

Theoretical Study of the Ruthenium-Catalyzed Cyclocotrimerization of Alkynes with Isocyanates and Isothiocyanates: Chemoselective Formation of Pyridine-2-one and Thiopyrane-2-imine

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Supporting Information

1. HNCO System

Complex C (N-attack)

Ru	0.053275	0.032588	0.269049
Cl	2.389467	0.419213	0.815485
C	0.248802	1.727832	-0.634297
C	-1.010276	-0.288131	-1.601918
C	-0.529083	2.049426	-1.777285
C	-1.238844	0.987587	-2.270213
C	-0.804133	-1.507532	1.979137
C	-1.837337	-0.947748	1.180687
C	-0.108392	-0.443547	2.587587
C	-1.826533	0.483774	1.353135
C	-0.740048	0.798456	2.222393
C	0.214223	-1.136553	-2.087906
N	0.828687	-1.450125	-0.932940
O	0.478931	-1.379882	-3.251933
H	0.980147	2.454348	-0.275915
H	-1.891404	-0.930953	-1.548674
H	-0.508669	3.027879	-2.252211
H	-1.923977	1.072580	-3.112681
H	-0.525498	-2.551293	2.013832
H	-2.543925	-1.506055	0.583333
H	0.790767	-0.530949	3.180822
H	-2.539857	1.179761	0.934269
H	-0.457691	1.778541	2.578983
H	1.812574	-1.705783	-0.965042

Zero-point correction=	0.177423
(Hartree/Particle)	
Thermal correction to Energy=	0.190653
Thermal correction to Enthalpy=	0.191598
Thermal correction to Gibbs Free Energy=	0.137035
Sum of electronic and zero-point Energies=	-1071.988032
Sum of electronic and thermal Energies=	-1071.974802
Sum of electronic and thermal Enthalpies=	-1071.973858
Sum of electronic and thermal Free Energies=	-1072.028420

Nimag = 0

Complex D (N-attack)

Ru	-0.036964	-0.046154	-0.544602
Ru	0.064353	-0.030817	-0.300953
Cl	2.350112	-0.124187	-1.126579

C	0.790914	-1.234297	1.266325
C	-1.137813	0.375528	1.571043
C	-0.315552	-1.791344	2.083423
C	-1.346121	-0.945293	2.236640
C	-1.467363	1.294141	-1.521654
C	-2.090952	0.085913	-0.986906
C	-0.456406	0.892485	-2.387286
C	-1.494872	-1.052106	-1.594817
C	-0.425508	-0.567452	-2.390630
C	0.128041	1.053714	1.969870
N	1.150963	0.147407	1.585006
O	0.331769	2.172658	2.398549
H	1.670569	-1.838581	1.074684
H	-1.980966	1.058225	1.526282
H	-0.261386	-2.790413	2.504103
H	-2.240757	-1.150501	2.816576
H	-1.721193	2.308609	-1.247338
H	-2.949215	0.062497	-0.331761
H	0.254449	1.529797	-2.892892
H	-1.762683	-2.085745	-1.430108
H	0.274406	-1.172777	-2.947557
H	2.116244	0.465158	1.562321

Zero-point correction=	0.179710
(Hartree/Particle)	
Thermal correction to Energy=	0.192457
Thermal correction to Enthalpy=	0.193402
Thermal correction to Gibbs Free Energy=	0.140192
Sum of electronic and zero-point Energies=	-1071.978436
Sum of electronic and thermal Energies=	-1071.965688
Sum of electronic and thermal Enthalpies=	-1071.964744
Sum of electronic and thermal Free Energies=	-1072.017953

Nimag = 0

Complex E (N-attack)

Ru	-0.036964	-0.046154	-0.544602
C	-1.614227	-1.150594	1.023879
C	-1.754273	0.241205	0.676854
C	-0.800389	1.142136	1.236964
C	-0.057699	0.799322	2.454339
Cl	2.048652	-0.545059	0.560226
N	-0.120297	-0.581136	2.798761
C	-0.767416	-1.504695	2.057144
O	0.575166	1.564258	3.159019
C	-0.077452	-0.953385	-2.628785
C	-1.207298	-0.089237	-2.419506
C	-0.712340	1.229467	-2.150032
C	0.725801	1.172170	-2.153720
C	1.098528	-0.183571	-2.470595
H	-2.214916	-1.914012	0.545815
H	-2.632608	0.592125	0.144136
H	-0.887875	2.208291	1.060883
H	0.544945	-0.864402	3.506763
H	-0.606332	-2.541881	2.331204
H	-0.118406	-2.016164	-2.825144
H	-2.247470	-0.378352	-2.490153
H	-1.309743	2.115843	-1.980690
H	1.403734	1.997649	-1.989689
H	2.109325	-0.565316	-2.487183

Zero-point correction=	0.180724
(Hartree/Particle)	
Thermal correction to Energy=	0.193714
Thermal correction to Enthalpy=	0.194659
Thermal correction to Gibbs Free Energy=	0.140394
Sum of electronic and zero-point Energies=	-1072.054919
Sum of electronic and thermal Energies=	-1072.041928
Sum of electronic and thermal Enthalpies=	-1072.040984
Sum of electronic and thermal Free Energies=	-1072.095249

Nimag = 0

Complex TSBC (N-attack)

Ru	0.019847	0.003957	0.258649
Cl	2.278294	0.889299	0.639795
C	-0.250512	1.834933	-0.543032
C	-1.217937	-0.355551	-1.395869
C	-1.078199	1.988381	-1.615835
C	-1.631809	0.755691	-2.081942
C	0.176511	-0.458213	2.600390
C	-0.327868	-1.649981	2.048410
C	-0.708638	0.626978	2.257648
C	-1.504755	-1.324077	1.313476
C	-1.779562	0.080568	1.486472
C	0.695781	-1.131878	-2.270527
N	1.140168	-1.204628	-1.085718
O	0.644900	-1.248599	-3.438471
H	0.267757	2.678095	-0.089230
H	-1.671025	-1.332797	-1.560947
H	-1.279899	2.944745	-2.094193
H	-2.328787	0.704290	-2.918711
H	1.111201	-0.350693	3.132339
H	0.147074	-2.620973	2.088704
H	-0.605100	1.653604	2.578748
H	-2.124885	-2.022692	0.769597
H	-2.644145	0.612489	1.116025
H	2.145073	-1.338169	-0.966742

Zero-point correction=	0.174319
(Hartree/Particle)	
Thermal correction to Energy=	0.188033
Thermal correction to Enthalpy=	0.188977
Thermal correction to Gibbs Free Energy=	0.133205
Sum of electronic and zero-point Energies=	-1071.970233
Sum of electronic and thermal Energies=	-1071.956519
Sum of electronic and thermal Enthalpies=	-1071.955575
Sum of electronic and thermal Free Energies=	-1072.011348

Nimag = 1

Complex TSCD (N-attack)

Ru	0.064690	0.057317	0.307123
Cl	2.228486	-0.288395	1.376388
C	1.138572	1.199143	-0.908084
C	-0.987433	0.083657	-1.685748
C	0.535556	1.897063	-2.010025
C	-0.647927	1.343898	-2.370313
C	-1.146156	-1.166403	1.947875
C	-1.995163	-0.700465	0.929665
C	-0.528749	-0.016370	2.535243

C	-1.939669	0.760290	0.915320
C	-1.053027	1.171929	1.944255
C	-0.069164	-1.091954	-2.049371
N	1.079642	-0.852090	-1.361757
O	-0.404964	-2.065339	-2.707271
H	2.201686	1.329274	-0.712454
H	-2.035882	-0.204621	-1.739077
H	1.037267	2.686920	-2.562428
H	-1.259191	1.708974	-3.194369
H	-0.929600	-2.196495	2.190157
H	-2.593547	-1.315738	0.272010
H	0.238503	-0.043687	3.294657
H	-2.533689	1.411991	0.291091
H	-0.797770	2.186339	2.213734
H	1.782777	-1.579544	-1.267769

Zero-point correction= 0.177161
 (Hartree/Particle)
 Thermal correction to Energy= 0.189735
 Thermal correction to Enthalpy= 0.190679
 Thermal correction to Gibbs Free Energy= 0.137431
 Sum of electronic and zero-point Energies= -1071.950548
 Sum of electronic and thermal Energies= -1071.937974
 Sum of electronic and thermal Enthalpies= -1071.937030
 Sum of electronic and thermal Free Energies= -1071.990278

Nimag = 1

Complex TSCD (N-attack)

Ru	0.064875	-0.032555	-0.324596
Cl	2.387970	-0.336572	-0.994156
C	0.372651	-1.484858	1.385100
C	-1.028424	0.729371	1.590431
C	-0.923225	-1.623171	2.024064
C	-1.647548	-0.481900	2.144422
C	0.382740	0.952102	1.953359
N	1.057691	-0.262027	1.593468
O	0.963068	1.932431	2.379820
C	-1.138310	1.454816	-1.545628
C	-2.050528	0.428336	-1.047850
C	-0.210765	0.818024	-2.382556
C	-1.681423	-0.815090	-1.610973
C	-0.504882	-0.605553	-2.386053
H	1.028114	-2.329256	1.213454
H	-1.619065	1.639117	1.540944
H	-1.279867	-2.601439	2.327975
H	-2.642831	-0.446451	2.576006
H	2.071949	-0.225717	1.499499
H	-1.172535	2.508446	-1.307392
H	-2.901942	0.598498	-0.405042
H	0.638962	1.279891	-2.863780
H	-2.157532	-1.766571	-1.418374
H	0.054663	-1.360089	-2.919170

Zero-point correction= 0.178504
 (Hartree/Particle)
 Thermal correction to Energy= 0.191090
 Thermal correction to Enthalpy= 0.192034
 Thermal correction to Gibbs Free Energy= 0.138904
 Sum of electronic and zero-point Energies= -1071.977374
 Sum of electronic and thermal Energies= -1071.964788
 Sum of electronic and thermal Enthalpies= -1071.963844

Sum of electronic and thermal Free Energies= -1072.016973

Nimag = 1

Complex C (O-attack)

Ru	0.052311	0.026686	0.267820
Cl	2.385519	0.259552	0.873335
C	0.400944	1.718070	-0.610425
C	-1.003871	-0.171708	-1.600341
C	-0.311092	2.111268	-1.771891
C	-1.096362	1.115015	-2.284457
C	-0.929800	-1.471389	1.947269
C	-1.907797	-0.823962	1.141810
C	-0.159295	-0.474214	2.573639
C	-1.784735	0.599919	1.325606
C	-0.678688	0.820098	2.204145
C	0.116622	-1.126650	-2.049460
O	0.767975	-1.486184	-0.957060
N	0.304739	-1.435430	-3.269350
H	1.173309	2.380754	-0.217362
H	-1.946915	-0.719544	-1.559001
H	-0.185659	3.082504	-2.245059
H	-1.743408	1.247986	-3.149823
H	-0.736273	-2.534746	1.976163
H	-2.650098	-1.320442	0.533167
H	0.723888	-0.639068	3.174018
H	-2.438516	1.354497	0.911011
H	-0.325037	1.771029	2.575666
H	1.120674	-2.050729	-3.343021

Zero-point correction= 0.177566

(Hartree/Particle)

Thermal correction to Energy=	0.190708
Thermal correction to Enthalpy=	0.191652
Thermal correction to Gibbs Free Energy=	0.137433
Sum of electronic and zero-point Energies=	-1071.970401
Sum of electronic and thermal Energies=	-1071.957259
Sum of electronic and thermal Enthalpies=	-1071.956315
Sum of electronic and thermal Free Energies=	-1072.010534

Nimag = 0

Complex D (O-attack)

Ru	0.137951	0.064451	-0.372772
Cl	2.433934	-0.346816	-0.357992
C	0.112912	-1.293954	1.253871
C	-1.108467	0.725306	1.268391
C	-1.318662	-1.569242	1.650723
C	-1.998537	-0.415110	1.670470
C	-0.476892	1.296684	-2.409091
C	-1.600189	0.888737	-1.613497
C	0.262516	0.152236	-2.720354
C	-1.613675	-0.538298	-1.523246
C	-0.412752	-1.005145	-2.149888
C	0.092247	0.788237	2.183968
O	0.677273	-0.433304	2.322089
N	0.497383	1.871547	2.722558
H	0.782936	-2.145162	1.162611
H	-1.564268	1.702603	1.128393
H	-1.680657	-2.536589	1.987627
H	-3.020262	-0.267468	2.007820

H	-0.196780	2.317505	-2.631131
H	-2.355366	1.550739	-1.212756
H	1.217950	0.126534	-3.225559
H	-2.369725	-1.147220	-1.051189
H	-0.116689	-2.037434	-2.277104
H	1.325257	1.685396	3.296428

Zero-point correction= 0.179045
 (Hartree/Particle)
 Thermal correction to Energy= 0.191745
 Thermal correction to Enthalpy= 0.192689
 Thermal correction to Gibbs Free Energy= 0.139338
 Sum of electronic and zero-point Energies= -1071.949126
 Sum of electronic and thermal Energies= -1071.936426
 Sum of electronic and thermal Enthalpies= -1071.935482
 Sum of electronic and thermal Free Energies= -1071.988833

Nimag = 0

Complex E (O-attack)

Ru	-0.080097	-0.015449	-0.435559
C	-1.783083	-0.845971	0.626474
C	-1.804335	0.581495	0.735006
C	-0.687646	1.150442	1.404869
C	-0.112463	0.416396	2.551186
Cl	2.132999	-0.212948	0.572102
O	-0.158644	-0.962316	2.426205
C	-0.644874	-1.445528	1.216900
N	0.352368	0.991840	3.578847
C	-0.804497	-0.688016	-2.435566
C	-1.032941	0.726293	-2.314444
C	0.237675	1.381601	-2.227913
C	1.230211	0.369219	-2.253525
C	0.599673	-0.916864	-2.386901
H	-2.503962	-1.399192	0.035561
H	-2.574911	1.179568	0.261590
H	-0.565635	2.225799	1.442936
H	-0.420981	-2.498513	1.103067
H	0.706278	0.298729	4.242307
H	-1.569200	-1.444669	-2.551249
H	-1.997989	1.214876	-2.336063
H	0.410462	2.444052	-2.134182
H	2.291036	0.529912	-2.132065
H	1.104444	-1.869475	-2.451142

Zero-point correction= 0.180356
 (Hartree/Particle)
 Thermal correction to Energy= 0.192953
 Thermal correction to Enthalpy= 0.193897
 Thermal correction to Gibbs Free Energy= 0.140410
 Sum of electronic and zero-point Energies= -1072.015927
 Sum of electronic and thermal Energies= -1072.003331
 Sum of electronic and thermal Enthalpies= -1072.002387
 Sum of electronic and thermal Free Energies= -1072.055874

Nimag = 0

Complex TSBC (O-attack)

Ru	0.031146	-0.002493	0.243785
Cl	2.192327	1.082496	0.215848
C	-0.503876	1.726383	-0.642826

C	-1.259881	-0.610201	-1.271505
C	-1.459707	1.708847	-1.618568
C	-1.899064	0.396809	-1.952737
C	0.441175	-0.220434	2.584283
C	-0.046790	-1.485069	2.209654
C	-0.531516	0.776662	2.215003
C	-1.308103	-1.300945	1.568712
C	-1.643989	0.096090	1.616167
C	0.697100	-1.130697	-2.039073
O	1.132929	-1.490376	-0.947745
N	0.706051	-0.956267	-3.257311
H	-0.027359	2.648108	-0.314558
H	-1.605327	-1.642333	-1.321349
H	-1.817696	2.601660	-2.127157
H	-2.663823	0.204783	-2.704550
H	1.415760	-0.013068	3.003091
H	0.492109	-2.420095	2.286025
H	-0.459831	1.835922	2.416436
H	-1.930742	-2.083721	1.158970
H	-2.570123	0.543940	1.285496
H	1.609160	-1.095727	-3.709882

Zero-point correction=	0.173605
(Hartree/Particle)	
Thermal correction to Energy=	0.187273
Thermal correction to Enthalpy=	0.188217
Thermal correction to Gibbs Free Energy=	0.133092
Sum of electronic and zero-point Energies=	-1071.946143
Sum of electronic and thermal Energies=	-1071.932475
Sum of electronic and thermal Enthalpies=	-1071.931531
Sum of electronic and thermal Free Energies=	-1071.986656

Nimag = 1

Complex TSCD (O-attack)

Ru	0.058674	0.021830	0.319518
Cl	2.265602	-0.212819	1.271920
C	1.034922	1.157041	-0.996990
C	-1.071056	0.015517	-1.605689
C	0.326259	1.885815	-2.020846
C	-0.862554	1.306875	-2.298973
C	-1.332547	-1.223543	1.880273
C	-2.080007	-0.407581	0.985566
C	-0.444004	-0.380433	2.567692
C	-1.698425	0.976631	1.173695
C	-0.654555	0.988473	2.140467
C	-0.062957	-1.007408	-2.078885
O	1.136311	-0.705516	-1.548150
N	-0.373829	-2.025844	-2.780284
H	2.100324	1.319467	-0.856072
H	-2.085582	-0.370412	-1.631152
H	0.766276	2.707138	-2.579396
H	-1.546497	1.643441	-3.075406
H	-1.375923	-2.301307	1.946792
H	-2.854621	-0.764929	0.323470
H	0.326395	-0.699638	3.253912
H	-2.144536	1.837190	0.695988
H	-0.140807	1.856146	2.528050
H	0.453955	-2.612973	-2.918268

Zero-point correction=	0.177625
(Hartree/Particle)	

Thermal correction to Energy=	0.190105
Thermal correction to Enthalpy=	0.191050
Thermal correction to Gibbs Free Energy=	0.138125
Sum of electronic and zero-point Energies=	-1071.931124
Sum of electronic and thermal Energies=	-1071.918643
Sum of electronic and thermal Enthalpies=	-1071.917699
Sum of electronic and thermal Free Energies=	-1071.970624

Nimag = 1

Complex TSDE (O-attack)

Ru	0.173684	-0.154581	-0.402394
Cl	2.323164	-0.223367	0.429956
C	-0.575358	-1.368670	1.129465
C	-0.814824	1.063782	1.193138
C	-1.993768	-0.930459	0.927007
C	-2.124465	0.421955	1.030519
C	-0.074278	0.495824	2.377739
O	-0.082128	-0.866263	2.397676
N	0.425418	1.241981	3.273275
C	0.445579	1.300924	-2.246288
C	-0.940389	1.230276	-1.876336
C	0.847503	-0.001417	-2.578663
C	-1.435049	-0.080856	-2.158068
C	-0.321540	-0.876902	-2.503847
H	-0.383099	-2.438836	1.105231
H	-0.741012	2.145258	1.128969
H	-2.807653	-1.620092	0.715676
H	-3.053404	0.971641	0.912192
H	0.848129	0.673748	4.011624
H	1.081596	2.170688	-2.163157
H	-1.540691	2.066133	-1.542045
H	1.850644	-0.314264	-2.835739
H	-2.452898	-0.419616	-2.032258
H	-0.338854	-1.926338	-2.766723

Zero-point correction=	0.177236
(Hartree/Particle)	
Thermal correction to Energy=	0.189858
Thermal correction to Enthalpy=	0.190802
Thermal correction to Gibbs Free Energy=	0.137047
Sum of electronic and zero-point Energies=	-1071.935540
Sum of electronic and thermal Energies=	-1071.922918
Sum of electronic and thermal Enthalpies=	-1071.921974
Sum of electronic and thermal Free Energies=	-1071.975729

Nimag = 1

2. HNCS System

Complex C (N-attack)

Ru	0.056035	0.052450	0.507890
Cl	2.388098	0.348010	1.110991
C	0.223846	1.889192	-0.046420
C	-1.054470	0.092934	-1.383832
C	-0.565651	2.428042	-1.100247
C	-1.265579	1.485832	-1.795738
C	-0.710616	-1.832609	1.876946
C	-1.773739	-1.182102	1.195843
C	-0.072886	-0.873329	2.691001
C	-1.835569	0.188361	1.644878
C	-0.767657	0.381188	2.571440

C	0.098496	-0.675943	-2.068471
N	0.837360	-1.052825	-1.041096
S	0.266388	-0.921540	-3.705213
H	0.957726	2.536386	0.437528
H	-1.962715	-0.511844	-1.416341
H	-0.550839	3.481691	-1.370503
H	-1.932575	1.728988	-2.621004
H	-0.382239	-2.849943	1.716299
H	-2.452331	-1.649372	0.496639
H	0.828898	-1.030095	3.265802
H	-2.585913	0.915128	1.366483
H	-0.538748	1.284403	3.118540
H	1.774736	-1.424288	-1.168763
Zero-point correction=			0.175127
(Hartree/Particle)			
Thermal correction to Energy=			0.188844
Thermal correction to Enthalpy=			0.189788
Thermal correction to Gibbs Free Energy=			0.133402
Sum of electronic and zero-point Energies=			-1394.946906
Sum of electronic and thermal Energies=			-1394.933190
Sum of electronic and thermal Enthalpies=			-1394.932246
Sum of electronic and thermal Free Energies=			-1394.988632

Nimag = 0

Complex D (N-attack)

Ru	0.056007	0.072268	0.466931
Cl	2.363013	0.497122	1.090811
C	0.270277	1.780436	-0.763811
C	-1.256748	-0.143282	-1.358943
C	-1.032647	2.218908	-1.314854
C	-1.849331	1.199465	-1.623823
C	-0.995749	-1.825101	1.399363
C	-1.920282	-0.704194	1.251978
C	0.017366	-1.422602	2.262518
C	-1.492656	0.361320	2.089539
C	-0.249568	-0.039376	2.647490
C	0.075234	-0.366493	-1.962587
N	0.880769	0.664522	-1.488863
S	0.594960	-1.607464	-2.935540
H	1.013381	2.519259	-0.485657
H	-1.906757	-1.008233	-1.433087
H	-1.264351	3.269658	-1.456742
H	-2.833615	1.299122	-2.070591
H	-1.065127	-2.770508	0.879179
H	-2.843423	-0.722636	0.691492
H	0.903786	-1.981700	2.524833
H	-1.984805	1.313664	2.223864
H	0.378042	0.559352	3.291186
H	1.887225	0.604431	-1.623750

Zero-point correction=			0.177343
(Hartree/Particle)			
Thermal correction to Energy=			0.190606
Thermal correction to Enthalpy=			0.191550
Thermal correction to Gibbs Free Energy=			0.136577
Sum of electronic and zero-point Energies=			-1394.936893
Sum of electronic and thermal Energies=			-1394.923630
Sum of electronic and thermal Enthalpies=			-1394.922686
Sum of electronic and thermal Free Energies=			-1394.977660

Nimag = 0

Complex E (N-attack)

Ru	0.035950	-0.047830	0.767241
C	2.001157	-0.866103	-0.560715
C	1.732458	0.537632	-0.386542
C	0.662445	1.086769	-1.156150
C	0.167392	0.423666	-2.344064
Cl	-1.696548	-1.265544	-0.356823
N	0.581572	-0.901615	-2.479066
C	1.383608	-1.537871	-1.596830
S	-0.806303	1.103688	-3.507020
C	0.146386	-0.609317	2.956390
C	1.011037	0.503506	2.674797
C	0.202178	1.578261	2.180126
C	-1.161251	1.118585	2.127238
C	-1.178944	-0.230644	2.630236
H	2.732755	-1.383194	0.047153
H	2.432904	1.172536	0.146614
H	0.448114	2.146712	-1.099586
H	0.128572	-1.420966	-3.220927
H	1.527383	-2.599212	-1.764039
H	0.457881	-1.580795	3.315681
H	2.080530	0.529950	2.835628
H	0.548064	2.565302	1.902243
H	-2.019816	1.689021	1.802181
H	-2.045847	-0.875184	2.661298

Zero-point correction=	0.178788
(Hartree/Particle)	
Thermal correction to Energy=	0.192155
Thermal correction to Enthalpy=	0.193099
Thermal correction to Gibbs Free Energy=	0.137426
Sum of electronic and zero-point Energies=	-1395.012585
Sum of electronic and thermal Energies=	-1394.999218
Sum of electronic and thermal Enthalpies=	-1394.998274
Sum of electronic and thermal Free Energies=	-1395.053947

Nimag = 0

Complex TSBC (N-attack)

Ru	0.016725	0.025113	0.490945
Cl	2.151739	1.160277	0.922055
C	-0.573627	1.901151	0.059964
C	-1.324853	-0.231227	-1.108519
C	-1.512720	2.110184	-0.908833
C	-1.940845	0.909979	-1.551259
C	0.469187	-0.862071	2.663543
C	0.069153	-1.983869	1.915986
C	-0.581803	0.126947	2.623449
C	-1.209323	-1.695897	1.355206
C	-1.646078	-0.409996	1.839609
C	0.604458	-0.620854	-2.286359
N	1.151006	-0.650657	-1.150820
S	0.473092	-0.731541	-3.862565
H	-0.132323	2.724406	0.619549
H	-1.646052	-1.222256	-1.421021
H	-1.882091	3.094290	-1.190637
H	-2.697121	0.902581	-2.336186
H	1.430602	-0.723825	3.137453

H	0.664984	-2.865223	1.720746
H	-0.577537	1.075051	3.141879
H	-1.786645	-2.358310	0.725875
H	-2.605227	0.050979	1.652248
H	2.168148	-0.714198	-1.086353

Zero-point correction=	0.172222
(Hartree/Particle)	
Thermal correction to Energy=	0.186166
Thermal correction to Enthalpy=	0.187110
Thermal correction to Gibbs Free Energy=	0.130561
Sum of electronic and zero-point Energies=	-1394.922118
Sum of electronic and thermal Energies=	-1394.908174
Sum of electronic and thermal Enthalpies=	-1394.907230
Sum of electronic and thermal Free Energies=	-1394.963779

Nimag = 1

Complex TSCD (N-attack)

Ru	0.079993	0.052044	0.510808
Cl	1.837160	-1.222240	1.612747
C	1.637846	1.000077	-0.284590
C	-0.582975	0.864350	-1.494231
C	1.465618	2.070722	-1.224858
C	0.242421	2.046546	-1.805811
C	-1.728356	-1.012762	1.642725
C	-2.185870	-0.027689	0.747166
C	-0.869006	-0.360346	2.575794
C	-1.641554	1.263169	1.159850
C	-0.844101	1.046199	2.314498
C	-0.034725	-0.440792	-2.037601
N	1.025781	-0.739869	-1.277585
S	-0.757187	-1.341620	-3.240089
H	2.642731	0.726078	0.032128
H	-1.644323	0.976209	-1.698743
H	2.269321	2.741313	-1.517315
H	-0.087576	2.760894	-2.558024
H	-1.918002	-2.074697	1.587064
H	-2.836679	-0.198758	-0.099095
H	-0.293961	-0.856111	3.343683
H	-1.866847	2.220884	0.713029
H	-0.307938	1.791728	2.883130
H	1.470597	-1.651211	-1.351258

Zero-point correction=	0.175157
(Hartree/Particle)	
Thermal correction to Energy=	0.188097
Thermal correction to Enthalpy=	0.189041
Thermal correction to Gibbs Free Energy=	0.134550
Sum of electronic and zero-point Energies=	-1394.912405
Sum of electronic and thermal Energies=	-1394.899464
Sum of electronic and thermal Enthalpies=	-1394.898520
Sum of electronic and thermal Free Energies=	-1394.953012

Nimag = 1

Complex TSDE (N-attack)

Ru	0.072858	0.069768	0.479074
Cl	2.371179	0.819306	0.744035
C	-0.339596	1.850242	-0.854337
C	-1.271877	-0.546392	-1.306090

C	-1.752138	1.791378	-1.190722
C	-2.239875	0.551676	-1.437258
C	0.038086	-0.349723	-1.933331
N	0.500285	0.902152	-1.492821
S	0.886156	-1.340083	-2.967502
C	-0.479335	-1.873457	1.518716
C	-1.666987	-1.026903	1.456906
C	0.478137	-1.197619	2.287633
C	-1.426292	0.144605	2.213897
C	-0.080407	0.087571	2.678556
H	0.162516	2.780920	-0.622670
H	-1.635086	-1.567385	-1.351363
H	-2.351075	2.695659	-1.199631
H	-3.274692	0.348517	-1.693286
H	1.490841	1.105839	-1.625637
H	-0.358649	-2.836272	1.042328
H	-2.597870	-1.279852	0.970443
H	1.491987	-1.520241	2.474922
H	-2.113162	0.968871	2.347042
H	0.430597	0.843943	3.255946

Zero-point correction= 0.176390
 (Hartree/Particle)
 Thermal correction to Energy= 0.189373
 Thermal correction to Enthalpy= 0.190317
 Thermal correction to Gibbs Free Energy= 0.135991
 Sum of electronic and zero-point Energies= -1394.936252
 Sum of electronic and thermal Energies= -1394.923269
 Sum of electronic and thermal Enthalpies= -1394.922324
 Sum of electronic and thermal Free Energies= -1394.976650

Nimag = 1

Complex C (S-attack)

Ru	0.032292	0.099804	0.376440
Cl	2.227467	-0.159923	1.425663
C	0.825337	1.762497	-0.197017
C	-0.808346	0.380479	-1.614344
C	0.447034	2.424530	-1.400618
C	-0.412754	1.695623	-2.160017
C	-1.321302	-1.450113	1.687165
C	-2.091932	-0.657863	0.797970
C	-0.638845	-0.572947	2.559471
C	-1.927212	0.731906	1.162831
C	-1.016982	0.778968	2.260367
C	-0.186299	-0.799111	-2.365444
S	0.865653	-1.549128	-1.163065
N	-0.466317	-1.063953	-3.575023
H	1.629173	2.201053	0.397411
H	-1.896856	0.268915	-1.645880
H	0.862718	3.382341	-1.705225
H	-0.786953	2.016629	-3.130897
H	-1.194337	-2.522024	1.636647
H	-2.722083	-1.036263	0.005757
H	0.100822	-0.862223	3.291927
H	-2.441989	1.572848	0.719753
H	-0.684728	1.660688	2.788900
H	0.048029	-1.884750	-3.906029

Zero-point correction= 0.175163
 (Hartree/Particle)
 Thermal correction to Energy= 0.188920

Thermal correction to Enthalpy=	0.189864
Thermal correction to Gibbs Free Energy=	0.133899
Sum of electronic and zero-point Energies=	-1394.949397
Sum of electronic and thermal Energies=	-1394.935641
Sum of electronic and thermal Enthalpies=	-1394.934696
Sum of electronic and thermal Free Energies=	-1394.990661

Nimag = 0

Complex D (S-attack)

Ru	0.021621	0.003599	0.415738
Cl	2.264788	-0.197686	1.389677
C	1.090225	1.099270	-0.985474
C	-1.218011	0.246529	-1.441401
C	0.316436	2.009179	-1.853044
C	-0.938512	1.585847	-2.049001
C	-1.234590	-1.252458	2.037263
C	-2.053342	-0.539237	1.125388
C	-0.406612	-0.306280	2.675132
C	-1.787247	0.885940	1.270104
C	-0.747573	1.025748	2.222026
C	-0.488113	-0.856051	-2.144735
S	1.265259	-0.700123	-1.669981
N	-1.035149	-1.805684	-2.783358
H	2.093985	1.398777	-0.697175
H	-2.275134	0.001130	-1.366207
H	0.759728	2.889437	-2.310596
H	-1.672461	2.072835	-2.686086
H	-1.179845	-2.326048	2.144982
H	-2.794767	-0.983614	0.477031
H	0.395195	-0.535775	3.360533
H	-2.305312	1.688737	0.765869
H	-0.306784	1.946767	2.574243
H	-0.361367	-2.499120	-3.113917

Zero-point correction=	0.176101
(Hartree/Particle)	
Thermal correction to Energy=	0.189520
Thermal correction to Enthalpy=	0.190464
Thermal correction to Gibbs Free Energy=	0.135617
Sum of electronic and zero-point Energies=	-1394.926350
Sum of electronic and thermal Energies=	-1394.912931
Sum of electronic and thermal Enthalpies=	-1394.911987
Sum of electronic and thermal Free Energies=	-1394.966834

Nimag = 0

Complex E (S-attack)

Ru	-0.078613	-0.000070	-0.580496
C	-1.892942	-0.571217	0.455404
C	-1.719888	0.843694	0.565580
C	-0.542225	1.337068	1.190118
C	0.017091	0.755807	2.435539
C	-0.967492	-0.521929	-2.551256
C	-0.853651	0.909414	-2.459957
C	0.534213	1.244654	-2.396877
C	1.259926	0.019383	-2.432111
C	0.347552	-1.076720	-2.536188
Cl	2.120392	-0.340785	0.410664
S	-0.224596	-1.014532	2.648203
C	-0.871230	-1.381355	1.014878

N	0.594407	1.516858	3.277558
H	-2.701020	-0.981156	-0.142847
H	-2.404040	1.514032	0.055300
H	-0.325197	2.397224	1.100771
H	-1.890444	-1.078566	-2.644660
H	-1.676551	1.611564	-2.473745
H	0.957826	2.235948	-2.326554
H	2.331150	-0.072079	-2.334247
H	0.610807	-2.122520	-2.597247
H	-0.874148	-2.447689	0.812310
H	0.948504	1.001365	4.086504

Zero-point correction= 0.177146
(Hartree/Particle)
Thermal correction to Energy= 0.190330
Thermal correction to Enthalpy= 0.191274
Thermal correction to Gibbs Free Energy= 0.136130
Sum of electronic and zero-point Energies= -1394.983195
Sum of electronic and thermal Energies= -1394.970011
Sum of electronic and thermal Enthalpies= -1394.969066
Sum of electronic and thermal Free Energies= -1395.024211

Nimag = 0

Complex TSBC (S-attack)

Ru	0.021043	0.042259	-0.363129
Cl	-1.869556	1.527410	-0.870729
C	0.804234	1.789054	0.285507
C	1.233110	-0.512663	1.271927
C	1.740685	1.786113	1.278510
C	1.993576	0.488234	1.815567
C	-0.342738	-0.555013	-2.638015
C	-0.184425	-1.790173	-1.981759
C	0.833233	0.248471	-2.413303
C	1.063914	-1.758980	-1.295633
C	1.726584	-0.515474	-1.602210
C	-0.634957	-0.690668	2.606050
S	-1.565423	-0.855832	1.258003
N	-0.344954	-0.645323	3.783522
H	0.474978	2.709060	-0.193483
H	1.415202	-1.559620	1.506652
H	2.225911	2.685858	1.652608
H	2.709985	0.310921	2.617228
H	-1.225769	-0.225522	-3.166352
H	-0.920637	-2.580571	-1.927069
H	1.015732	1.231328	-2.823282
H	1.473677	-2.557364	-0.693500
H	2.718654	-0.224944	-1.287864
H	-0.968986	-0.337335	4.522575

Zero-point correction= 0.170980
(Hartree/Particle)
Thermal correction to Energy= 0.185307
Thermal correction to Enthalpy= 0.186251
Thermal correction to Gibbs Free Energy= 0.129057
Sum of electronic and zero-point Energies= -1394.909814
Sum of electronic and thermal Energies= -1394.895487
Sum of electronic and thermal Enthalpies= -1394.894543
Sum of electronic and thermal Free Energies= -1394.951737

Nimag = 1

Complex TSCD (S-attack)

Ru	0.016047	0.047662	0.416879
Cl	2.207152	-0.187029	1.508683
C	1.088575	1.270462	-0.761779
C	-1.100334	0.297429	-1.508540
C	0.452949	2.082978	-1.770626
C	-0.768126	1.614531	-2.105080
C	-1.235003	-1.327195	1.913384
C	-2.056041	-0.663119	0.973313
C	-0.538304	-0.327037	2.635942
C	-1.914874	0.775752	1.167088
C	-0.969708	0.976315	2.204089
C	-0.366377	-0.823429	-2.223986
S	1.272610	-0.912427	-1.512161
N	-0.949003	-1.596494	-3.047565
H	2.131461	1.456984	-0.515233
H	-2.167568	0.080439	-1.500175
H	0.947876	2.922960	-2.251051
H	-1.415930	2.061575	-2.856587
H	-1.090547	-2.394232	2.001024
H	-2.709706	-1.145387	0.260429
H	0.232535	-0.509381	3.369302
H	-2.468187	1.546412	0.650074
H	-0.634014	1.921641	2.604257
H	-0.328844	-2.344450	-3.367638

Zero-point correction= 0.175335
(Hartree/Particle)

Thermal correction to Energy= 0.188311
Thermal correction to Enthalpy= 0.189256
Thermal correction to Gibbs Free Energy= 0.135099
Sum of electronic and zero-point Energies= -1394.923925
Sum of electronic and thermal Energies= -1394.910949
Sum of electronic and thermal Enthalpies= -1394.910005
Sum of electronic and thermal Free Energies= -1394.964161

Nimag = 1

Complex TSDE (S-attack)

Ru	0.020083	-0.130588	-0.496470
Cl	2.307344	-0.213751	-0.042691
C	-1.226261	-1.046108	0.935156
C	-0.194812	1.266803	1.171031
C	-2.233382	0.054223	0.992147
C	-1.672628	1.284933	1.118935
C	0.872373	0.046737	-2.854314
C	0.280348	1.230784	-2.374906
C	-0.086280	-1.003496	-2.793714
C	-1.088095	0.928745	-2.022424
C	-1.308222	-0.466387	-2.300743
C	0.364472	0.532103	2.365201
S	-0.249177	-1.166268	2.479506
N	1.186755	1.086384	3.158681
H	-1.608808	-2.034222	0.677805
H	0.303853	2.229193	1.066303
H	-3.304651	-0.126080	0.929722
H	-2.244591	2.209910	1.142627
H	1.917829	-0.078223	-3.098400
H	0.761723	2.192347	-2.265251
H	0.091244	-2.036392	-3.062161
H	-1.838488	1.649097	-1.728893

H	-2.243524	-0.999449	-2.198557
H	1.491361	0.459033	3.906141

Zero-point correction=	0.174150
(Hartree/Particle)	
Thermal correction to Energy=	0.187413
Thermal correction to Enthalpy=	0.188357
Thermal correction to Gibbs Free Energy=	0.133411
Sum of electronic and zero-point Energies=	-1394.907296
Sum of electronic and thermal Energies=	-1394.894032
Sum of electronic and thermal Enthalpies=	-1394.893088
Sum of electronic and thermal Free Energies=	-1394.948035

Nimag = 1