2.034139	4.623756	-3.363488
C	-0.821716	3.083953	1.597610
C	-1.804083	2.624755	2.701142
C	0.593019	3.243968	2.206251
H	-1.174139	4.084837	1.244260
C	-1.809822	3.620248	3.879608
H	-1.493667	1.619334	3.059036
H	-2.836819	2.533578	2.306141
C	0.591267	4.247484	3.374842
H	0.917190	2.246403	2.569067
H	1.332692	3.554152	1.442621
C	-0.405555	3.830240	4.468232
H	-2.510999	3.260753	4.664282
H	-2.211239	4.600645	3.530209
H	1.616867	4.332061	3.795959
H	0.324176	5.264103	2.999887
H	-0.434867	4.586390	5.283115
H	-0.058254	2.878885	4.931132
H	2.421859	0.917372	-1.163987
H	2.593601	0.935416	0.720388

14e1-1

Ru	0.079657	0.468600	-1.401147
Cl	0.234259	2.758165	-0.989250
Cl	1.162148	-1.339852	-2.377836
C	-0.082662	-0.060496	0.451648
C	-1.596014	0.297463	-2.059731
H	-1.695233	0.630987	-3.125683
H	-2.512532	-0.097116	-1.580690
N	1.010283	-0.207016	1.283146
N	-1.204944	-0.243198	1.227568
C	0.624959	-0.326957	2.701746
C	-0.875739	-0.637954	2.612350
H	1.208243	-1.127624	3.200679
H	0.823662	0.627222	3.240675
H	-1.483821	-0.059500	3.337416
H	-1.098202	-1.718433	2.771118
C	2.404480	-0.205411	0.916290
C	-2.582248	-0.266255	0.823638
C	3.015678	-1.445585	0.581181
C	4.383375	-1.447826	0.252633
C	5.159367	-0.271262	0.267779
C	4.538288	0.924449	0.673642
C	3.173117	0.984407	1.023487
C	-3.355341	0.917710	0.941970
C	-4.717636	0.857177	0.590218
C	-5.322946	-0.333327	0.135982
C	-4.523468	-1.489283	0.036130
C	-3.154474	-1.483547	0.374552
C	2.233345	-2.737472	0.593127
H	4.858597	-2.405054	-0.020148
C	6.613715	-0.296599	-0.144922
H	5.136469	1.849101	0.735625
C	2.594186	2.271350	1.563025
C	-2.728294	2.210971	1.405319
H	-5.325183	1.774160	0.673885
C	-6.786706	-0.355926	-0.244850
H	-4.976170	-2.429496	-0.321222
C	-2.312963	-2.728746	0.212011
H	-3.481364	3.021288	1.457219
H	-2.271310	2.110823	2.413302
H	-1.915525	2.531569	0.718241
H	-2.913940	-3.562943	-0.199226
H	-1.457844	-2.548114	-0.473707
H	-1.883728	-3.073058	1.177583
H	-7.140073	-1.384523	-0.456488
H	-7.422006	0.065207	0.562653
H	-6.974411	0.257430	-1.152631
H	1.511384	-2.764427	-0.249635
H	2.910700	-3.607709	0.489697
H	1.656260	-2.864775	1.533333
H	3.255810	3.128102	1.328079
H	1.594997	2.492312	1.138990
H	2.500332	2.228907	2.671401
H	7.176030	0.560778	0.276574
H	7.114825	-1.232547	0.177231
H	6.710721	-0.242069	-1.251680

Cl1-1

Ru	0.228142	1.356257	-0.081340
C	-0.114903	-0.674731	0.088168
Cl	0.149636	1.377839	2.367434
Cl	0.011659	1.065173	-2.504076
C	-1.487558	1.947761	-0.075981
H	-1.991085	2.216104	0.877874
H	-2.047526	2.078327	-1.026924
C	1.520944	3.117765	0.468986
C	1.498682	3.018400	-0.922178
H	2.308454	2.508612	-1.470129
H	0.837354	3.644575	-1.540532
N	0.938996	-1.529908	0.174463
N	-1.266353	-1.388753	0.165921
C	0.521301	-2.941002	0.331269
C	-1.017481	-2.842820	0.324196
H	0.920478	-3.555721	-0.503212
H	0.922483	-3.358263	1.278890
H	-1.478149	-3.206747	1.266516
H	-1.482682	-3.402476	-0.514625
H	0.878566	3.830217	1.009456
C	2.336366	-1.171228	0.093812
C	-2.630208	-0.925321	0.086643
C	2.978410	-1.164665	-1.177846
C	4.342104	-0.813578	-1.228475
C	5.085476	-0.513488	-0.069507
C	4.438884	-0.620543	1.176462
C	3.076998	-0.968398	1.291988
C	-3.332800	-0.618805	1.284853
C	-4.676550	-0.211362	1.176932
C	-5.340111	-0.127666	-0.064131
C	-4.628011	-0.495579	-1.220867
C	-3.280683	-0.910445	-1.175437
C	2.252464	-1.554006	-2.441509
H	4.841499	-0.794690	-2.211765
C	6.538127	-0.104894	-0.166207
H	5.015032	-0.446308	2.100539
C	2.459333	-1.160212	2.654844
C	-2.677921	-0.735198	2.639393
H	-5.224014	0.039677	2.101181
C	-6.777065	0.337881	-0.141177
H	-5.136343	-0.469322	-2.199314
C	-2.571794	-1.327231	-2.440632
H	2.960354	-1.633171	-3.289489
H	1.740631	-2.534355	-2.338084
H	1.473541	-0.803723	-2.703547
H	3.199903	-0.954965	3.452185
H	1.590610	-0.482210	2.800860
H	2.101792	-2.203491	2.796402
H	7.058490	-0.202888	0.807494
H	7.085146	-0.715603	-0.914066
H	6.632710	0.955964	-0.486477
H	-3.390985	-0.469668	3.444131
H	-2.327260	-1.771852	2.837190
H	-1.788498	-0.071736	2.721807
H	-3.267701	-1.318672	-3.302058
H	-1.722661	-0.644043	-2.665595
H	-2.151273	-2.353006	-2.362093
H	-7.201982	0.190665	-1.153868
H	-7.420135	-0.204091	0.583868
H	-6.860485	1.419245	0.103172
H	2.350958	2.693940	1.057791

TS1-1

Ru	0.188614	1.324403	0.021309
C	-0.098516	-0.697541	0.053094
Cl	0.016113	1.216715	2.443940
Cl	0.278929	1.311152	-2.421665
C	-1.535975	1.880753	-0.132053
H	-2.166440	2.022010	0.774685
H	-1.980120	2.139490	-1.118716
C	0.860914	3.545994	0.595116
C	1.692238	2.963055	-0.347975
H	2.574521	2.379607	-0.015731
H	1.668865	3.239756	-1.412664
N	0.960555	-1.551846	0.101668
N	-1.245755	-1.425427	0.105772
C	0.548969	-2.963189	0.267460
C	-0.985257	-2.884433	0.143718
H	1.016092	-3.598920	-0.513329
H	0.879466	-3.344478	1.257903
H	-1.512303	-3.349392	1.002126
H	-1.367877	-3.360942	-0.785305
H	0.097438	4.277846	0.284845
C	2.354994	-1.181607	0.039740
C	-2.606270	-0.961213	0.013650
C	2.997802	-1.142231	-1.229028
C	4.359052	-0.779756	-1.271751
C	5.096969	-0.492528	-0.107025
C	4.448319	-0.625327	1.136630
C	3.090487	-0.989606	1.243495
C	-3.366002	-0.799245	1.203800
C	-4.710495	-0.396367	1.080197
C	-5.316417	-0.173291	-0.172576
C	-4.544094	-0.389464	-1.330597
C	-3.194996	-0.793280	-1.269159
C	2.269005	-1.497549	-2.500493
H	4.859496	-0.735954	-2.253579
C	6.543852	-0.060182	-0.187493
H	5.020482	-0.459777	2.064990
C	2.474776	-1.220751	2.601910
C	-2.764579	-1.053368	2.564589
H	-5.304265	-0.259273	1.999631
C	-6.750699	0.296702	-0.268776
H	-5.005801	-0.250366	-2.322606
C	-2.411447	-1.039916	-2.534640
H	2.977987	-1.586657	-3.346616
H	1.723970	-2.460972	-2.411031
H	1.520275	-0.713608	-2.751900
H	3.177533	-0.924949	3.405243
H	1.537187	-0.639483	2.732788
H	2.236094	-2.296461	2.756156
H	7.126605	-0.411967	0.688131
H	7.034622	-0.439246	-1.106583
H	6.625791	1.049100	-0.207442
H	-3.496774	-0.832919	3.365818
H	-2.453263	-2.114299	2.685063
H	-1.861418	-0.425643	2.728669
H	-3.057804	-0.925757	-3.426623
H	-1.557959	-0.330973	-2.628753
H	-1.983211	-2.065241	-2.562023
H	-7.216646	-0.001911	-1.229460
H	-7.370574	-0.106664	0.557787
H	-6.810080	1.405935	-0.207287
H	1.033980	3.441606	1.676452

MCy-1

Ru	-0.000896	1.231220	-0.009611
C	0.000263	-0.779961	0.029645
Cl	0.022885	1.302097	-2.418199
Cl	-0.025499	1.358434	2.397334
C	1.348548	2.673154	-0.011816
H	1.938458	2.763401	-0.942726
H	1.917427	2.789257	0.929242
C	-1.351887	2.671441	-0.038433
C	-0.002185	3.504847	-0.037870
H	-0.011359	4.118479	0.883466
H	0.006600	4.092674	-0.975868
N	-1.107115	-1.562968	0.051098
N	1.108626	-1.561565	0.055216
C	-0.770218	-3.005516	0.072979
C	0.773438	-3.003148	0.119061
H	-1.227841	-3.493864	0.959058
H	-1.173379	-3.506051	-0.833535
H	1.232555	-3.542440	-0.736338
H	1.176304	-3.449419	1.053492
H	-1.924017	2.761563	-0.980403
C	-2.480357	-1.118726	0.018186
C	2.481571	-1.116102	0.028685
C	-3.176034	-0.930574	1.243125
C	-4.522332	-0.520443	1.180851
C	-5.189614	-0.316563	-0.043584
C	-4.481055	-0.565381	-1.235057
C	-3.132769	-0.976622	-1.235467
C	3.140824	-0.990582	-1.224740
C	4.487245	-0.578581	-1.224330
C	5.190277	-0.312087	-0.031749
C	4.517280	-0.497657	1.190749
C	3.169901	-0.909601	1.253236
C	-2.509136	-1.164078	2.576507
H	-5.068337	-0.365521	2.126687
C	-6.623733	0.162591	-0.074473
H	-4.994085	-0.446592	-2.204226
C	-2.421638	-1.256234	-2.536674
C	2.432790	-1.287073	-2.523789
H	5.004193	-0.472157	-2.192983
C	6.627656	0.156675	-0.072832
H	5.058335	-0.326157	2.136426
C	2.499993	-1.125047	2.588328
H	-3.240336	-1.071240	3.403122
H	-2.055542	-2.176315	2.641921
H	-1.692266	-0.427555	2.747454
H	-3.129534	-1.217122	-3.387488
H	-1.616524	-0.509222	-2.718270
H	-1.944461	-2.259490	-2.543322
H	-7.128608	-0.113326	-1.022081
H	-7.213683	-0.254678	0.767202
H	-6.673594	1.270463	0.013371
H	3.144776	-1.272756	-3.371984
H	1.942144	-2.283675	-2.512853
H	1.638143	-0.532973	-2.721568
H	3.224679	-0.996807	3.415935
H	1.666233	-0.403444	2.739836
H	2.069966	-2.145909	2.676339
H	7.102251	0.115280	0.927758
H	7.236942	-0.456893	-0.769098
H	6.693920	1.207617	-0.429975
H	-1.939072	2.785507	0.891571

TS2-1

Ru	0.188614	1.324403	0.021309
C	-0.098516	-0.697541	0.053094
Cl	0.016113	1.216715	2.443940
Cl	0.278929	1.311152	-2.421665
C	-1.535975	1.880753	-0.132053
H	-2.166440	2.022010	0.774685
H	-1.980120	2.139490	-1.118716
C	0.860914	3.545994	0.595116
C	1.692238	2.963055	-0.347975
H	2.574521	2.379607	-0.015731
H	1.668865	3.239756	-1.412664
N	0.960555	-1.551846	0.101668
N	-1.245755	-1.425427	0.105772
C	0.548969	-2.963189	0.267460
C	-0.985257	-2.884433	0.143718
H	1.016092	-3.598920	-0.513329
H	0.879466	-3.344478	1.257903
H	-1.512303	-3.349392	1.002126
H	-1.367877	-3.360942	-0.785305
H	0.097438	4.277846	0.284845
C	2.354994	-1.181607	0.039740
C	-2.606270	-0.961213	0.013650
C	2.997802	-1.142231	-1.229028
C	4.359052	-0.779756	-1.271751
C	5.096969	-0.492528	-0.107025
C	4.448319	-0.625327	1.136630
C	3.090487	-0.989606	1.243495
C	-3.366002	-0.799245	1.203800
C	-4.710495	-0.396367	1.080197
C	-5.316417	-0.173291	-0.172576
C	-4.544094	-0.389464	-1.330597
C	-3.194996	-0.793280	-1.269159
C	2.269005	-1.497549	-2.500493
H	4.859496	-0.735954	-2.253579
C	6.543852	-0.060182	-0.187493
H	5.020482	-0.459777	2.064990
C	2.474776	-1.220751	2.601910
C	-2.764579	-1.053368	2.564589
H	-5.304265	-0.259273	1.999631
C	-6.750699	0.296702	-0.268776
H	-5.005801	-0.250366	-2.322606
C	-2.411447	-1.039916	-2.534640
H	2.977987	-1.586657	-3.346616
H	1.723970	-2.460972	-2.411031
H	1.520275	-0.713608	-2.751900
H	3.177533	-0.924949	3.405243
H	1.537187	-0.639483	2.732788
H	2.236094	-2.296461	2.756156
H	7.126605	-0.411967	0.688131
H	7.034622	-0.439246	-1.106583
H	6.625791	1.049100	-0.207442
H	-3.496774	-0.832919	3.365818
H	-2.453263	-2.114299	2.685063
H	-1.861418	-0.425643	2.728669
H	-3.057804	-0.925757	-3.426623
H	-1.557959	-0.330973	-2.628753
H	-1.983211	-2.065241	-2.562023
H	-7.216646	-0.001911	-1.229460
H	-7.370574	-0.106664	0.557787
H	-6.810080	1.405935	-0.207287
H	1.033980	3.441606	1.676452

Cl2-1

Ru	0.228142	1.356257	-0.081340
C	-0.114903	-0.674731	0.088168
Cl	0.149636	1.377839	2.367434
Cl	0.011659	1.065173	-2.504076
C	-1.487558	1.947761	-0.075981
H	-1.991085	2.216104	0.877874
H	-2.047526	2.078327	-1.026924
C	1.520944	3.117765	0.468986
C	1.498682	3.018400	-0.922178
H	2.308454	2.508612	-1.470129
H	0.837354	3.644575	-1.540532
N	0.938996	-1.529908	0.174463
N	-1.266353	-1.388753	0.165921
C	0.521301	-2.941002	0.331269
C	-1.017481	-2.842820	0.324196
H	0.920478	-3.555721	-0.503212
H	0.922483	-3.358263	1.278890
H	-1.478149	-3.206747	1.266516
H	-1.482682	-3.402476	-0.514625
H	0.878566	3.830217	1.009456
C	2.336366	-1.171228	0.093812
C	-2.630208	-0.925321	0.086643
C	2.978410	-1.164665	-1.177846
C	4.342104	-0.813578	-1.228475
C	5.085476	-0.513488	-0.069507
C	4.438884	-0.620543	1.176462
C	3.076998	-0.968398	1.291988
C	-3.332800	-0.618805	1.284853
C	-4.676550	-0.211362	1.176932
C	-5.340111	-0.127666	-0.064131
C	-4.628011	-0.495579	-1.220867
C	-3.280683	-0.910445	-1.175437
C	2.252464	-1.554006	-2.441509
H	4.841499	-0.794690	-2.211765
C	6.538127	-0.104894	-0.166207
H	5.015032	-0.446308	2.100539
C	2.459333	-1.160212	2.654844
C	-2.677921	-0.735198	2.639393
H	-5.224014	0.039677	2.101181
C	-6.777065	0.337881	-0.141177
H	-5.136343	-0.469322	-2.199314
C	-2.571794	-1.327231	-2.440632
H	2.960354	-1.633171	-3.289489
H	1.740631	-2.534355	-2.338084
H	1.473541	-0.803723	-2.703547
H	3.199903	-0.954965	3.452185
H	1.590610	-0.482210	2.800860
H	2.101792	-2.203491	2.796402
H	7.058490	-0.202888	0.807494
H	7.085146	-0.715603	-0.914066
H	6.632710	0.955964	-0.486477
H	-3.390985	-0.469668	3.444131
H	-2.327260	-1.771852	2.837190
H	-1.788498	-0.071736	2.721807
H	-3.267701	-1.318672	-3.302058
H	-1.722661	-0.644043	-2.665595
H	-2.151273	-2.353006	-2.362093
H	-7.201982	0.190665	-1.153868
H	-7.420135	-0.204091	0.583868
H	-6.860485	1.419245	0.103172
H	2.350958	2.693940	1.057791

14e2-1

Ru	0.079657	0.468600	-1.401147
Cl	0.234259	2.758165	-0.989250
Cl	1.162148	-1.339852	-2.377836
C	-0.082662	-0.060496	0.451648
C	-1.596014	0.297463	-2.059731
H	-1.695233	0.630987	-3.125683
H	-2.512532	-0.097116	-1.580690
N	1.010283	-0.207016	1.283146
N	-1.204944	-0.243198	1.227568
C	0.624959	-0.326957	2.701746
C	-0.875739	-0.637954	2.612350
H	1.208243	-1.127624	3.200679
H	0.823662	0.627222	3.240675
H	-1.483821	-0.059500	3.337416
H	-1.098202	-1.718433	2.771118
C	2.404480	-0.205411	0.916290
C	-2.582248	-0.266255	0.823638
C	3.015678	-1.445585	0.581181
C	4.383375	-1.447826	0.252633
C	5.159367	-0.271262	0.267779
C	4.538288	0.924449	0.673642
C	3.173117	0.984407	1.023487
C	-3.355341	0.917710	0.941970
C	-4.717636	0.857177	0.590218
C	-5.322946	-0.333327	0.135982
C	-4.523468	-1.489283	0.036130
C	-3.154474	-1.483547	0.374552
C	2.233345	-2.737472	0.593127
H	4.858597	-2.405054	-0.020148
C	6.613715	-0.296599	-0.144922
H	5.136469	1.849101	0.735625
C	2.594186	2.271350	1.563025
C	-2.728294	2.210971	1.405319
H	-5.325183	1.774160	0.673885
C	-6.786706	-0.355926	-0.244850
H	-4.976170	-2.429496	-0.321222
C	-2.312963	-2.728746	0.212011
H	-3.481364	3.021288	1.457219
H	-2.271310	2.110823	2.413302
H	-1.915525	2.531569	0.718241
H	-2.913940	-3.562943	-0.199226
H	-1.457844	-2.548114	-0.473707
H	-1.883728	-3.073058	1.177583
H	-7.140073	-1.384523	-0.456488
H	-7.422006	0.065207	0.562653
H	-6.974411	0.257430	-1.152631
H	1.511384	-2.764427	-0.249635
H	2.910700	-3.607709	0.489697
H	1.656260	-2.864775	1.533333
H	3.255810	3.128102	1.328079
H	1.594997	2.492312	1.138990
H	2.500332	2.228907	2.671401
H	7.176030	0.560778	0.276574
H	7.114825	-1.232547	0.177231
H	6.710721	-0.242069	-1.251680

Precat-2

Ru	-0.002929	-0.328337	-0.056133
Cl	-0.293995	-0.328627	2.348918
Cl	-0.215947	-0.536341	-2.484029
P	-0.747209	2.069224	-0.212863
N	-1.015070	-3.225232	0.095517
N	1.172636	-3.198198	-0.146051
C	0.072168	-2.395410	-0.012679
C	-0.672744	-4.656519	-0.063584
H	-1.089000	-5.043774	-1.019609
H	-1.111573	-5.255509	0.760931
C	0.859208	-4.641779	-0.050635
H	1.286343	-5.060895	0.887833
H	1.308994	-5.196484	-0.899853
C	-2.411008	-2.906315	0.275373
C	-2.947684	-2.916722	1.593615
C	-2.085499	-3.213649	2.795846
H	-2.684604	-3.181971	3.726942
H	-1.259367	-2.477078	2.883591
H	-1.628003	-4.225025	2.728045
C	-4.329594	-2.693601	1.753974
H	-4.744665	-2.685391	2.775960
C	-5.193603	-2.515822	0.656019
C	-6.667866	-2.247775	0.860719
H	-7.272237	-2.595751	-0.001482
H	-6.861574	-1.158213	0.976781
H	-7.051700	-2.743453	1.775735
C	-4.641036	-2.596588	-0.636652
H	-5.305183	-2.516591	-1.513746
C	-3.263283	-2.803305	-0.858430
C	-2.745724	-2.961987	-2.268223
H	-3.552484	-2.773393	-3.003692
H	-2.375431	-3.995132	-2.450520
H	-1.903670	-2.269058	-2.484710
C	2.566720	-2.852427	-0.203595
C	3.220352	-2.852082	-1.465893
C	2.448096	-3.065053	-2.745732
H	3.112576	-2.976812	-3.627707
H	1.621352	-2.327464	-2.848045
H	1.981570	-4.074185	-2.782574
C	4.612701	-2.644365	-1.490935
H	5.126749	-2.638374	-2.467315
C	5.365334	-2.460701	-0.311910
C	6.858580	-2.231408	-0.380686
H	7.352057	-2.959635	-1.058093
H	7.333487	-2.313579	0.617238
H	7.089229	-1.217705	-0.775025
C	4.685612	-2.486222	0.920437
H	5.255767	-2.350788	1.854527
C	3.292449	-2.685887	1.004649
C	2.601006	-2.724554	2.346145
H	2.116969	-3.708291	2.531693
H	1.797939	-1.959447	2.419655
H	3.323430	-2.551399	3.167315
C	1.798257	0.029534	-0.294287
C	4.071104	0.987123	-0.187958
C	2.854285	0.688751	0.490880
C	5.130685	1.631480	0.466151
C	2.754640	1.042637	1.862358
C	5.010631	1.974182	1.825713
H	6.056811	1.863839	-0.083856
C	3.823001	1.668689	2.519212
H	1.823202	0.800629	2.394993
H	5.842541	2.476662	2.345284
H	3.728259	1.927989	3.586040
C	-2.430311	2.150610	-1.113603
C	-2.408878	2.345369	-2.647397
C	-3.291296	0.914286	-0.768212
H	-2.916434	3.056065	-0.676568
C	-3.841121	2.503519	-3.197005
H	-1.920916	1.463007	-3.115083
H	-1.813679	3.237942	-2.930680
C	-4.725821	1.063397	-1.306857
H	-2.812668	0.022256	-1.230371
H	-3.312858	0.724393	0.324098
C	-4.735939	1.310373	-2.824001
H	-3.804004	2.631361	-4.300954
H	-4.290462	3.440079	-2.790505
H	-5.314805	0.156194	-1.054188
H	-5.224610	1.916647	-0.789671
H	-5.774305	1.473980	-3.187238
H	-4.361019	0.398801	-3.343025
C	0.272663	3.349322	-1.213034
C	1.266321	4.230752	-0.421769
C	0.987933	2.717476	-2.426956
H	-0.522287	4.033496	-1.594918
C	1.910684	5.298483	-1.331479
H	2.065493	3.594229	0.018789
H	0.760569	4.743729	0.419900
C	1.623549	3.785947	-3.336284
H	1.786678	2.038997	-2.054584
H	0.305743	2.065980	-3.005253
C	2.599291	4.681506	-2.558021
H	2.632850	5.901226	-0.738424
H	1.121302	6.008553	-1.672447
H	2.138436	3.290781	-4.188156
H	0.821069	4.417451	-3.784463
H	3.014292	5.478360	-3.213331
H	3.466375	4.069486	-2.218911
C	-1.182359	3.075248	1.358075
C	-2.498365	2.660922	2.059587
C	-0.054449	3.123628	2.415973
H	-1.333373	4.105716	0.948853
C	-2.846898	3.634267	3.205359
H	-2.375429	1.630906	2.462309
H	-3.347982	2.638522	1.347766
C	-0.385939	4.126409	3.537142
H	0.042682	2.106896	2.849103
H	0.924944	3.365253	1.963333
C	-1.709183	3.765234	4.230428
H	-3.783279	3.299908	3.703445
H	-3.066975	4.638851	2.773808
H	0.445342	4.151995	4.275175
H	-0.457137	5.155821	3.112498
H	-1.968724	4.520586	5.004283
H	-1.584573	2.796058	4.764949
H	4.169690	0.701852	-1.247836
H	2.175285	-0.253957	-1.305628

14e1-2

Ru	-0.229244	0.878736	0.091096
Cl	-0.972340	1.556755	-2.007499
N	-1.798072	-1.551861	0.152394
C	-0.519565	-1.026598	0.092993
C	-1.805921	-2.995101	0.445091
C	-3.038441	-0.830419	0.026820
C	-3.601070	-0.672565	-1.271184
C	-4.822348	0.014823	-1.389421
C	-5.506345	0.525683	-0.267297
C	-4.959064	0.285203	1.006355
C	-3.743534	-0.407791	1.185730
C	-2.923649	-1.239000	-2.496178
C	-6.787953	1.310506	-0.433667
C	-3.273917	-0.745417	2.581347
H	-2.099835	-3.176964	1.503966
H	-2.533240	-3.524196	-0.204649
H	-5.255323	0.151301	-2.394662
H	-5.500095	0.636076	1.901302
H	-2.025590	-0.639252	-2.755961
H	-2.591775	-2.286893	-2.339454
H	-3.608489	-1.223141	-3.366642
H	-7.429125	0.883114	-1.232153
H	-6.571923	2.362843	-0.721947
H	-7.377065	1.340618	0.504878
H	-3.598854	-1.771654	2.866124
H	-3.712824	-0.050633	3.324204
H	-2.172948	-0.686314	2.679736
N	0.350653	-2.093070	0.159065
C	-0.349247	-3.394550	0.169897
C	1.779609	-2.106671	0.029736
C	2.577109	-2.122157	1.202853
C	3.975586	-2.204032	1.053357
C	4.590695	-2.277827	-0.213419
C	3.765296	-2.254365	-1.356244
C	2.361382	-2.171552	-1.263068
C	1.945365	-2.014522	2.570349
C	6.092686	-2.407155	-0.338621
C	1.508188	-2.088918	-2.508068
H	-0.226348	-3.909345	-0.811087
H	0.075181	-4.057697	0.951340
H	4.603888	-2.207923	1.959992
H	4.226818	-2.299176	-2.357163
H	1.376084	-1.065805	2.674884
H	1.224917	-2.839211	2.759639
H	2.713747	-2.050263	3.367058
H	6.454068	-2.060640	-1.327690
H	6.411475	-3.467083	-0.225908
H	6.620009	-1.826352	0.445516
H	0.732409	-2.883099	-2.538920
H	2.126702	-2.189016	-3.421109
H	0.970026	-1.117812	-2.560925
Cl	-0.390480	1.173078	2.401300
C	1.594742	1.021750	-0.147854
H	2.233667	0.150946	-0.391759
C	2.296402	2.302019	-0.099191
C	3.672019	2.349348	-0.463688
C	1.665447	3.518573	0.290405
C	4.381194	3.558138	-0.449417
H	4.174315	1.414792	-0.762243
C	2.377088	4.723311	0.304034
H	0.607793	3.510908	0.601968
C	3.736431	4.749047	-0.066799
H	5.444619	3.574019	-0.737163
H	1.871711	5.652806	0.610268
H	4.293477	5.699435	-0.053578

Cl1-2

Ru	0.393947	0.981342	-0.468894
C	0.635354	-0.972359	0.252971
Cl	0.287400	1.503210	1.910118
Cl	0.705191	-0.033077	-2.683499
C	-1.417393	0.970789	-0.857505
H	-1.675790	0.338766	-1.737683
C	0.726680	3.217349	-0.458399
C	1.060077	2.721817	-1.719534
H	2.106692	2.479759	-1.974228
H	0.381004	2.807881	-2.581513
N	1.869056	-1.453991	0.576040
N	-0.282939	-1.934502	0.527501
C	1.810882	-2.791580	1.209160
C	0.339510	-3.191871	1.011280
H	2.522762	-3.485792	0.717488
H	2.093682	-2.714793	2.281647
H	-0.151390	-3.528254	1.947044
H	0.208109	-3.993868	0.252086
H	-0.242150	3.710310	-0.275915
C	3.143509	-0.793388	0.404737
C	-1.713381	-1.910829	0.346935
C	3.871437	-1.012737	-0.800410
C	5.106564	-0.354605	-0.958972
C	5.655515	0.468044	0.044818
C	4.961074	0.569628	1.264472
C	3.723817	-0.071451	1.484321
C	-2.538627	-1.551435	1.446710
C	-3.934450	-1.596253	1.269856
C	-4.524810	-2.004273	0.056923
C	-3.674735	-2.399113	-0.993322
C	-2.269265	-2.376049	-0.873783
C	3.379865	-1.962698	-1.863543
H	5.664832	-0.507058	-1.897923
C	6.955562	1.206648	-0.180049
H	5.402128	1.152735	2.090384
C	3.119086	-0.058692	2.868155
C	-1.948614	-1.149690	2.776501
H	-4.580628	-1.305705	2.115102
C	-6.028299	-2.010766	-0.104213
H	-4.115010	-2.750373	-1.941801
C	-1.400696	-2.844383	-2.016360
H	4.147161	-2.101405	-2.650120
H	3.146555	-2.963263	-1.440151
H	2.452092	-1.578193	-2.339685
H	3.472449	0.818412	3.445366
H	2.013741	-0.017222	2.842962
H	3.433575	-0.965659	3.432685
H	7.473627	1.427855	0.774931
H	7.648459	0.629124	-0.825595
H	6.775086	2.179729	-0.688125
H	-2.747218	-0.908823	3.505024
H	-1.334191	-1.966643	3.215096
H	-1.281919	-0.265996	2.675908
H	-2.021741	-3.166078	-2.875204
H	-0.709593	-2.043792	-2.362937
H	-0.769092	-3.711514	-1.723671
H	-6.342638	-2.562241	-1.012751
H	-6.530155	-2.473909	0.770940
H	-6.421208	-0.973933	-0.187986
H	1.498232	3.400501	0.306467
C	-2.584760	1.708537	-0.364931
C	-3.790674	1.552409	-1.111715
C	-2.607311	2.580279	0.759400
C	-4.957797	2.244346	-0.762160
H	-3.790100	0.875869	-1.981492
C	-3.779543	3.263114	1.109971
H	-1.693029	2.682823	1.363205
C	-4.955766	3.104314	0.352000
H	-5.873376	2.116040	-1.361531
H	-3.777130	3.930842	1.986500
H	-5.871221	3.651453	0.629602

TS1-2

Ru	-0.394652	-0.970982	-0.392457
C	-0.636589	0.947431	0.271656
Cl	-0.389761	-1.644689	1.928889
Cl	-0.830020	-0.248600	-2.674172
C	1.418750	-0.868845	-0.821199
H	1.642614	-0.174456	-1.661226
C	-0.096391	-3.335362	-0.706444
C	-1.326857	-2.900144	-1.161663
H	-2.203965	-2.907826	-0.486993
H	-1.528544	-2.755657	-2.234491
N	-1.870796	1.450707	0.580013
N	0.288220	1.900682	0.577987
C	-1.804050	2.777152	1.231266
C	-0.322479	3.156350	1.072704
H	-2.493297	3.490883	0.734210
H	-2.111171	2.694079	2.296737
H	0.151932	3.467796	2.026083
H	-0.163428	3.973834	0.334819
H	0.724818	-3.525682	-1.415802
C	-3.152644	0.816753	0.377796
C	1.709087	1.881819	0.357147
C	-3.847015	1.056916	-0.842566
C	-5.097368	0.436419	-1.028459
C	-5.689661	-0.373412	-0.038941
C	-5.021354	-0.503459	1.192814
C	-3.771710	0.102343	1.440444
C	2.568304	1.501769	1.422260
C	3.957703	1.581529	1.212475
C	4.507020	2.031878	-0.005422
C	3.623006	2.416533	-1.032409
C	2.222675	2.360044	-0.876941
C	-3.296294	1.979685	-1.900991
H	-5.630921	0.606105	-1.978791
C	-7.006853	-1.071232	-0.293089
H	-5.493641	-1.080601	2.005553
C	-3.185278	0.055692	2.831424
C	2.009821	1.021759	2.739104
H	4.632357	1.279655	2.031102
C	6.005762	2.082588	-0.199300
H	4.032954	2.781333	-1.989373
C	1.304395	2.773736	-2.002685
H	-4.062628	2.192299	-2.671973
H	-2.967872	2.949718	-1.471097
H	-2.414082	1.521448	-2.398835
H	-3.603299	-0.793158	3.407584
H	-2.084343	-0.059660	2.818525
H	-3.441634	0.983772	3.390967
H	-7.531190	-1.317301	0.652229
H	-7.685096	-0.451762	-0.915203
H	-6.849617	-2.026774	-0.840528
H	2.823796	0.753427	3.440419
H	1.387528	1.801220	3.230650
H	1.353501	0.134747	2.600819
H	1.885498	3.131033	-2.875203
H	0.656628	1.931129	-2.335995
H	0.620849	3.596176	-1.699709
H	6.283617	2.628585	-1.122804
H	6.510327	2.576491	0.657441
H	6.429451	1.057322	-0.273599
H	0.043261	-3.679028	0.329258
C	2.622261	-1.582366	-0.383092
C	3.789308	-1.428729	-1.187102
C	2.711492	-2.402894	0.775663
C	4.985165	-2.084691	-0.863089
H	3.736324	-0.785853	-2.080475
C	3.914328	-3.038648	1.107024
H	1.821047	-2.508232	1.414851
C	5.051841	-2.890701	0.288281
H	5.870035	-1.966341	-1.508798
H	3.967918	-3.663773	2.012829
H	5.991030	-3.405032	0.548777

MCy-2

Ru	-0.263403	-0.737245	-0.546896
C	-0.733583	1.050397	0.254931
Cl	-0.298251	-1.842131	1.590103
Cl	-0.367672	0.287363	-2.742527
C	1.334709	-1.726978	-1.298263
H	1.616143	-1.225889	-2.244803
C	-1.332328	-2.227776	-1.280102
C	0.136012	-2.746039	-1.541792
H	0.187701	-2.953033	-2.629362
H	0.311529	-3.645079	-0.923649
N	-1.990157	1.465014	0.565488
N	0.148392	2.040745	0.544243
C	-2.009098	2.875708	1.019087
C	-0.513138	3.203453	1.181228
H	-2.506338	3.513808	0.255825
H	-2.580786	2.970481	1.964923
H	-0.202520	3.279700	2.246850
H	-0.216061	4.144128	0.674320
H	-1.875143	-2.824299	-0.522774
C	-3.221618	0.721838	0.434426
C	1.586129	1.999182	0.425457
C	-3.969837	0.804055	-0.771105
C	-5.178432	0.083046	-0.847617
C	-5.669432	-0.679788	0.230347
C	-4.931081	-0.683042	1.429560
C	-3.714936	0.015997	1.564505
C	2.358604	1.470681	1.496010
C	3.761239	1.513631	1.380566
C	4.406521	2.080521	0.263321
C	3.607397	2.625690	-0.759272
C	2.198434	2.609732	-0.700729
C	-3.516569	1.649891	-1.936195
H	-5.760766	0.134686	-1.783052
C	-6.949050	-1.475226	0.099784
H	-5.314850	-1.241987	2.299514
C	-2.973588	0.005978	2.878572
C	1.715094	0.889599	2.731676
H	4.367552	1.096756	2.201955
C	5.916316	2.107507	0.180162
H	4.092215	3.092877	-1.632894
C	1.381442	3.230109	-1.807206
H	-4.252303	1.603176	-2.762750
H	-3.408982	2.719086	-1.650809
H	-2.530395	1.315178	-2.327729
H	-3.583575	-0.470626	3.670704
H	-2.020583	-0.560043	2.781363
H	-2.716434	1.031022	3.220893
H	-7.440898	-1.626402	1.081963
H	-7.673138	-0.978910	-0.578191
H	-6.747337	-2.484215	-0.323270
H	2.478438	0.668719	3.502958
H	0.975577	1.586232	3.180852
H	1.168410	-0.053158	2.506169
H	2.037496	3.707386	-2.561213
H	0.758755	2.460790	-2.315224
H	0.688026	4.010499	-1.425842
H	6.269258	2.646552	-0.721376
H	6.362567	2.600643	1.069873
H	6.331756	1.077487	0.144848
H	-1.899633	-2.009187	-2.203867
C	2.544268	-2.162102	-0.547800
C	3.782967	-1.592450	-0.941367
C	2.558576	-3.136850	0.481487
C	4.988187	-1.982428	-0.337390
H	3.790911	-0.836294	-1.742982
C	3.763688	-3.528302	1.081504
H	1.611508	-3.570422	0.832679
C	4.984553	-2.955577	0.676923
H	5.937354	-1.533322	-0.671195
H	3.749791	-4.289450	1.878035
H	5.928867	-3.270109	1.149522

TS2-2

Ru	-0.209934	-0.823987	-0.472098
C	-0.708672	0.986887	0.283080
Cl	-0.029700	-1.741736	1.760236
Cl	-0.332137	-0.004808	-2.751570
C	1.226952	-2.330410	-1.419977
H	1.345840	-1.884550	-2.423005
C	-1.799605	-1.710830	-0.712299
C	0.053160	-3.082652	-1.213588
H	-0.577631	-3.306226	-2.087852
H	-0.055239	-3.740499	-0.337379
N	-1.963745	1.411261	0.612269
N	0.170031	1.984001	0.579848
C	-1.973565	2.781229	1.174078
C	-0.484093	3.175134	1.164182
H	-2.601397	3.449476	0.546149
H	-2.410610	2.776108	2.195420
H	-0.083614	3.372716	2.181640
H	-0.277579	4.072770	0.543010
H	-2.257273	-2.312049	0.105763
C	-3.217322	0.731010	0.419786
C	1.599694	1.978476	0.389170
C	-3.920627	0.911481	-0.802837
C	-5.175658	0.286076	-0.943919
C	-5.750188	-0.484976	0.086508
C	-5.041351	-0.607536	1.297880
C	-3.782599	-0.004357	1.496291
C	2.441909	1.563984	1.457688
C	3.835579	1.643689	1.268766
C	4.405522	2.141608	0.080511
C	3.539216	2.575933	-0.940920
C	2.136437	2.520810	-0.809821
C	-3.348911	1.743754	-1.923794
H	-5.725378	0.418051	-1.891196
C	-7.083382	-1.172072	-0.109656
H	-5.483539	-1.186032	2.126472
C	-3.063591	-0.145917	2.815180
C	1.876879	1.068783	2.766386
H	4.495593	1.313025	2.088005
C	5.906766	2.254151	-0.068513
H	3.963864	2.988882	-1.871506
C	1.248196	3.037890	-1.914801
H	-4.083004	1.856949	-2.745427
H	-3.068043	2.762619	-1.581180
H	-2.425577	1.280156	-2.339745
H	-3.668237	-0.734295	3.532829
H	-2.080942	-0.652169	2.683263
H	-2.859341	0.841652	3.282864
H	-7.601285	-1.346614	0.855048
H	-7.757058	-0.580207	-0.762432
H	-6.952317	-2.164719	-0.594715
H	2.687917	0.872524	3.494515
H	1.187425	1.810273	3.224689
H	1.295229	0.130166	2.628811
H	1.850591	3.520494	-2.709143
H	0.660000	2.211876	-2.373284
H	0.518300	3.789114	-1.544024
H	6.210486	2.318774	-1.132718
H	6.291111	3.166335	0.439406
H	6.428017	1.388379	0.389096
H	-2.347788	-1.682088	-1.680894
C	2.482414	-2.402656	-0.633882
C	3.586219	-1.638201	-1.089149
C	2.665388	-3.244309	0.492163
C	4.831524	-1.712984	-0.446133
H	3.457826	-0.983400	-1.966025
C	3.908941	-3.316361	1.132652
H	1.823863	-3.838825	0.874084
C	4.997925	-2.553351	0.667620
H	5.677004	-1.116205	-0.822697
H	4.032766	-3.978010	2.004724
H	5.975393	-2.620335	1.171710

Cl2-2

Ru	0.178956	-0.813456	-0.746045
C	0.764376	0.858245	0.349343
Cl	0.564547	0.587758	-2.714666
Cl	0.039175	-1.971205	1.400599
C	-1.289202	-2.575595	-1.242413
H	-0.702354	-3.446581	-0.908552
C	1.832043	-1.533649	-0.948686
C	-0.893089	-1.904475	-2.404581
H	-0.080533	-2.298483	-3.032164
H	-1.561482	-1.192041	-2.912320
N	2.011911	1.211996	0.765204
N	-0.114744	1.802338	0.777290
C	2.020276	2.492698	1.512867
C	0.530074	2.867073	1.580536
H	2.477682	2.348707	2.513797
H	2.631057	3.245046	0.969425
H	0.310223	3.863667	1.144090
H	0.126538	2.857292	2.615825
H	2.460129	-1.283051	-1.832164
C	3.275605	0.555941	0.538719
C	-1.541937	1.870133	0.560788
C	3.777555	-0.339884	1.522980
C	5.040989	-0.924792	1.304449
C	5.821723	-0.626081	0.170439
C	5.320836	0.317924	-0.747462
C	4.064862	0.935130	-0.582720
C	-2.035961	2.657597	-0.518295
C	-3.430969	2.787344	-0.657942
C	-4.335266	2.200249	0.250144
C	-3.807725	1.476917	1.334682
C	-2.420236	1.310537	1.527469
C	2.999487	-0.653642	2.776760
H	5.428812	-1.630861	2.057881
C	7.154218	-1.303082	-0.058586
H	5.931284	0.597597	-1.622531
C	3.595349	1.977712	-1.567100
C	-1.110310	3.371372	-1.472439
H	-3.819393	3.388590	-1.497425
C	-5.826865	2.379511	0.074405
H	-4.495000	1.030810	2.071996
C	-1.909988	0.588696	2.749844
H	3.561684	-1.355369	3.423340
H	2.800554	0.262187	3.375193
H	2.012636	-1.107167	2.535333
H	4.344976	2.127413	-2.368524
H	2.630224	1.687568	-2.037904
H	3.436938	2.962617	-1.075551
H	7.854200	-0.651493	-0.620024
H	7.638019	-1.590954	0.896719
H	7.028185	-2.234417	-0.653950
H	-1.687559	3.963831	-2.208859
H	-0.432216	4.073522	-0.940117
H	-0.467869	2.650068	-2.023209
H	-2.750940	0.278224	3.399838
H	-1.325256	-0.317256	2.476475
H	-1.239539	1.234454	3.357915
H	-6.400385	1.817301	0.837627
H	-6.116133	3.449769	0.154480
H	-6.161139	2.035032	-0.927443
H	2.236116	-2.265261	-0.215346
C	-2.617953	-2.449650	-0.599457
C	-2.954376	-3.331352	0.458422
C	-3.599864	-1.527584	-1.039561
C	-4.227156	-3.301289	1.046675
H	-2.197722	-4.046433	0.815423
C	-4.873135	-1.500141	-0.451430
H	-3.371704	-0.826164	-1.857111
C	-5.194623	-2.387084	0.592215
H	-4.467693	-4.000407	1.863596
H	-5.624361	-0.781942	-0.815756
H	-6.197930	-2.368189	1.047243

14e2-2

Ru	0.079657	0.468600	-1.401147
Cl	0.234259	2.758165	-0.989250
Cl	1.162148	-1.339852	-2.377836
C	-0.082662	-0.060496	0.451648
C	-1.596014	0.297463	-2.059731
H	-1.695233	0.630987	-3.125683
H	-2.512532	-0.097116	-1.580690
N	1.010283	-0.207016	1.283146
N	-1.204944	-0.243198	1.227568
C	0.624959	-0.326957	2.701746
C	-0.875739	-0.637954	2.612350
H	1.208243	-1.127624	3.200679
H	0.823662	0.627222	3.240675
H	-1.483821	-0.059500	3.337416
H	-1.098202	-1.718433	2.771118
C	2.404480	-0.205411	0.916290
C	-2.582248	-0.266255	0.823638
C	3.015678	-1.445585	0.581181
C	4.383375	-1.447826	0.252633
C	5.159367	-0.271262	0.267779
C	4.538288	0.924449	0.673642
C	3.173117	0.984407	1.023487
C	-3.355341	0.917710	0.941970
C	-4.717636	0.857177	0.590218
C	-5.322946	-0.333327	0.135982
C	-4.523468	-1.489283	0.036130
C	-3.154474	-1.483547	0.374552
C	2.233345	-2.737472	0.593127
H	4.858597	-2.405054	-0.020148
C	6.613715	-0.296599	-0.144922
H	5.136469	1.849101	0.735625
C	2.594186	2.271350	1.563025
C	-2.728294	2.210971	1.405319
H	-5.325183	1.774160	0.673885
C	-6.786706	-0.355926	-0.244850
H	-4.976170	-2.429496	-0.321222
C	-2.312963	-2.728746	0.212011
H	-3.481364	3.021288	1.457219
H	-2.271310	2.110823	2.413302
H	-1.915525	2.531569	0.718241
H	-2.913940	-3.562943	-0.199226
H	-1.457844	-2.548114	-0.473707
H	-1.883728	-3.073058	1.177583
H	-7.140073	-1.384523	-0.456488
H	-7.422006	0.065207	0.562653
H	-6.974411	0.257430	-1.152631
H	1.511384	-2.764427	-0.249635
H	2.910700	-3.607709	0.489697
H	1.656260	-2.864775	1.533333
H	3.255810	3.128102	1.328079
H	1.594997	2.492312	1.138990
H	2.500332	2.228907	2.671401
H	7.176030	0.560778	0.276574
H	7.114825	-1.232547	0.177231
H	6.710721	-0.242069	-1.251680

Precat-3

Ru	-0.505235	-0.351580	0.080933
Cl	-1.345768	-0.483848	2.348053
Cl	-0.286163	-0.436390	-2.358786
P	-1.245513	2.048194	-0.122352
N	-1.735340	-3.170943	0.065707
N	0.450033	-3.311478	0.279296
C	-0.581962	-2.428858	0.123697
C	-1.494305	-4.630811	0.126744
H	-1.767970	-5.101341	-0.843631
H	-2.124304	-5.093098	0.913828
C	0.002959	-4.716497	0.429248
H	0.217047	-5.070657	1.461651
H	0.555473	-5.375144	-0.272318
C	-3.108616	-2.770432	-0.125965
C	-3.978387	-2.718049	0.997938
C	-3.511916	-3.056425	2.394019
H	-4.176971	-2.600069	3.153755
H	-2.482573	-2.697615	2.583825
H	-3.544797	-4.157780	2.558621
C	-5.341150	-2.432790	0.773851
H	-6.013622	-2.369996	1.646110
C	-5.872875	-2.268773	-0.518431
C	-7.336083	-1.949376	-0.727622
H	-7.730353	-2.421807	-1.650692
H	-7.493587	-0.852909	-0.832703
H	-7.956548	-2.287363	0.126804
C	-4.998622	-2.416408	-1.613657
H	-5.400176	-2.349967	-2.638977
C	-3.623121	-2.675138	-1.450018
C	-2.748609	-2.899750	-2.659420
H	-3.339366	-2.811073	-3.592294
H	-2.294080	-3.914413	-2.650903
H	-1.909126	-2.171321	-2.703747
C	1.868188	-3.105502	0.392745
C	2.666858	-3.281593	-0.770163
C	2.030301	-3.471683	-2.127119
H	2.799829	-3.507051	-2.923052
H	1.317107	-2.651229	-2.361588
H	1.452192	-4.420494	-2.184638
C	4.064842	-3.274213	-0.622003
H	4.693183	-3.407378	-1.518605
C	4.681583	-3.099550	0.635039
C	6.187946	-3.136478	0.760766
H	6.583483	-4.149018	0.527054
H	6.520931	-2.875035	1.785009
H	6.669041	-2.431489	0.050697
C	3.857328	-2.914775	1.760882
H	4.321089	-2.769830	2.750926
C	2.449545	-2.933832	1.673545
C	1.599253	-2.819382	2.916543
H	1.172898	-3.806731	3.205041
H	0.745113	-2.125060	2.778256
H	2.201646	-2.463435	3.774835
H	2.158737	-0.494873	-1.652039
C	2.358962	-0.093714	-0.654010
C	3.569422	0.407508	-0.215635
C	1.319036	0.003344	0.383619
C	3.392204	0.846039	1.194230
C	2.037621	0.575533	1.579245
C	4.272578	1.470999	2.087654
C	1.619342	0.866117	2.883118
C	3.832943	1.768937	3.399063
H	5.293752	1.742538	1.781478
C	2.527167	1.450841	3.797242
H	0.588157	0.633062	3.181391
H	4.525253	2.252005	4.107361
H	2.194895	1.671195	4.824271
C	4.789748	0.512467	-1.033339
C	6.089717	0.413964	-0.470735
C	4.691818	0.697336	-2.439049
C	7.236739	0.499698	-1.276370
H	6.200057	0.231589	0.607758
C	5.838224	0.784695	-3.241076
H	3.695726	0.793853	-2.898103
C	7.118691	0.689350	-2.664439
H	8.233478	0.413801	-0.814180
H	5.732242	0.937043	-4.327188
H	8.019459	0.763917	-3.294176
C	-2.679173	2.211181	-1.375243
C	-2.324805	2.531220	-2.846288
C	-3.602702	0.973504	-1.333242
H	-3.244962	3.090417	-0.983779
C	-3.605406	2.776700	-3.671364
H	-1.756953	1.676740	-3.273894
H	-1.675108	3.427472	-2.917752
C	-4.890512	1.215371	-2.142042
H	-3.046734	0.117959	-1.774519
H	-3.853074	0.679249	-0.292929
C	-4.576353	1.587701	-3.599876
H	-3.331068	2.992150	-4.727203
H	-4.117034	3.691709	-3.290673
H	-5.532383	0.310178	-2.100835
H	-5.475144	2.037694	-1.666287
H	-5.511631	1.815334	-4.156976
H	-4.114453	0.710033	-4.106957
C	-0.040573	3.387979	-0.771664
C	0.789016	4.138774	0.293421
C	0.892619	2.861072	-1.882229
H	-0.741067	4.132693	-1.221375
C	1.625967	5.268607	-0.343000
H	1.464317	3.421808	0.811883
H	0.134582	4.584314	1.067657
C	1.706780	3.998698	-2.526921
H	1.591474	2.126973	-1.428605
H	0.332989	2.292542	-2.648291
C	2.528304	4.763839	-1.478029
H	2.229882	5.767885	0.445833
H	0.934994	6.046899	-0.743576
H	2.370853	3.581885	-3.314945
H	1.016650	4.705593	-3.044972
H	3.074924	5.611814	-1.945675
H	3.303891	4.084719	-1.056363
C	-2.044241	2.962607	1.361889
C	-3.498223	2.545721	1.691613
C	-1.216443	2.930767	2.667686
H	-2.077882	4.016403	0.986991
C	-4.111217	3.466579	2.767634
H	-3.493343	1.493283	2.051209
H	-4.146539	2.581078	0.793768
C	-1.806662	3.882602	3.724960
H	-1.242742	1.891291	3.052560
H	-0.151477	3.169376	2.489101
C	-3.264255	3.517409	4.048338
H	-5.146053	3.129942	2.996874
H	-4.205581	4.496699	2.350739
H	-1.184189	3.851337	4.645656
H	-1.760905	4.934035	3.354024
H	-3.700713	4.237436	4.774905
H	-3.286742	2.519016	4.541552

14e1-3

Ru	1.022871	0.842987	-0.228882
Cl	1.569718	1.142018	-2.476424
Cl	1.452099	1.638930	1.902667
N	2.775284	-1.436085	-0.203115
N	0.731664	-2.174340	-0.648227
C	1.450923	-1.054744	-0.303868
C	2.989858	-2.868818	-0.471804
H	3.352489	-3.384460	0.445755
H	3.758998	-3.009615	-1.259742
C	1.596161	-3.345223	-0.912632
H	1.556825	-3.605670	-1.993357
H	1.239303	-4.230076	-0.344762
C	3.861022	-0.653390	0.333316
C	4.820200	-0.080475	-0.544688
C	4.761213	-0.289702	-2.039077
H	5.466754	0.387719	-2.558990
H	3.744787	-0.104975	-2.441160
H	5.049706	-1.330103	-2.310289
C	5.879809	0.656523	0.023493
H	6.617158	1.121491	-0.652302
C	6.032577	0.803504	1.414951
C	7.150143	1.640889	1.994072
H	7.522330	1.222494	2.951678
H	6.797706	2.674259	2.207086
H	8.006716	1.724207	1.295124
C	5.106322	0.153850	2.255564
H	5.228401	0.222020	3.349528
C	4.025071	-0.586190	1.744650
C	3.076204	-1.294726	2.682183
H	3.447660	-1.250858	3.724496
H	2.945652	-2.364515	2.413904
H	2.075627	-0.816110	2.659809
C	-0.687625	-2.378120	-0.753736
C	-1.367718	-2.914529	0.371583
C	-0.651522	-3.134933	1.685940
H	-1.358458	-3.468700	2.470439
H	-0.153379	-2.208673	2.042574
H	0.142229	-3.909565	1.607013
C	-2.737997	-3.215334	0.247946
H	-3.273626	-3.621206	1.122360
C	-3.441123	-3.000440	-0.953893
C	-4.922882	-3.283365	-1.053219
H	-5.197417	-3.679893	-2.052253
H	-5.512009	-2.353376	-0.896669
H	-5.253739	-4.013457	-0.287502
C	-2.727258	-2.490925	-2.056396
H	-3.254696	-2.331120	-3.011912
C	-1.352755	-2.185500	-1.991354
C	-0.621655	-1.687199	-3.213718
H	0.187625	-2.386040	-3.519127
H	-0.136324	-0.705275	-3.035917
H	-1.313161	-1.585465	-4.072650
H	-1.785848	-0.606239	0.975950
C	-1.894438	0.363508	0.482960
C	-3.057256	1.122563	0.480492
C	-0.834748	1.050177	-0.232298
C	-2.794049	2.365861	-0.288182
C	-1.433252	2.325352	-0.734096
C	-3.592278	3.482528	-0.565915
C	-0.903676	3.378977	-1.491540
C	-3.046248	4.548117	-1.320915
H	-4.626529	3.547379	-0.194850
C	-1.723415	4.493945	-1.785052
H	0.131604	3.335288	-1.862678
H	-3.670323	5.428147	-1.544305
H	-1.313801	5.327133	-2.377472
C	-4.317829	0.762750	1.149240
C	-5.577786	1.043101	0.557573
C	-4.304523	0.100130	2.404776
C	-6.772237	0.673046	1.195766
H	-5.615782	1.524148	-0.431434
C	-5.499492	-0.261131	3.043341
H	-3.337356	-0.100676	2.891546
C	-6.740140	0.023722	2.442859
H	-7.738011	0.892171	0.712548
H	-5.463987	-0.760819	4.024781
H	-7.678562	-0.256933	2.946936

Cl1-3

Ru	0.984728	0.774422	0.492340
Cl	1.797942	1.586051	-1.650022
Cl	0.547236	-0.632166	2.466229
N	2.762550	-1.505108	-0.409914
N	0.685103	-2.051037	-0.911857
C	1.465638	-1.084431	-0.368694
C	2.898939	-2.878815	-0.945453
H	3.224630	-3.570078	-0.137522
H	3.664118	-2.907314	-1.747389
C	1.481438	-3.181677	-1.453339
H	1.409749	-3.186502	-2.563130
H	1.081732	-4.147585	-1.084787
C	3.942347	-0.778725	0.001966
C	4.709627	-0.093522	-0.981292
C	4.413518	-0.196310	-2.459588
H	4.698099	0.735936	-2.985767
H	3.342962	-0.375598	-2.662499
H	5.010501	-1.021334	-2.911214
C	5.842944	0.627906	-0.558086
H	6.423967	1.181799	-1.314665
C	6.260092	0.652902	0.786332
C	7.446665	1.484000	1.218907
H	7.923481	1.074919	2.132488
H	7.135830	2.526747	1.450688
H	8.216612	1.545304	0.422882
C	5.541868	-0.128643	1.711635
H	5.890271	-0.185219	2.756642
C	4.401640	-0.874102	1.346692
C	3.765261	-1.804999	2.350051
H	4.266469	-1.718158	3.334015
H	3.862303	-2.864339	2.024886
H	2.683002	-1.598115	2.491450
C	-0.742173	-2.086627	-1.111893
C	-1.534050	-2.867861	-0.227436
C	-0.929700	-3.574559	0.963742
H	-1.720806	-4.028401	1.592261
H	-0.340023	-2.872158	1.591259
H	-0.247097	-4.397922	0.656114
C	-2.911905	-2.976497	-0.493376
H	-3.534376	-3.574711	0.193149
C	-3.514259	-2.348220	-1.602112
C	-5.001498	-2.472113	-1.843564
H	-5.281094	-2.133704	-2.861301
H	-5.572633	-1.856235	-1.114874
H	-5.347299	-3.519834	-1.720778
C	-2.691073	-1.606398	-2.469513
H	-3.136319	-1.123995	-3.355679
C	-1.302789	-1.472577	-2.260956
C	-0.452283	-0.725801	-3.259757
H	0.297270	-1.396226	-3.735386
H	0.119230	0.104899	-2.793610
H	-1.078514	-0.305309	-4.070505
H	-1.775019	-0.494250	1.537766
C	-1.938788	0.362907	0.878726
C	-3.162864	0.942229	0.604004
C	-0.850628	1.052593	0.175717
C	-2.931895	2.072566	-0.335843
C	-1.529318	2.130335	-0.628503
C	-3.808414	3.031565	-0.855474
C	-1.043532	3.129880	-1.481614
C	-3.304595	4.034109	-1.719514
H	-4.875195	3.029472	-0.585485
C	-1.941438	4.074058	-2.036661
H	0.027353	3.162593	-1.729800
H	-3.992224	4.786944	-2.137254
H	-1.555651	4.851902	-2.714653
C	-4.451725	0.520688	1.175825
C	-5.666332	0.618473	0.446679
C	-4.506415	-0.024221	2.486596
C	-6.881317	0.190281	1.005677
H	-5.649417	1.001365	-0.584224
C	-5.720985	-0.448339	3.042877
H	-3.579815	-0.087495	3.077951
C	-6.916130	-0.341573	2.306698
H	-7.809501	0.269655	0.417099
H	-5.737988	-0.857537	4.065737
H	-7.871013	-0.669714	2.747220
C	1.508990	2.896291	0.982561
C	1.209076	2.226349	2.174353
H	0.776030	3.561564	0.499132
H	2.553129	3.030442	0.655521
H	0.232711	2.332782	2.672774
H	2.011279	1.811082	2.807167

TS1-3

Ru	0.904381	-0.580165	0.615944
Cl	1.719103	0.909044	2.331305
Cl	0.664628	-2.293211	-1.104801
N	2.899676	0.630683	-1.339296
N	0.858972	1.394553	-1.710944
C	1.609723	0.604114	-0.899597
C	3.040171	1.381793	-2.608651
H	3.244151	0.678071	-3.445152
H	3.888702	2.093831	-2.547194
C	1.673836	2.074681	-2.744800
H	1.718713	3.166856	-2.534519
H	1.218389	1.942380	-3.747282
C	4.058206	0.032692	-0.717166
C	4.785987	0.800454	0.234177
C	4.385072	2.212006	0.586877
H	5.172050	2.703200	1.192021
H	3.442822	2.213509	1.175876
H	4.214784	2.833371	-0.317817
C	5.921078	0.218253	0.830898
H	6.480338	0.804514	1.579281
C	6.366881	-1.074201	0.491645
C	7.557349	-1.694492	1.188111
H	8.074337	-2.431280	0.540530
H	7.240986	-2.233221	2.108648
H	8.295651	-0.927634	1.499532
C	5.671019	-1.768890	-0.516149
H	6.032680	-2.760415	-0.836854
C	4.531539	-1.234986	-1.152848
C	3.897696	-1.976792	-2.304760
H	4.283617	-3.013555	-2.363270
H	4.140174	-1.485741	-3.273808
H	2.792950	-2.026089	-2.209156
C	-0.523755	1.765691	-1.549429
C	-1.506982	1.127076	-2.345938
C	-1.144548	0.010137	-3.294867
H	-2.051457	-0.418498	-3.764357
H	-0.598405	-0.804024	-2.769851
H	-0.484436	0.366208	-4.116492
C	-2.841741	1.567069	-2.226062
H	-3.616247	1.070481	-2.834086
C	-3.209755	2.615770	-1.362312
C	-4.647215	3.072440	-1.246932
H	-4.742683	4.163730	-1.431522
H	-5.043108	2.886367	-0.225129
H	-5.303845	2.546961	-1.968517
C	-2.199853	3.236647	-0.599303
H	-2.465532	4.062651	0.081460
C	-0.852827	2.837390	-0.676665
C	0.202164	3.530507	0.152958
H	1.041723	3.907383	-0.470067
H	0.648749	2.843212	0.905185
H	-0.228205	4.397028	0.691795
H	-1.678130	-2.262767	-0.397770
C	-1.971558	-1.481160	0.311292
C	-3.260182	-1.097579	0.606040
C	-0.983363	-0.628295	1.008741
C	-3.195921	0.011927	1.593823
C	-1.819728	0.301338	1.858895
C	-4.213186	0.685617	2.280965
C	-1.487382	1.285451	2.796300
C	-3.864955	1.678098	3.226852
H	-5.271265	0.435921	2.109398
C	-2.518272	1.974346	3.478118
H	-0.429330	1.508681	2.997679
H	-4.659440	2.213051	3.771738
H	-2.253193	2.745540	4.218768
C	-4.481101	-1.696155	0.037412
C	-5.621030	-0.911299	-0.274549
C	-4.532167	-3.086777	-0.241715
C	-6.764757	-1.495352	-0.842002
H	-5.592190	0.174964	-0.104113
C	-5.677482	-3.668665	-0.802983
H	-3.662644	-3.714658	0.007569
C	-6.800785	-2.876089	-1.104302
H	-7.634791	-0.864728	-1.085829
H	-5.697000	-4.752073	-1.002097
H	-7.701528	-3.334352	-1.542709
C	1.476697	-2.188557	1.881498
C	0.141828	-1.961656	2.343118
H	2.306835	-1.782520	2.486523
H	1.686333	-3.082552	1.270154
H	-0.017681	-1.356323	3.249099
H	-0.623807	-2.721354	2.121722

MCy-3

Ru	0.870832	-0.747401	-0.047788
Cl	1.336281	-0.940587	2.307818
Cl	0.753512	-0.610513	-2.465335
N	2.913465	1.480522	-0.041241
N	0.863558	2.247677	0.297111
C	1.602548	1.134124	0.066209
C	3.110857	2.945888	0.066522
H	3.480616	3.350780	-0.900660
H	3.871087	3.175962	0.841007
C	1.705876	3.459911	0.429712
H	1.646414	3.849222	1.469114
H	1.341848	4.256385	-0.251836
C	4.048658	0.621560	-0.295248
C	4.810933	0.142487	0.805563
C	4.482138	0.521762	2.228885
H	5.201660	0.059683	2.932802
H	3.458317	0.191660	2.508291
H	4.532107	1.622424	2.379645
C	5.924001	-0.677780	0.532879
H	6.510671	-1.064725	1.383037
C	6.316954	-1.000348	-0.780657
C	7.485620	-1.924148	-1.040061
H	7.992206	-1.687080	-1.997696
H	7.147021	-2.982003	-1.104369
H	8.238191	-1.872990	-0.227149
C	5.589054	-0.434473	-1.844927
H	5.910403	-0.626955	-2.882409
C	4.466778	0.392450	-1.634807
C	3.767204	1.024456	-2.812828
H	4.331173	0.838868	-3.747746
H	3.667670	2.124564	-2.695025
H	2.741230	0.612745	-2.934615
C	-0.566089	2.358828	0.465254
C	-1.369548	2.603586	-0.679864
C	-0.779895	2.637995	-2.069033
H	-1.537294	2.961251	-2.809421
H	-0.396573	1.639164	-2.374612
H	0.079068	3.339914	-2.135673
C	-2.747021	2.834791	-0.484841
H	-3.379534	3.021129	-1.368359
C	-3.328425	2.855428	0.796698
C	-4.797937	3.157991	0.989129
H	-4.941829	4.147479	1.475659
H	-5.284255	2.407867	1.647866
H	-5.342886	3.174737	0.024816
C	-2.495457	2.621171	1.909023
H	-2.929518	2.635555	2.922883
C	-1.114795	2.380718	1.777219
C	-0.260050	2.175901	3.004482
H	0.473871	3.000939	3.140526
H	0.313570	1.225445	2.947210
H	-0.888360	2.145598	3.916002
H	-1.559955	-1.356234	-2.032679
C	-1.873600	-1.503690	-0.992996
C	-3.149514	-1.359527	-0.498726
C	-0.903895	-1.813039	0.088135
C	-3.114720	-1.657974	0.954944
C	-1.767614	-1.960092	1.321960
C	-4.154411	-1.792477	1.889117
C	-1.484235	-2.422437	2.613752
C	-3.852222	-2.225281	3.197585
H	-5.199148	-1.602188	1.600738
C	-2.531892	-2.544036	3.552804
H	-0.452658	-2.664210	2.904354
H	-4.662460	-2.332063	3.936750
H	-2.305957	-2.897336	4.571444
C	-4.341765	-1.022946	-1.300437
C	-5.394870	-0.230938	-0.776292
C	-4.455312	-1.474020	-2.641260
C	-6.512157	0.097548	-1.561155
H	-5.317952	0.158094	0.249349
C	-5.571918	-1.146277	-3.423414
H	-3.659142	-2.108017	-3.061489
C	-6.608271	-0.359617	-2.886988
H	-7.314313	0.720117	-1.132922
H	-5.638790	-1.515211	-4.459497
H	-7.487949	-0.106569	-3.499999
C	1.731196	-2.507617	-0.277479
C	0.217703	-2.931851	-0.194806
H	2.338210	-2.848184	0.582551
H	2.179730	-2.684244	-1.273116
H	0.114123	-3.640473	0.647731
H	-0.056301	-3.382311	-1.167424

TS2-3

Ru	-0.755197	0.556981	-0.327519
Cl	-0.691165	1.384512	1.931417
Cl	-0.779183	-0.319260	-2.599749
N	-2.930136	-1.424579	0.442209
N	-0.915249	-2.235570	0.848093
C	-1.592421	-1.159711	0.363542
C	-3.213056	-2.739243	1.063071
H	-3.857142	-3.351839	0.397764
H	-3.758650	-2.598341	2.021446
C	-1.810087	-3.339962	1.260703
H	-1.605401	-3.629802	2.312457
H	-1.629105	-4.233417	0.624338
C	-4.038607	-0.591683	0.055332
C	-4.627066	0.278425	1.013477
C	-4.086777	0.385970	2.418120
H	-4.667452	1.121642	3.008332
H	-3.017522	0.695768	2.422913
H	-4.144463	-0.586648	2.953808
C	-5.746662	1.039628	0.617573
H	-6.203141	1.723584	1.352797
C	-6.304469	0.940734	-0.671719
C	-7.486122	1.791715	-1.080637
H	-8.196471	1.225657	-1.717760
H	-7.155563	2.674082	-1.671919
H	-8.040486	2.174967	-0.200580
C	-5.724843	0.028785	-1.577314
H	-6.163381	-0.087726	-2.582804
C	-4.603837	-0.754514	-1.239785
C	-4.025595	-1.731151	-2.233536
H	-4.648148	-1.778295	-3.148362
H	-3.963563	-2.758845	-1.815787
H	-2.992305	-1.436443	-2.524321
C	0.512933	-2.433544	0.913804
C	1.179937	-3.041611	-0.186438
C	0.448510	-3.418685	-1.451933
H	1.119437	-3.965687	-2.142844
H	0.058202	-2.521380	-1.981382
H	-0.424664	-4.074831	-1.246191
C	2.555335	-3.314094	-0.056963
H	3.080043	-3.781353	-0.907170
C	3.270065	-3.031525	1.124423
C	4.746951	-3.337563	1.222448
H	5.107329	-3.289013	2.269492
H	5.339583	-2.609448	0.627175
H	4.979935	-4.346901	0.823306
C	2.566703	-2.466551	2.204630
H	3.099702	-2.261654	3.148167
C	1.189327	-2.172290	2.135397
C	0.469667	-1.622069	3.342107
H	-0.379963	-2.270203	3.649053
H	0.050567	-0.613562	3.132025
H	1.157300	-1.543760	4.206721
H	1.706762	0.580959	-2.259271
C	1.919782	1.256518	-1.421121
C	3.129123	1.414915	-0.769542
C	0.904108	2.147896	-0.825922
C	2.960510	2.452324	0.279741
C	1.604762	2.893504	0.257710
C	3.883429	3.072942	1.139127
C	1.170963	3.926911	1.094881
C	3.438899	4.106736	1.989372
H	4.945350	2.785111	1.134879
C	2.097476	4.528949	1.970962
H	0.123016	4.262149	1.081415
H	4.155863	4.596075	2.667985
H	1.767189	5.336438	2.643222
C	4.387404	0.728658	-1.118195
C	5.341197	0.373283	-0.130198
C	4.679180	0.406894	-2.469260
C	6.539967	-0.268655	-0.482328
H	5.122575	0.573083	0.929257
C	5.874431	-0.237964	-2.818344
H	3.962200	0.693760	-3.254174
C	6.814752	-0.574619	-1.827080
H	7.266721	-0.533213	0.302689
H	6.080497	-0.468820	-3.875822
H	7.758915	-1.070943	-2.102377
C	-2.193909	1.647006	-0.695086
C	-0.292998	2.575756	-1.461851
H	-2.582372	2.369393	0.057495
H	-2.730642	1.614076	-1.669769
H	-0.738445	3.520713	-1.109722
H	-0.473789	2.296551	-2.511124

Cl2-3

Ru	0.561910	-0.001961	-0.886881
Cl	-0.191904	-1.237147	1.055710
Cl	1.788145	1.288899	-2.586104
N	2.842971	0.970480	1.027946
N	1.155097	2.380421	0.801370
C	1.638867	1.163730	0.432528
C	3.280024	2.163930	1.794634
H	4.156568	2.629881	1.294105
H	3.589781	1.872906	2.818879
C	2.034453	3.067842	1.773890
H	1.530058	3.131745	2.763250
H	2.255053	4.101326	1.438174
C	3.706083	-0.184826	0.991645
C	3.603940	-1.144031	2.036287
C	2.599105	-0.996347	3.152056
H	2.718238	-1.805136	3.899165
H	1.562303	-1.035270	2.752340
H	2.713009	-0.028557	3.687038
C	4.484406	-2.243194	2.013789
H	4.403217	-2.996836	2.814988
C	5.464655	-2.401345	1.014081
C	6.364710	-3.616339	0.994020
H	7.329269	-3.405031	0.489737
H	5.885002	-4.456304	0.444493
H	6.581338	-3.982185	2.018385
C	5.575978	-1.397355	0.033037
H	6.361203	-1.478073	-0.737414
C	4.725979	-0.272551	0.006244
C	4.936243	0.812425	-1.022394
H	5.710316	0.512320	-1.755577
H	5.287098	1.755272	-0.546752
H	4.002461	1.052527	-1.575740
C	-0.112051	2.955673	0.411855
C	-0.140847	3.929213	-0.628028
C	1.118369	4.405367	-1.309908
H	0.878049	5.124636	-2.116941
H	1.678650	3.555212	-1.754030
H	1.794199	4.925895	-0.596153
C	-1.386590	4.480661	-0.984081
H	-1.416774	5.223311	-1.799006
C	-2.581367	4.132883	-0.321182
C	-3.906084	4.717687	-0.756540
H	-4.668442	4.649647	0.045084
H	-4.307208	4.176173	-1.641501
H	-3.805698	5.782789	-1.050420
C	-2.499441	3.236298	0.760505
H	-3.410552	2.993153	1.332265
C	-1.280006	2.650791	1.165214
C	-1.243636	1.764188	2.384779
H	-0.421048	2.047743	3.074407
H	-1.076127	0.698068	2.110832
H	-2.195866	1.834013	2.945118
H	-2.807428	0.725685	-0.681619
C	-2.619510	-0.334940	-0.899575
C	-3.298274	-1.406098	-0.353481
C	-1.539410	-0.806989	-1.771503
C	-2.706071	-2.651838	-0.897842
C	-1.632838	-2.291857	-1.765975
C	-3.074701	-4.001896	-0.761189
C	-0.928088	-3.268600	-2.479088
C	-2.355322	-4.981434	-1.473739
H	-3.922350	-4.294814	-0.122892
C	-1.291682	-4.621320	-2.324554
H	-0.097785	-2.989340	-3.148614
H	-2.634035	-6.042370	-1.369634
H	-0.744175	-5.401133	-2.877373
C	-4.423392	-1.319205	0.595829
C	-4.537084	-2.219884	1.685493
C	-5.408235	-0.307512	0.461512
C	-5.591877	-2.107644	2.605310
H	-3.763408	-2.988928	1.830824
C	-6.462819	-0.198666	1.380675
H	-5.350013	0.384065	-0.393901
C	-6.561111	-1.099581	2.456879
H	-5.653206	-2.811142	3.451275
H	-7.221904	0.589631	1.250357
H	-7.391622	-1.017226	3.176060
C	1.764793	-1.335748	-1.164281
C	-0.777365	-0.001237	-2.643305
H	1.732309	-2.266240	-0.558222
H	2.525012	-1.252971	-1.971037
H	-0.236895	-0.444364	-3.493161
H	-1.054065	1.058582	-2.774089

14e2-3

Ru	0.079657	0.468600	-1.401147
Cl	0.234259	2.758165	-0.989250
Cl	1.162148	-1.339852	-2.377836
C	-0.082662	-0.060496	0.451648
C	-1.596014	0.297463	-2.059731
H	-1.695233	0.630987	-3.125683
H	-2.512532	-0.097116	-1.580690
N	1.010283	-0.207016	1.283146
N	-1.204944	-0.243198	1.227568
C	0.624959	-0.326957	2.701746
C	-0.875739	-0.637954	2.612350
H	1.208243	-1.127624	3.200679
H	0.823662	0.627222	3.240675
H	-1.483821	-0.059500	3.337416
H	-1.098202	-1.718433	2.771118
C	2.404480	-0.205411	0.916290
C	-2.582248	-0.266255	0.823638
C	3.015678	-1.445585	0.581181
C	4.383375	-1.447826	0.252633
C	5.159367	-0.271262	0.267779
C	4.538288	0.924449	0.673642
C	3.173117	0.984407	1.023487
C	-3.355341	0.917710	0.941970
C	-4.717636	0.857177	0.590218
C	-5.322946	-0.333327	0.135982
C	-4.523468	-1.489283	0.036130
C	-3.154474	-1.483547	0.374552
C	2.233345	-2.737472	0.593127
H	4.858597	-2.405054	-0.020148
C	6.613715	-0.296599	-0.144922
H	5.136469	1.849101	0.735625
C	2.594186	2.271350	1.563025
C	-2.728294	2.210971	1.405319
H	-5.325183	1.774160	0.673885
C	-6.786706	-0.355926	-0.244850
H	-4.976170	-2.429496	-0.321222
C	-2.312963	-2.728746	0.212011
H	-3.481364	3.021288	1.457219
H	-2.271310	2.110823	2.413302
H	-1.915525	2.531569	0.718241
H	-2.913940	-3.562943	-0.199226
H	-1.457844	-2.548114	-0.473707
H	-1.883728	-3.073058	1.177583
H	-7.140073	-1.384523	-0.456488
H	-7.422006	0.065207	0.562653
H	-6.974411	0.257430	-1.152631
H	1.511384	-2.764427	-0.249635
H	2.910700	-3.607709	0.489697
H	1.656260	-2.864775	1.533333
H	3.255810	3.128102	1.328079
H	1.594997	2.492312	1.138990
H	2.500332	2.228907	2.671401
H	7.176030	0.560778	0.276574
H	7.114825	-1.232547	0.177231
H	6.710721	-0.242069	-1.251680

Precat-4

Ru	0.347501	-0.017140	-0.038060
Cl	0.112775	-0.179671	-2.438878
C	1.273525	-1.866687	-0.184607
N	2.580466	-2.147701	-0.469928
N	0.582295	-3.041555	-0.192746
C	2.765672	-3.570416	-0.865994
C	1.466323	-4.217066	-0.395912
C	3.790293	-1.375153	-0.373599
C	-0.804053	-3.329817	0.097113
C	4.531900	-1.475586	0.837750
C	5.828264	-0.926294	0.877735
C	6.400146	-0.272022	-0.236240
C	5.632288	-0.183230	-1.413653
C	4.344026	-0.755206	-1.524465
H	6.411829	-1.015747	1.809602
H	6.066633	0.304254	-2.302934
C	-1.647186	-3.717999	-0.983205
C	-2.936730	-4.192528	-0.681488
C	-3.413926	-4.287625	0.642516
C	-2.540528	-3.925768	1.685152
C	-1.221099	-3.484337	1.448063
H	-3.588254	-4.509807	-1.512675
H	-2.875739	-4.037614	2.729612
H	1.573445	-4.771115	0.563441
H	3.669503	-3.993059	-0.385074
Cl	0.650150	0.074616	2.364648
C	1.690553	1.190813	-0.279860
H	2.034331	1.402311	-1.319766
H	2.901648	-3.631054	-1.968146
H	1.026402	-4.908531	-1.139783
P	2.586710	2.289316	0.897323
C	3.616698	3.361200	-0.173768
H	4.185647	4.083438	0.445179
H	4.327022	2.727908	-0.742848
H	2.975159	3.917072	-0.886286
C	3.732626	1.535855	2.092295
H	4.228802	2.358254	2.647293
H	3.152176	0.894839	2.781373
H	4.487287	0.928877	1.557539
C	1.506402	3.391271	1.865173
H	0.911462	4.028756	1.186105
H	0.835688	2.755268	2.473762
H	2.137811	4.026932	2.518239
C	-0.285483	-3.266425	2.611950
H	-0.018785	-2.196530	2.739638
H	-0.745037	-3.623261	3.553771
H	0.669158	-3.817422	2.476406
C	-4.806542	-4.802444	0.925233
H	-5.575439	-4.201306	0.395549
H	-4.924058	-5.849953	0.574164
H	-5.041738	-4.780451	2.007230
C	-1.174036	-3.666442	-2.417681
H	-0.502580	-4.520905	-2.658127
H	-2.030199	-3.734054	-3.116729
H	-0.615895	-2.732502	-2.635267
C	3.641411	-0.770834	-2.860369
H	3.974611	0.074064	-3.495675
H	3.895428	-1.699681	-3.418780
H	2.537467	-0.730309	-2.768444
C	7.810428	0.268735	-0.176220
H	8.549204	-0.549753	-0.320542
H	7.998591	1.021825	-0.966800
H	8.034449	0.730493	0.807041
C	3.944289	-2.153142	2.053871
H	4.626569	-2.074840	2.922332
H	2.965224	-1.707359	2.332305
H	3.763728	-3.235525	1.877010
P	-1.784469	1.409866	-0.093107
C	-2.815659	1.587362	1.500648
C	-3.524411	0.285393	1.943790
C	-2.066084	2.201066	2.705083
H	-3.608689	2.304143	1.172744
C	-4.467256	0.538425	3.139161
H	-2.757389	-0.470917	2.225169
H	-4.115696	-0.149343	1.115058
C	-3.025684	2.477559	3.879772
H	-1.282272	1.485222	3.027952
H	-1.546921	3.136449	2.422787
C	-3.747165	1.196587	4.324651
H	-4.934217	-0.421774	3.446460
H	-5.303285	1.195463	2.805469
H	-2.456152	2.919098	4.725603
H	-3.777533	3.243509	3.578125
H	-4.466745	1.416042	5.141957
H	-3.001147	0.484816	4.745830
C	-3.126499	0.733275	-1.288846
C	-3.106745	1.235204	-2.754547
C	-3.237917	-0.805091	-1.306212
H	-4.046383	1.147522	-0.807370
C	-4.391650	0.804608	-3.492306
H	-2.215616	0.812330	-3.263829
H	-3.023481	2.338421	-2.824649
C	-4.530820	-1.247944	-2.020459
H	-2.356636	-1.199115	-1.852826
H	-3.197416	-1.241999	-0.288608
C	-4.592042	-0.717033	-3.460831
H	-4.351466	1.172101	-4.540100
H	-5.270080	1.304140	-3.021868
H	-4.599683	-2.355703	-2.008947
H	-5.413356	-0.877773	-1.448330
H	-5.556291	-0.992436	-3.939096
H	-3.792226	-1.203147	-4.064416
C	-1.671073	3.213286	-0.750041
C	-1.804189	4.398712	0.230557
C	-0.495288	3.418427	-1.724409
H	-2.601840	3.243434	-1.356833
C	-1.928251	5.727180	-0.547131
H	-0.922147	4.461563	0.902678
H	-2.689726	4.277037	0.886052
C	-0.599854	4.760307	-2.474815
H	0.454066	3.393923	-1.140202
H	-0.425680	2.572651	-2.439409
C	-0.751057	5.946288	-1.509647
H	-2.009901	6.568834	0.173386
H	-2.880464	5.722653	-1.125266
H	0.287451	4.893065	-3.130450
H	-1.480233	4.726548	-3.156305
H	-0.883166	6.894041	-2.073467
H	0.188339	6.068055	-0.920231

14e1-4

Ru	-0.265975	0.905966	-0.004350
Cl	-1.066158	1.406003	-2.096243
C	-0.358470	-1.052595	0.009870
N	0.621903	-2.002628	0.011467
N	-1.571117	-1.675514	0.043144
C	0.065546	-3.378966	0.002337
C	-1.453375	-3.147627	0.121458
C	2.049502	-1.841373	-0.007876
C	-2.867541	-1.040477	0.027222
C	2.751590	-1.768550	1.223661
C	4.156031	-1.654795	1.178574
C	4.868707	-1.629806	-0.039099
C	4.133428	-1.706819	-1.241447
C	2.728162	-1.820572	-1.255144
H	4.711945	-1.599434	2.129532
H	4.671320	-1.689934	-2.204192
C	-3.527087	-0.850643	-1.220738
C	-4.792201	-0.236685	-1.212475
C	-5.430608	0.155911	-0.017332
C	-4.782685	-0.123057	1.201130
C	-3.516099	-0.738931	1.256478
H	-5.302727	-0.069827	-2.175561
H	-5.285804	0.130202	2.149063
H	-1.871701	-3.511026	1.084519
H	0.483661	-3.964094	0.847058
Cl	-0.689627	1.314128	2.223300
C	1.536088	1.183004	-0.145957
H	2.331024	0.417703	-0.270503
H	0.351303	-3.897961	-0.937533
H	-2.029914	-3.621785	-0.699124
P	2.166712	2.881556	-0.053768
C	3.258000	3.215850	-1.479970
H	3.681359	4.238416	-1.409269
H	4.082607	2.475457	-1.490279
H	2.673373	3.119492	-2.416710
C	3.139497	3.073267	1.479651
H	3.553155	4.099747	1.550098
H	2.477398	2.874895	2.346361
H	3.967602	2.336872	1.481005
C	0.810502	4.095726	-0.045237
H	0.206996	3.978035	-0.968534
H	0.165184	3.913395	0.839021
H	1.224188	5.122905	0.004959
C	-2.950058	-1.141890	2.598838
H	-1.856650	-1.301945	2.576603
H	-3.159521	-0.373068	3.368343
H	-3.430780	-2.083654	2.945354
C	-6.770822	0.851937	-0.049583
H	-6.645974	1.935342	-0.267536
H	-7.426818	0.437824	-0.842015
H	-7.301025	0.769534	0.919646
C	-2.953309	-1.361513	-2.522778
H	-3.340754	-2.382315	-2.738875
H	-3.254870	-0.717986	-3.372059
H	-1.848810	-1.411798	-2.514177
C	1.969668	-1.883153	-2.561190
H	2.652685	-1.763313	-3.424000
H	1.448155	-2.855819	-2.690606
H	1.193589	-1.091168	-2.621946
C	6.378879	-1.570252	-0.054932
H	6.809012	-2.595804	-0.045628
H	6.763758	-1.068613	-0.965448
H	6.781966	-1.044266	0.833638
C	2.017516	-1.791633	2.544328
H	2.722139	-1.698252	3.392950
H	1.276957	-0.967254	2.616341
H	1.455881	-2.739762	2.686430

Cl1-4

Ru	-0.552668	0.896857	-0.342176
Cl	-0.780459	0.132473	-2.635271
C	-0.301161	-1.134827	0.030337
N	0.752941	-1.977032	0.071221
N	-1.451153	-1.826667	0.190546
C	0.295890	-3.396816	0.145240
C	-1.214048	-3.270030	0.423663
C	2.173182	-1.720080	0.073667
C	-2.757831	-1.217242	0.267255
C	2.839492	-1.678487	1.329191
C	4.244267	-1.564500	1.331416
C	4.994878	-1.493270	0.138791
C	4.296328	-1.544900	-1.084551
C	2.893214	-1.687741	-1.149913
H	4.768723	-1.537072	2.301222
H	4.863274	-1.514032	-2.030147
C	-3.629413	-1.295551	-0.862420
C	-4.879029	-0.659390	-0.772220
C	-5.309923	0.000599	0.401891
C	-4.464163	-0.030960	1.525392
C	-3.198385	-0.657626	1.500368
H	-5.551301	-0.696301	-1.645631
H	-4.809382	0.418156	2.471695
H	-1.490372	-3.534557	1.467740
H	0.845833	-3.934209	0.942784
Cl	0.077879	1.305302	1.977068
C	1.021642	1.644683	-0.902118
H	1.270968	1.536781	-1.982743
H	0.514559	-3.900623	-0.820198
H	-1.833770	-3.880444	-0.262479
P	2.243335	2.701760	-0.055917
C	3.321209	3.308849	-1.405554
H	4.092812	3.993775	-1.000242
H	3.820075	2.447481	-1.893330
H	2.714967	3.848533	-2.160431
C	3.329692	1.862670	1.137100
H	4.132151	2.564992	1.442023
H	2.721784	1.555194	2.007896
H	3.770284	0.963057	0.663461
C	1.517494	4.177050	0.735666
H	0.923382	4.745234	-0.006886
H	0.872252	3.843802	1.571578
H	2.336280	4.819340	1.118881
C	-2.430558	-0.795663	2.794467
H	-1.426601	-1.235695	2.660232
H	-2.289935	0.184831	3.291137
H	-3.003530	-1.440362	3.495116
C	-6.659920	0.675999	0.449235
H	-6.727605	1.489559	-0.304011
H	-7.473273	-0.042410	0.213395
H	-6.868689	1.113890	1.444507
C	-3.278833	-2.099088	-2.091157
H	-3.599047	-3.157229	-1.960386
H	-3.807590	-1.712252	-2.983806
H	-2.194876	-2.080404	-2.307470
C	2.214115	-1.867360	-2.486546
H	2.897924	-1.600499	-3.315860
H	1.927947	-2.931413	-2.642205
H	1.287775	-1.264862	-2.585154
C	6.504315	-1.420620	0.173081
H	6.943184	-2.441804	0.209106
H	6.915050	-0.924188	-0.728722
H	6.872079	-0.881162	1.069008
C	2.079634	-1.754134	2.633043
H	2.771946	-1.716325	3.496049
H	1.357916	-0.914678	2.726997
H	1.497768	-2.696705	2.723067
C	-1.927971	2.548227	0.207742
C	-2.156688	2.203038	-1.134926
H	-1.750798	2.801052	-1.966228
H	-2.982570	1.524477	-1.406790
H	-1.343391	3.439324	0.482461
H	-2.572051	2.146388	1.007136

TS1-4

Ru	-0.474640	0.776744	-0.357293
Cl	-0.793063	0.149816	-2.649414
C	-0.341298	-1.217053	0.098496
N	0.689602	-2.086642	0.159052
N	-1.508914	-1.872019	0.289572
C	0.207472	-3.488011	0.322099
C	-1.314435	-3.322497	0.524129
C	2.107737	-1.833064	0.100326
C	-2.798086	-1.218220	0.303579
C	2.815776	-1.688945	1.323497
C	4.218865	-1.560299	1.267156
C	4.924789	-1.570322	0.045583
C	4.183977	-1.716093	-1.145488
C	2.781820	-1.874869	-1.149111
H	4.777395	-1.457739	2.212688
H	4.716762	-1.743517	-2.110860
C	-3.606149	-1.230291	-0.869521
C	-4.827558	-0.528295	-0.831526
C	-5.291906	0.116839	0.333509
C	-4.511479	0.014668	1.504505
C	-3.277840	-0.663456	1.527886
H	-5.449165	-0.507682	-1.742139
H	-4.885200	0.458198	2.442140
H	-1.649525	-3.595324	1.547589
H	0.712655	-3.966593	1.185290
Cl	-0.065716	1.417825	1.952300
C	1.003756	1.756246	-0.879768
H	1.291234	1.706423	-1.957135
H	0.459240	-4.074788	-0.586320
H	-1.911772	-3.912264	-0.200225
P	2.215988	2.785531	0.053699
C	3.368722	3.409027	-1.224421
H	4.139114	4.055219	-0.757422
H	3.867917	2.553090	-1.721770
H	2.816064	3.995400	-1.985688
C	3.222423	1.849047	1.242448
H	4.057366	2.494467	1.584263
H	2.574424	1.555681	2.089540
H	3.623101	0.937038	0.756001
C	1.517171	4.251297	0.890467
H	1.101684	4.959632	0.147336
H	0.731735	3.913224	1.594167
H	2.333353	4.754835	1.447693
C	-2.536968	-0.847524	2.830198
H	-1.543305	-0.354986	2.815998
H	-3.114005	-0.416876	3.670838
H	-2.379199	-1.924188	3.054073
C	-6.624579	0.828424	0.347774
H	-6.873115	1.255961	-0.644049
H	-7.441587	0.120871	0.610410
H	-6.648052	1.643790	1.097911
C	-3.246672	-2.037044	-2.093560
H	-3.701766	-3.050460	-2.022443
H	-3.647281	-1.567252	-3.012635
H	-2.155391	-2.146757	-2.225877
C	2.047309	-2.124682	-2.444433
H	2.726081	-2.006520	-3.311156
H	1.650809	-3.162961	-2.485636
H	1.181449	-1.443215	-2.582358
C	6.433702	-1.482774	0.016600
H	6.884248	-2.499230	0.040812
H	6.801083	-0.990677	-0.906366
H	6.833942	-0.931852	0.891221
C	2.095785	-1.660931	2.651864
H	2.812390	-1.556877	3.489284
H	1.373610	-0.817536	2.702200
H	1.515517	-2.591136	2.831292
C	-1.977321	2.314493	-0.320098
C	-1.075006	2.927426	-1.218744
H	-0.533353	3.831478	-0.900253
H	-1.140492	2.732689	-2.301367
H	-2.121616	2.716051	0.696496
H	-2.807598	1.716833	-0.748200

MCy-4

Ru	-0.350065	0.784483	-0.258403
Cl	-0.726180	0.394168	-2.588248
C	-0.466149	-1.214433	0.049810
N	0.512079	-2.144620	0.074846
N	-1.675814	-1.799134	0.174933
C	-0.056068	-3.520429	0.132545
C	-1.563675	-3.269498	0.344976
C	1.942765	-1.956592	0.060769
C	-2.941942	-1.101264	0.221063
C	2.630945	-1.929633	1.305213
C	4.038693	-1.872908	1.282639
C	4.770339	-1.849093	0.076654
C	4.050695	-1.882117	-1.135666
C	2.641678	-1.963204	-1.176499
H	4.581180	-1.860088	2.242820
H	4.603500	-1.885306	-2.090106
C	-3.757870	-1.062178	-0.946512
C	-4.975763	-0.363060	-0.870610
C	-5.423851	0.247888	0.321030
C	-4.627063	0.113520	1.473878
C	-3.394407	-0.572211	1.461802
H	-5.607659	-0.311044	-1.772907
H	-4.986045	0.533026	2.428232
H	-1.916213	-3.561826	1.357419
H	0.412225	-4.091288	0.959578
Cl	0.154635	1.285294	2.044393
C	0.924428	2.190414	-0.879069
H	1.225981	2.015577	-1.934217
H	0.162112	-4.055213	-0.816119
H	-2.196862	-3.789026	-0.401221
P	2.393100	2.833279	0.016022
C	3.407412	3.673822	-1.253696
H	4.326334	4.088616	-0.792545
H	3.693297	2.949542	-2.042642
H	2.829256	4.499108	-1.715794
C	3.390063	1.489588	0.710833
H	4.352411	1.895293	1.081981
H	2.810242	1.033816	1.536238
H	3.581068	0.721444	-0.065945
C	2.043499	4.064230	1.312555
H	1.550322	4.956758	0.879233
H	1.393818	3.598205	2.079150
H	3.008253	4.372691	1.764969
C	-2.626413	-0.757356	2.748922
H	-1.769722	-0.053728	2.824851
H	-3.285549	-0.582895	3.621176
H	-2.210453	-1.781608	2.841221
C	-6.744577	0.980620	0.357868
H	-6.771746	1.798779	-0.392576
H	-7.586008	0.297759	0.113257
H	-6.944801	1.421899	1.353597
C	-3.384625	-1.795372	-2.212579
H	-3.605676	-2.882341	-2.118918
H	-3.974963	-1.422610	-3.071849
H	-2.312999	-1.675683	-2.462567
C	1.926752	-2.107975	-2.499084
H	2.633943	-1.992262	-3.343102
H	1.470755	-3.117488	-2.597648
H	1.107181	-1.369653	-2.626670
C	6.281974	-1.844788	0.084476
H	6.674162	-2.884392	0.130749
H	6.699295	-1.383045	-0.832660
H	6.689776	-1.308676	0.965034
C	1.887313	-1.962752	2.619995
H	2.593163	-1.962822	3.472830
H	1.213839	-1.085225	2.726315
H	1.255542	-2.871269	2.717061
C	-1.699234	2.220475	-0.310764
C	-0.418594	3.027417	-0.791528
H	-0.292015	3.862640	-0.075870
H	-0.636384	3.369651	-1.821958
H	-2.079586	2.539628	0.677692
H	-2.460134	2.113369	-1.105725

TS2-4

Ru	-0.135757	0.956287	-0.114504
Cl	0.004881	0.693769	-2.508158
C	-0.581021	-1.056217	0.067464
N	0.301576	-2.084391	0.144284
N	-1.842758	-1.558228	0.146991
C	-0.373617	-3.406184	0.220993
C	-1.857940	-3.026907	0.359258
C	1.745419	-2.048960	0.092769
C	-3.094272	-0.852311	0.081224
C	2.479089	-2.024645	1.313303
C	3.887303	-2.071500	1.240753
C	4.575543	-2.192993	0.016227
C	3.811007	-2.277498	-1.164924
C	2.401480	-2.230835	-1.157853
H	4.461580	-2.048484	2.182081
H	4.324877	-2.412900	-2.131315
C	-3.763537	-0.762637	-1.180946
C	-5.045080	-0.185797	-1.210108
C	-5.696966	0.259175	-0.038874
C	-5.034255	0.097441	1.196049
C	-3.751297	-0.473069	1.292647
H	-5.561600	-0.099494	-2.180256
H	-5.543078	0.405774	2.124114
H	-2.270927	-3.260605	1.363671
H	0.012002	-3.982386	1.086087
Cl	0.032067	1.022256	2.299034
C	0.966515	2.852610	-0.608378
H	0.889063	2.972744	-1.706018
H	-0.161235	-3.992486	-0.698193
H	-2.505966	-3.518719	-0.394319
P	2.690585	2.809303	-0.067953
C	3.548790	4.176007	-0.923502
H	4.617359	4.192832	-0.627584
H	3.475799	4.032740	-2.020289
H	3.075710	5.140315	-0.650887
C	3.475598	1.254765	-0.579186
H	4.572983	1.325181	-0.443428
H	3.086744	0.412795	0.030893
H	3.235247	1.061381	-1.643580
C	2.856908	3.034649	1.723639
H	2.546702	4.060605	2.004037
H	2.196840	2.297157	2.233659
H	3.914732	2.876972	2.014822
C	-3.111795	-0.690491	2.640249
H	-2.088529	-0.261307	2.687132
H	-3.719458	-0.231895	3.443710
H	-3.023696	-1.773701	2.876161
C	-7.066092	0.890461	-0.109947
H	-6.987291	1.969944	-0.366599
H	-7.692818	0.418802	-0.893466
H	-7.602083	0.821007	0.857021
C	-3.114966	-1.263267	-2.446512
H	-2.859473	-2.342445	-2.377169
H	-3.790937	-1.136530	-3.313516
H	-2.165543	-0.724885	-2.661461
C	1.635623	-2.418931	-2.444793
H	2.326433	-2.475073	-3.308040
H	1.054013	-3.366338	-2.434150
H	0.922678	-1.587767	-2.624918
C	6.082866	-2.302641	-0.023112
H	6.399153	-3.366561	0.047065
H	6.501609	-1.905257	-0.969554
H	6.559118	-1.769100	0.823901
C	1.792088	-2.011489	2.657645
H	2.534858	-2.006918	3.478622
H	1.131513	-1.127902	2.777155
H	1.158696	-2.914521	2.794858
C	-1.915184	1.446583	-0.270403
C	-0.088388	3.269724	0.222297
H	0.025529	3.400464	1.309976
H	-0.957999	3.766380	-0.237546
H	-2.490774	1.857036	0.587999
H	-2.410093	1.492612	-1.262901

Cl2-4

Ru	0.039115	0.874045	-0.474167
Cl	-0.477897	1.206799	1.885494
C	0.688066	-1.053660	0.069174
N	-0.161413	-2.104874	0.168410
N	1.958963	-1.482937	0.256461
C	0.565866	-3.393807	0.300985
C	2.012924	-2.938475	0.554183
C	-1.606547	-2.094996	0.159945
C	3.180232	-0.717210	0.287349
C	-2.319831	-2.276574	-1.057718
C	-3.730751	-2.319788	-0.995902
C	-4.436886	-2.257594	0.221004
C	-3.689449	-2.147155	1.412603
C	-2.282490	-2.080459	1.415074
H	-4.290368	-2.452224	-1.937233
H	-4.217526	-2.135700	2.380855
C	3.553373	-0.056532	1.494426
C	4.770433	0.654073	1.511179
C	5.632478	0.695022	0.397789
C	5.265114	-0.038167	-0.750232
C	4.065098	-0.769448	-0.828402
H	5.062565	1.173046	2.438968
H	5.947330	-0.057757	-1.616506
H	2.745379	-3.438815	-0.108754
H	0.456640	-3.977670	-0.637904
Cl	0.799914	0.030409	-2.619959
C	-1.185056	2.749839	-0.671294
H	-0.552585	3.599913	-0.359167
H	0.142443	-3.995723	1.129427
H	2.342298	-3.091358	1.604666
P	-2.831228	2.867570	0.066735
C	-3.875392	3.855834	-1.064387
H	-4.885700	3.992229	-0.627876
H	-3.411092	4.848919	-1.227389
H	-3.965281	3.339020	-2.040612
C	-2.753393	3.759658	1.647732
H	-3.776405	3.882204	2.056472
H	-2.119332	3.172980	2.341583
H	-2.301078	4.758336	1.484197
C	-3.638360	1.258022	0.293112
H	-3.647847	0.691637	-0.659967
H	-3.073212	0.678741	1.049825
H	-4.681760	1.417658	0.630351
C	3.791956	-1.629785	-2.039662
H	2.712483	-1.694674	-2.271401
H	4.306425	-1.226865	-2.933919
H	4.186291	-2.659217	-1.883303
C	6.919726	1.484634	0.430215
H	6.824412	2.421561	-0.160982
H	7.202310	1.770114	1.462450
H	7.759196	0.911156	-0.013652
C	2.715456	-0.152296	2.746833
H	2.589965	-1.208895	3.068564
H	3.199175	0.388565	3.582858
H	1.697035	0.266873	2.609749
C	-1.529601	-2.037440	2.723479
H	-2.230841	-2.031720	3.580164
H	-0.871488	-2.924390	2.846307
H	-0.890536	-1.133419	2.791725
C	-5.943260	-2.379550	0.256863
H	-6.245716	-3.442340	0.382719
H	-6.384026	-1.819190	1.106013
H	-6.410293	-2.020632	-0.682067
C	-1.627725	-2.528338	-2.376735
H	-2.315359	-2.342993	-3.225260
H	-0.724026	-1.904360	-2.522047
H	-1.318823	-3.595056	-2.448920
C	1.664464	1.674310	-0.260823
C	-0.962211	2.149556	-1.936247
H	-1.744632	1.537010	-2.421331
H	-0.220647	2.562043	-2.637150
H	2.408578	1.693576	-1.085219
H	1.920867	2.200023	0.684656

14e2-4

Ru	0.079657	0.468600	-1.401147
Cl	0.234259	2.758165	-0.989250
Cl	1.162148	-1.339852	-2.377836
C	-0.082662	-0.060496	0.451648
C	-1.596014	0.297463	-2.059731
H	-1.695233	0.630987	-3.125683
H	-2.512532	-0.097116	-1.580690
N	1.010283	-0.207016	1.283146
N	-1.204944	-0.243198	1.227568
C	0.624959	-0.326957	2.701746
C	-0.875739	-0.637954	2.612350
H	1.208243	-1.127624	3.200679
H	0.823662	0.627222	3.240675
H	-1.483821	-0.059500	3.337416
H	-1.098202	-1.718433	2.771118
C	2.404480	-0.205411	0.916290
C	-2.582248	-0.266255	0.823638
C	3.015678	-1.445585	0.581181
C	4.383375	-1.447826	0.252633
C	5.159367	-0.271262	0.267779
C	4.538288	0.924449	0.673642
C	3.173117	0.984407	1.023487
C	-3.355341	0.917710	0.941970
C	-4.717636	0.857177	0.590218
C	-5.322946	-0.333327	0.135982
C	-4.523468	-1.489283	0.036130
C	-3.154474	-1.483547	0.374552
C	2.233345	-2.737472	0.593127
H	4.858597	-2.405054	-0.020148
C	6.613715	-0.296599	-0.144922
H	5.136469	1.849101	0.735625
C	2.594186	2.271350	1.563025
C	-2.728294	2.210971	1.405319
H	-5.325183	1.774160	0.673885
C	-6.786706	-0.355926	-0.244850
H	-4.976170	-2.429496	-0.321222
C	-2.312963	-2.728746	0.212011
H	-3.481364	3.021288	1.457219
H	-2.271310	2.110823	2.413302
H	-1.915525	2.531569	0.718241
H	-2.913940	-3.562943	-0.199226
H	-1.457844	-2.548114	-0.473707
H	-1.883728	-3.073058	1.177583
H	-7.140073	-1.384523	-0.456488
H	-7.422006	0.065207	0.562653
H	-6.974411	0.257430	-1.152631
H	1.511384	-2.764427	-0.249635
H	2.910700	-3.607709	0.489697
H	1.656260	-2.864775	1.533333
H	3.255810	3.128102	1.328079
H	1.594997	2.492312	1.138990
H	2.500332	2.228907	2.671401
H	7.176030	0.560778	0.276574
H	7.114825	-1.232547	0.177231
H	6.710721	-0.242069	-1.251680

Precat-5

Ru	0.020958	-0.223692	0.024553
Cl	-0.045845	-0.156411	-2.375879
C	0.932028	-2.136331	-0.437171
N	2.185984	-2.450570	-0.925675
N	0.137121	-3.221638	-0.683568
C	2.174524	-3.700322	-1.732177
C	0.866016	-4.352360	-1.310800
C	3.493188	-1.869321	-0.730564
C	-1.211442	-3.541919	-0.269245
C	4.326808	-2.421503	0.286817
C	5.633144	-1.911742	0.445800
C	6.160740	-0.922191	-0.405950
C	5.356159	-0.493305	-1.481301
C	4.050488	-0.979658	-1.694016
H	6.270304	-2.330458	1.243017
H	5.775155	0.214562	-2.216118
C	-2.231346	-3.609856	-1.255150
C	-3.496276	-4.102423	-0.870222
C	-3.768733	-4.536254	0.440297
C	-2.715469	-4.501826	1.377518
C	-1.428425	-4.043215	1.044021
H	-4.290984	-4.158570	-1.632400
H	-2.891244	-4.875347	2.400059
H	0.995728	-5.167001	-0.563423
H	3.067393	-4.317423	-1.513881
Cl	-0.869861	-0.808025	2.182153
C	1.387721	0.821387	0.694917
H	2.191939	-3.437877	-2.812820
H	0.287110	-4.761646	-2.160351
P	2.280874	0.416693	2.344058
C	4.053014	0.870497	2.218463
H	4.564581	0.570493	3.155561
H	4.507923	0.327392	1.365709
H	4.170235	1.958626	2.061818
C	2.256916	-1.331311	2.833180
H	3.035488	-1.490979	3.605568
H	1.248641	-1.570174	3.219080
H	2.464560	-1.958450	1.953365
C	1.629510	1.272527	3.833720
H	1.630854	2.372495	3.731408
H	0.598396	0.913360	4.011348
H	2.277469	0.984710	4.687466
C	-0.301636	-4.177579	2.040415
H	0.290557	-3.247294	2.109937
H	-0.693498	-4.407559	3.050001
H	0.384154	-5.008350	1.759775
C	-5.140925	-5.029364	0.837249
H	-5.690071	-4.253159	1.414280
H	-5.758357	-5.284253	-0.046622
H	-5.079025	-5.926435	1.486952
C	-1.979215	-3.240414	-2.699301
H	-1.513371	-4.085425	-3.254766
H	-2.930433	-3.014986	-3.220189
H	-1.308557	-2.363601	-2.798667
C	3.360731	-0.679748	-3.002925
H	3.696004	0.288214	-3.424524
H	3.639891	-1.456532	-3.749830
H	2.256557	-0.676881	-2.924996
C	7.560880	-0.383247	-0.222830
H	8.185454	-0.582524	-1.119297
H	7.554864	0.718248	-0.079920
H	8.068276	-0.838322	0.650234
C	3.927809	-3.638311	1.098860
H	4.334948	-3.597294	2.128742
H	2.833745	-3.792823	1.161731
H	4.356492	-4.553235	0.632698
C	1.968550	2.069195	0.113354
C	2.353018	2.111587	-1.249890
C	2.213578	3.229277	0.901221
C	2.988086	3.240450	-1.789529
H	2.134849	1.241020	-1.879785
C	2.828434	4.365880	0.354913
H	1.893206	3.262525	1.952048
C	3.233952	4.371821	-0.992061
H	3.285820	3.238352	-2.849955
H	2.987774	5.254333	0.985883
H	3.729126	5.258065	-1.418391
P	-1.787024	1.609421	-0.108469
C	-3.405328	0.912308	-0.828691
C	-3.589761	0.960671	-2.361336
C	-3.723439	-0.506458	-0.311510
H	-4.153224	1.618529	-0.394471
C	-5.028811	0.555726	-2.743163
H	-2.857443	0.277779	-2.844090
H	-3.394900	1.975773	-2.759975
C	-5.164935	-0.908513	-0.675593
H	-3.012137	-1.220685	-0.780755

14e1-5

Ru	-0.621434	0.794806	-0.028513
Cl	-0.743481	1.178696	-2.301701
C	-0.635402	-1.156143	-0.362139
N	0.315545	-2.110490	-0.637671
N	-1.867036	-1.714189	-0.564461
C	-0.308055	-3.319478	-1.244819
C	-1.795198	-3.145532	-0.921130
C	1.750970	-2.126594	-0.507743
C	-3.140382	-1.091282	-0.286428
C	2.314271	-2.945722	0.514518
C	3.716776	-3.085720	0.576659
C	4.573196	-2.477870	-0.362111
C	3.980808	-1.714004	-1.389572
C	2.585461	-1.541125	-1.503742
H	4.149529	-3.716663	1.371262
H	4.626222	-1.266849	-2.164140
C	-3.924628	-0.588534	-1.360096
C	-5.170969	-0.006013	-1.048059
C	-5.669819	0.046792	0.266262
C	-4.896051	-0.535662	1.293714
C	-3.643599	-1.119819	1.045703
H	-5.778489	0.404633	-1.871419
H	-5.285212	-0.537814	2.325307
H	-2.130995	-3.770421	-0.063295
H	0.127250	-4.243230	-0.818465
Cl	-1.767986	1.518595	1.847467
C	1.102016	1.307612	0.403483
H	-0.105693	-3.322064	-2.338791
H	-2.455651	-3.364934	-1.783173
P	1.958571	0.825489	1.954602
C	1.851233	2.298668	3.032782
H	2.295725	2.061790	4.020792
H	2.392753	3.145900	2.569622
H	0.782807	2.567915	3.158930
C	3.728141	0.418222	1.773631
H	4.153718	0.202470	2.775028
H	3.844145	-0.469665	1.120406
H	4.259374	1.282715	1.330556
C	1.126941	-0.508967	2.859728
H	0.093330	-0.182743	3.086568
H	1.102880	-1.426690	2.248510
H	1.682516	-0.700539	3.799747
C	-2.891671	-1.801762	2.165898
H	-1.803425	-1.599572	2.124191
H	-3.261946	-1.465219	3.153479
H	-3.029322	-2.905338	2.127247
C	-6.991162	0.708525	0.577663
H	-6.830682	1.728249	0.991270
H	-7.622497	0.814402	-0.326376
H	-7.563534	0.139049	1.338066
C	-3.521431	-0.744528	-2.807111
H	-4.019267	-1.637366	-3.247270
H	-3.843988	0.128797	-3.407840
H	-2.429237	-0.854522	-2.935736
C	2.025740	-0.803646	-2.692664
H	2.778817	-0.736929	-3.501290
H	1.123607	-1.300978	-3.100925
H	1.703162	0.226241	-2.437734
C	6.068383	-2.691980	-0.314722
H	6.364199	-3.522796	-0.992031
H	6.624650	-1.793106	-0.648981
H	6.416434	-2.961477	0.702130
C	1.464205	-3.744578	1.481914
H	1.936581	-3.800470	2.483274
H	0.439281	-3.341300	1.599187
H	1.360291	-4.795791	1.132827
C	1.623012	2.574658	-0.179248
C	0.864017	3.774751	-0.114388
C	2.875227	2.595011	-0.850956
C	1.346844	4.953565	-0.701267
H	-0.104831	3.776751	0.410707
C	3.345750	3.777949	-1.442068
H	3.460822	1.666845	-0.943750
C	2.586713	4.959786	-1.365992
H	0.747627	5.875284	-0.639543
H	4.310476	3.774740	-1.973258
H	2.960448	5.886205	-1.828810

Cl1-5

Ru	-0.637037	0.684043	0.282294
Cl	-0.633977	0.953583	-2.124357
C	-0.697887	-1.361552	-0.254976
N	0.206407	-2.342749	-0.462932
N	-1.946752	-1.852373	-0.437393
C	-0.451731	-3.611735	-0.892225
C	-1.951623	-3.302547	-0.742935
C	1.648186	-2.336092	-0.392416
C	-3.174363	-1.096972	-0.333909
C	2.274404	-2.819724	0.786182
C	3.683278	-2.905921	0.801559
C	4.470138	-2.560961	-0.315196
C	3.805138	-2.132209	-1.483273
C	2.401195	-2.030780	-1.559814
H	4.178048	-3.276689	1.714919
H	4.396931	-1.891925	-2.382457
C	-3.773887	-0.581573	-1.521681
C	-4.953119	0.175050	-1.388463
C	-5.580126	0.384956	-0.141176
C	-5.021400	-0.239666	0.991363
C	-3.843764	-1.012191	0.921521
H	-5.412354	0.594360	-2.299162
H	-5.537407	-0.155435	1.962302
H	-2.430533	-3.861021	0.089566
H	-0.112494	-4.449682	-0.251492
Cl	-0.509007	-0.186707	2.553519
C	1.035114	1.476597	0.414050
H	-0.157441	-3.842867	-1.937716
H	-2.531795	-3.497162	-1.667331
P	2.045744	1.650619	2.001994
C	3.509293	2.697972	1.642478
H	4.069510	2.844232	2.588544
H	4.161793	2.205942	0.896320
H	3.196034	3.679242	1.238309
C	2.768152	0.116435	2.676585
H	3.492326	0.395569	3.469188
H	1.963624	-0.520492	3.083903
H	3.291945	-0.425942	1.864480
C	1.182933	2.561268	3.334603
H	0.890603	3.562996	2.962052
H	0.294819	1.988830	3.659098
H	1.887198	2.684750	4.182629
C	-3.414144	-1.816334	2.125680
H	-2.332460	-2.038812	2.131104
H	-3.650900	-1.287544	3.069713
H	-3.973413	-2.778241	2.147083
C	-6.827447	1.229925	-0.035800
H	-6.574417	2.312591	-0.054638
H	-7.514950	1.047211	-0.886605
H	-7.378901	1.035350	0.904986
C	-3.256494	-0.909470	-2.902297
H	-3.831034	-1.766057	-3.321070
H	-3.396607	-0.057146	-3.595318
H	-2.182484	-1.165495	-2.905868
C	1.736029	-1.652252	-2.861413
H	2.490649	-1.385480	-3.626220
H	1.146352	-2.500968	-3.272474
H	1.036004	-0.797825	-2.745560
C	5.975292	-2.697652	-0.288885
H	6.298526	-3.600364	-0.851588
H	6.474062	-1.829386	-0.766585
H	6.363764	-2.797042	0.743808
C	1.474042	-3.276608	1.984393
H	2.131372	-3.437515	2.861145
H	0.685095	-2.548659	2.264165
H	0.970394	-4.248704	1.785788
C	-1.921673	2.130875	1.358828
C	-1.996952	2.386965	-0.023297
H	-1.457488	3.220927	-0.496761
H	-2.832148	1.981316	-0.619660
H	-1.323840	2.769852	2.026370
H	-2.698258	1.531775	1.860887
C	1.717207	2.223026	-0.689299
C	1.404219	3.583685	-0.929650
C	2.748659	1.618457	-1.447940
C	2.091774	4.313517	-1.912517
H	0.611684	4.074182	-0.342365
C	3.429220	2.352213	-2.432505
H	3.000997	0.560840	-1.273882
C	3.104731	3.699852	-2.669951
H	1.828559	5.367991	-2.090768
H	4.219484	1.863975	-3.024369
H	3.639416	4.270987	-3.444557

TS1-5

Ru	-0.590959	-0.662407	0.054532
Cl	-0.529340	-0.485170	2.432136
C	-0.775241	1.410781	-0.070193
N	0.111067	2.424942	-0.177133
N	-2.032596	1.918276	-0.033365
C	-0.568505	3.747715	-0.276524
C	-2.051554	3.400114	-0.054058
C	1.552248	2.403477	-0.216184
C	-3.246387	1.149541	0.124017
C	2.214760	2.396010	-1.472779
C	3.621580	2.492880	-1.477375
C	4.369528	2.646618	-0.290487
C	3.670415	2.680763	0.932770
C	2.266661	2.562533	1.000920
H	4.147073	2.486502	-2.447410
H	4.231929	2.812271	1.872489
C	-3.747118	0.889056	1.430086
C	-4.904013	0.088658	1.544172
C	-5.598273	-0.397163	0.419578
C	-5.133851	-0.018470	-0.859427
C	-3.984162	0.771683	-1.037711
H	-5.286161	-0.139651	2.552912
H	-5.700638	-0.330112	-1.752676
H	-2.711399	3.765242	-0.866833
H	-0.373850	4.191111	-1.275667
Cl	-0.797567	-0.625359	-2.371805
C	0.975622	-1.679952	-0.090218
H	-0.161378	4.441244	0.486891
H	-2.447661	3.785449	0.909679
P	1.646949	-2.525817	-1.661030
C	2.990446	-3.672262	-1.160608
H	3.379556	-4.172879	-2.071001
H	3.808465	-3.117684	-0.663197
H	2.607290	-4.439338	-0.459859
C	2.458245	-1.308008	-2.753073
H	3.027719	-1.851999	-3.533972
H	1.679596	-0.665571	-3.202583
H	3.151419	-0.689576	-2.149060
C	0.517271	-3.593566	-2.632052
H	0.319375	-4.530689	-2.075065
H	-0.420242	-3.052327	-2.853542
H	1.033257	-3.849100	-3.580537
C	-3.619977	1.273908	-2.414982
H	-2.531053	1.233324	-2.606946
H	-4.124814	0.677621	-3.199559
H	-3.958127	2.326709	-2.542754
C	-6.826781	-1.264322	0.566433
H	-7.127179	-1.378003	1.626158
H	-7.687435	-0.839152	0.008697
H	-6.651285	-2.280708	0.152864
C	-3.160024	1.518546	2.671250
H	-3.710249	2.456536	2.909063
H	-3.267114	0.849677	3.547062
H	-2.085802	1.754543	2.568909
C	1.556577	2.599589	2.332323
H	2.272158	2.775653	3.158036
H	0.796071	3.408611	2.373096
H	1.020281	1.646309	2.532249
C	5.870017	2.824075	-0.339505
H	6.347251	2.582715	0.630877
H	6.334432	2.192205	-1.123691
H	6.131729	3.877946	-0.579136
C	1.449812	2.347176	-2.776102
H	2.128143	2.129157	-3.624388
H	0.639792	1.588820	-2.766087
H	0.976789	3.329444	-2.998338
C	-2.056181	-2.199874	-0.050027
C	-0.977756	-2.942715	0.495970
H	-0.518666	-3.745399	-0.101260
H	-0.847072	-2.998982	1.587973
H	-2.418819	-2.385117	-1.074458
H	-2.794655	-1.777702	0.660537
C	2.007469	-1.782511	0.987456
C	2.035087	-2.851683	1.918419
C	3.044143	-0.818068	1.030051
C	3.060641	-2.941348	2.870052
H	1.243275	-3.614134	1.910889
C	4.072498	-0.920440	1.982414
H	3.032301	0.029032	0.328243
C	4.085870	-1.978591	2.905708
H	3.055493	-3.770646	3.594584
H	4.862621	-0.154020	2.004080
H	4.889297	-2.052615	3.654759

H	-3.559379	-0.597194	0.779580			
C	-5.415093	-0.824437	-2.189585			
H	-5.137784	0.577666	-3.848796			
H	-5.736510	1.320820	-2.348033			
H	-5.371467	-1.933104	-0.301174			
H	-5.876159	-0.234284	-0.143955			
H	-6.476717	-1.053366	-2.424484			
H	-4.807772	-1.604799	-2.702344			
C	-1.612529	3.218328	-1.153810			
C	-1.037379	4.463153	-0.436970			
C	-0.915504	3.045727	-2.520009			
H	-2.692049	3.436097	-1.343834			
C	-1.198692	5.725365	-1.311263			
H	0.040573	4.303594	-0.220190			
H	-1.539795	4.645574	0.533528			
C	-1.077723	4.303176	-3.396273			
H	0.163263	2.853870	-2.344919			
H	-1.290454	2.155607	-3.055282			
C	-0.550169	5.562239	-2.692860			
H	-0.769373	6.599771	-0.776005			
H	-2.284542	5.943103	-1.436100			
H	-0.557266	4.146939	-4.365611			
H	-2.155434	4.442695	-3.645358			
H	-0.728503	6.465313	-3.315048			
H	0.553905	5.477988	-2.570174			
C	-2.443915	2.370254	1.520287			
C	-3.535551	1.597028	2.296334			
C	-1.300839	2.761576	2.477643			
H	-2.924938	3.305634	1.146679			
C	-4.052670	2.430176	3.488087			
H	-3.114798	0.637699	2.664231			
H	-4.393599	1.349586	1.639757			
C	-1.809200	3.585024	3.677292			
H	-0.844173	1.817071	2.837602			
H	-0.507843	3.319274	1.938896			
C	-2.919959	2.845217	4.438857			
H	-4.826484	1.849566	4.034538			
H	-4.564301	3.343238	3.104663			
H	-0.962785	3.826885	4.357346			
H	-2.198180	4.564082	3.313531			
H	-3.314309	3.477981	5.262489			
H	-2.493995	1.935203	4.920583			

MCy-5

Ru	0.492845	-0.601496	-0.053941
Cl	0.394876	-0.501030	-2.424943
C	0.962313	1.379849	0.060898
N	0.148254	2.454529	0.153512
N	2.253757	1.779087	0.003608
C	0.930302	3.717787	0.252473
C	2.365367	3.258364	-0.061400
C	-1.292598	2.505530	0.213981
C	3.418478	0.930046	-0.134160
C	-1.937766	2.535630	1.480795
C	-3.338959	2.688465	1.504274
C	-4.097812	2.862581	0.327379
C	-3.415009	2.867645	-0.905305
C	-2.017627	2.697492	-0.993533
H	-3.849028	2.712008	2.482156
H	-3.983168	3.025718	-1.836847
C	3.908972	0.612769	-1.429820
C	5.036850	-0.230527	-1.516619
C	5.709030	-0.710638	-0.376939
C	5.248715	-0.289296	0.889436
C	4.125769	0.543740	1.041240
H	5.414443	-0.498464	-2.517317
H	5.796779	-0.601422	1.794086
H	3.111537	3.620497	0.673500
H	0.827342	4.140595	1.274835
Cl	0.698100	-0.668464	2.360548
C	-1.035940	-1.939254	0.021346
H	0.541228	4.464778	-0.467852
H	2.703765	3.562910	-1.074928
P	-1.883261	-2.478725	1.634664
C	-3.280962	-3.577323	1.180590
H	-3.735324	-3.965266	2.115287
H	-4.041607	-3.023196	0.599402
H	-2.918577	-4.429077	0.572013
C	-2.631244	-1.104447	2.565854
H	-3.259692	-1.532374	3.373244
H	-1.819512	-0.481520	2.984678
H	-3.263562	-0.497301	1.889730
C	-0.882568	-3.519006	2.762150
H	-0.689300	-4.504411	2.292979
H	0.063976	-3.007397	3.013741
H	-1.479040	-3.681275	3.683613
C	3.730847	1.045149	2.409463
H	2.719774	0.692459	2.698495
H	4.449689	0.696932	3.175938
H	3.718773	2.155770	2.447756
C	6.911430	-1.617965	-0.495488
H	6.708384	-2.613150	-0.044747
H	7.204585	-1.778228	-1.551282
H	7.786625	-1.197971	0.043532
C	3.334860	1.217275	-2.689324
H	3.786129	2.217546	-2.876270
H	3.571541	0.590708	-3.571075
H	2.234986	1.326499	-2.649491
C	-1.328415	2.727121	-2.335551
H	-2.042799	2.985293	-3.140493
H	-0.508300	3.475646	-2.363351
H	-0.872302	1.742413	-2.577784
C	-5.589627	3.096993	0.396955
H	-5.807757	4.159123	0.643503
H	-6.088840	2.877471	-0.567535
H	-6.067365	2.480861	1.185706
C	-1.159718	2.470213	2.774786
H	-1.838992	2.317223	3.636288
H	-0.403552	1.658413	2.774416
H	-0.620325	3.424319	2.964710
C	1.647780	-2.187413	-0.151543
C	0.216144	-2.858735	-0.321975
H	0.226502	-3.717384	0.378412
H	0.120562	-3.177623	-1.375555
H	2.175484	-2.471205	0.778213
H	2.249448	-2.260117	-1.077222
C	-2.132665	-1.837707	-1.019075
C	-2.367078	-2.860335	-1.969435
C	-3.014431	-0.731392	-0.992794
C	-3.440475	-2.772887	-2.869837
H	-1.709999	-3.742307	-2.016490
C	-4.090926	-0.650171	-1.890562
H	-2.834485	0.099535	-0.292905
C	-4.310855	-1.670052	-2.832046
H	-3.596715	-3.576663	-3.606156
H	-4.752351	0.229086	-1.859821
H	-5.152989	-1.603667	-3.538077

TS2-5

Ru	-0.176758	0.402563	0.326682
Cl	-0.028163	1.100798	-1.945453
C	-1.112367	-1.298505	-0.332733
N	-0.497960	-2.446317	-0.721386
N	-2.456594	-1.452622	-0.485357
C	-1.453709	-3.428527	-1.292784
C	-2.818142	-2.821902	-0.929411
C	0.908015	-2.772388	-0.674840
C	-3.503811	-0.503552	-0.217208
C	1.399038	-3.498288	0.447889
C	2.758650	-3.871458	0.454357
C	3.623268	-3.584826	-0.621903
C	3.084884	-2.918874	-1.741303
C	1.730050	-2.530405	-1.811379
H	3.145278	-4.430621	1.322843
H	3.729458	-2.726883	-2.615581
C	-4.041524	0.249928	-1.309214
C	-5.143655	1.083984	-1.056922
C	-5.751347	1.166196	0.216030
C	-5.237429	0.361423	1.252779
C	-4.138270	-0.498681	1.063319
H	-5.553929	1.679636	-1.889064
H	-5.722659	0.383979	2.242393
H	-3.326187	-3.366310	-0.103859
H	-1.289035	-4.431318	-0.850546
Cl	-0.179456	-0.583505	2.550827
C	1.473804	2.087851	0.831355
H	-1.297467	-3.508957	-2.390172
H	-3.518132	-2.779374	-1.787600
P	2.888514	1.289671	1.715097
C	4.358074	2.358117	1.523944
H	5.179749	1.940348	2.140478
H	4.669808	2.409406	0.463811
H	4.117001	3.382227	1.870892
C	3.325390	-0.365518	1.099586
H	4.241251	-0.710254	1.620464
H	2.494883	-1.068473	1.314009
H	3.511561	-0.344849	0.008194
C	2.589079	1.165131	3.505593
H	2.422096	2.174994	3.929196
H	1.700800	0.520832	3.676532
H	3.484623	0.711186	3.976415
C	-3.670910	-1.395502	2.181448
H	-2.591678	-1.255222	2.404309
H	-4.245515	-1.202206	3.107568
H	-3.812846	-2.468115	1.925915
C	-6.925140	2.086507	0.448120
H	-6.597558	3.148969	0.458389
H	-7.677840	1.993888	-0.361888
H	-7.426593	1.881421	1.413949
C	-3.440518	0.167767	-2.689029
H	-3.440218	-0.873298	-3.077391
H	-4.009393	0.790588	-3.405474
H	-2.381318	0.508269	-2.688037
C	1.177664	-1.962905	-3.096598
H	1.996355	-1.668920	-3.782008
H	0.571871	-2.726930	-3.632532
H	0.536145	-1.074906	-2.925799
C	5.063184	-4.045926	-0.610050
H	5.158375	-5.041691	-1.096073
H	5.723988	-3.352665	-1.168744
H	5.456148	-4.151437	0.420995
C	0.496110	-3.912607	1.585546
H	1.068183	-4.454435	2.363324
H	0.005816	-3.037705	2.059783
H	-0.307162	-4.596442	1.235499
C	-1.775870	1.323691	0.492113
C	0.303943	2.318476	1.586470
H	0.175069	1.965205	2.620539
H	-0.337904	3.162604	1.285985
H	-2.292956	1.446578	1.469141
H	-2.188882	1.907255	-0.357291
C	1.910802	2.998900	-0.277154
C	2.695713	2.527513	-1.358171
C	1.584684	4.375458	-0.236317
C	3.146578	3.402979	-2.356490
H	2.923512	1.453592	-1.439166
C	2.023988	5.249521	-1.244482
H	0.998289	4.777311	0.605120
C	2.809971	4.767804	-2.304754
H	3.747631	3.013654	-3.192876
H	1.759708	6.317187	-1.191705
H	3.159510	5.454361	-3.091381

Cl2-5

Ru	0.049362	0.260661	-0.425966
Cl	-0.429851	0.550205	1.942669
C	0.311326	-1.773481	0.060584
N	-0.721206	-2.646945	0.154908
N	1.478421	-2.439156	0.238257
C	-0.254281	-4.050081	0.296826
C	1.259671	-3.883295	0.514368
C	-2.139519	-2.370029	0.123366
C	2.823521	-1.921185	0.259842
C	-2.845182	-2.400256	-1.112343
C	-4.240566	-2.185711	-1.081184
C	-4.952771	-2.007438	0.121025
C	-4.227020	-2.053139	1.329425
C	-2.832098	-2.251860	1.363152
H	-4.791880	-2.201139	-2.036507
H	-4.765955	-1.956175	2.286791
C	3.338131	-1.375470	1.472227
C	4.667137	-0.906253	1.474846
C	5.500675	-1.000419	0.343248
C	4.980620	-1.622906	-0.811188
C	3.662013	-2.110675	-0.876902
H	5.069260	-0.473462	2.405799
H	5.629591	-1.748346	-1.693869
H	1.866206	-4.501317	-0.176497
H	-0.496887	-4.617638	-0.626876
Cl	0.612613	-0.623081	-2.620193
C	-0.708211	2.436325	-0.563304
H	-0.766514	-4.544753	1.146059
H	1.580014	-4.117248	1.552315
P	-2.357876	2.757428	0.171533
C	-3.135940	4.057754	-0.854211
H	-4.124562	4.332549	-0.434106
H	-2.481622	4.952203	-0.865882
H	-3.265172	3.691816	-1.891897
C	-2.311789	3.406492	1.869519
H	-3.351164	3.625895	2.187824
H	-1.855102	2.643288	2.528639
H	-1.711664	4.336286	1.896944
C	-3.445847	1.301938	0.125549
H	-3.526666	0.902607	-0.904379
H	-3.039852	0.516200	0.794068
H	-4.455185	1.601710	0.471402
C	3.201960	-2.865633	-2.101441
H	2.128163	-2.701926	-2.310804
H	3.772725	-2.550597	-2.996697
H	3.380937	-3.957494	-1.977607
C	6.913392	-0.466053	0.362444
H	6.984706	0.483696	-0.211392
H	7.261701	-0.259408	1.393403
H	7.623062	-1.177270	-0.107867
C	2.523459	-1.349146	2.743348
H	2.261684	-2.378505	3.072368
H	3.097130	-0.880864	3.566306
H	1.570686	-0.793180	2.627537
C	-2.124510	-2.395240	2.690016
H	-2.801284	-2.134196	3.526511
H	-1.795763	-3.444324	2.857833
H	-1.231462	-1.742636	2.752573
C	-6.455814	-1.846076	0.120143
H	-6.955504	-2.838266	0.172761
H	-6.809960	-1.261804	0.993169
H	-6.818076	-1.352648	-0.804069
C	-2.173828	-2.743287	-2.420445
H	-2.851504	-2.545631	-3.273709
H	-1.232566	-2.180417	-2.584593
H	-1.923054	-3.826569	-2.456671
C	1.804642	0.711829	-0.222477
C	-0.705722	1.756070	-1.812582
H	-1.626624	1.308305	-2.229763
H	0.050962	1.997626	-2.574949
H	2.529851	0.598588	-1.055519
H	2.171108	1.160337	0.725206
C	0.276271	3.547917	-0.279061
C	0.869032	3.726259	0.995008
C	0.594049	4.468876	-1.308044
C	1.760674	4.786565	1.224927
H	0.651271	3.000410	1.793822
C	1.488870	5.526929	-1.073891
H	0.137776	4.356659	-2.304602
C	2.073841	5.690258	0.193176
H	2.222213	4.902290	2.218293
H	1.727012	6.228601	-1.888624
H	2.773628	6.520360	0.376715

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Ru	0.079657	0.468600	-1.401147
Cl	0.234259	2.758165	-0.989250
Cl	1.162148	-1.339852	-2.377836
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C	-1.596014	0.297463	-2.059731
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H	-2.512532	-0.097116	-1.580690
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C	0.624959	-0.326957	2.701746
C	-0.875739	-0.637954	2.612350
H	1.208243	-1.127624	3.200679
H	0.823662	0.627222	3.240675
H	-1.483821	-0.059500	3.337416
H	-1.098202	-1.718433	2.771118
C	2.404480	-0.205411	0.916290
C	-2.582248	-0.266255	0.823638
C	3.015678	-1.445585	0.581181
C	4.383375	-1.447826	0.252633
C	5.159367	-0.271262	0.267779
C	4.538288	0.924449	0.673642
C	3.173117	0.984407	1.023487
C	-3.355341	0.917710	0.941970
C	-4.717636	0.857177	0.590218
C	-5.322946	-0.333327	0.135982
C	-4.523468	-1.489283	0.036130
C	-3.154474	-1.483547	0.374552
C	2.233345	-2.737472	0.593127
H	4.858597	-2.405054	-0.020148
C	6.613715	-0.296599	-0.144922
H	5.136469	1.849101	0.735625
C	2.594186	2.271350	1.563025
C	-2.728294	2.210971	1.405319
H	-5.325183	1.774160	0.673885
C	-6.786706	-0.355926	-0.244850
H	-4.976170	-2.429496	-0.321222
C	-2.312963	-2.728746	0.212011
H	-3.481364	3.021288	1.457219
H	-2.271310	2.110823	2.413302
H	-1.915525	2.531569	0.718241
H	-2.913940	-3.562943	-0.199226
H	-1.457844	-2.548114	-0.473707
H	-1.883728	-3.073058	1.177583
H	-7.140073	-1.384523	-0.456488
H	-7.422006	0.065207	0.562653
H	-6.974411	0.257430	-1.152631
H	1.511384	-2.764427	-0.249635
H	2.910700	-3.607709	0.489697
H	1.656260	-2.864775	1.533333
H	3.255810	3.128102	1.328079
H	1.594997	2.492312	1.138990
H	2.500332	2.228907	2.671401
H	7.176030	0.560778	0.276574
H	7.114825	-1.232547	0.177231
H	6.710721	-0.242069	-1.251680