Supporting information

Mechanism investigation of ketone hydrogenation catalyzed by ruthenium bifunctional catalysts: insights from a DFT study

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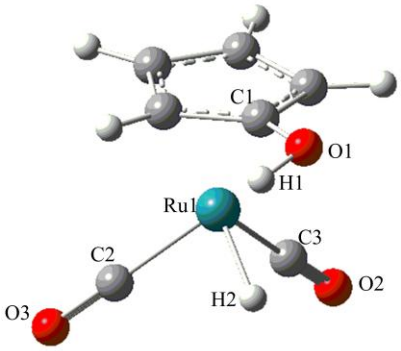
Abbreviations:

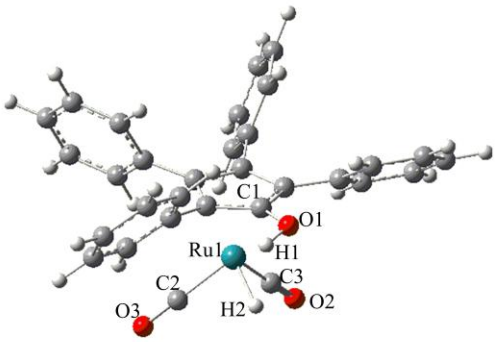
DFT: density function theory; HT: hydrogen transfer; DH: dehydrogenation; DA: dihydrogen activation; AHT: alcohol-assisted hydrogen transfer; DHT: direct hydrogen transfer; ADH: alcohol-assisted dehydrogenation; DDH: direct dehydrogenation; ADA: alcohol-assisted dihydrogen activation; DDA: direct dihydrogen activation; CD: charge difference; DPT: distance of proton transfer.

Index:

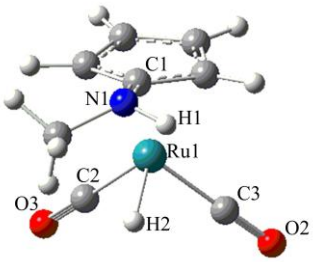
Fig. S1 Structural data of simplified and full models of **D** and **E**.



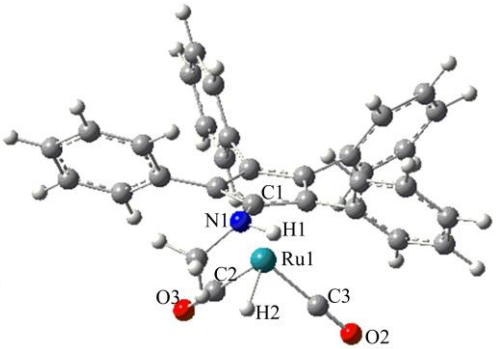
D (simplified model)



D (full model)



E (simplified model)

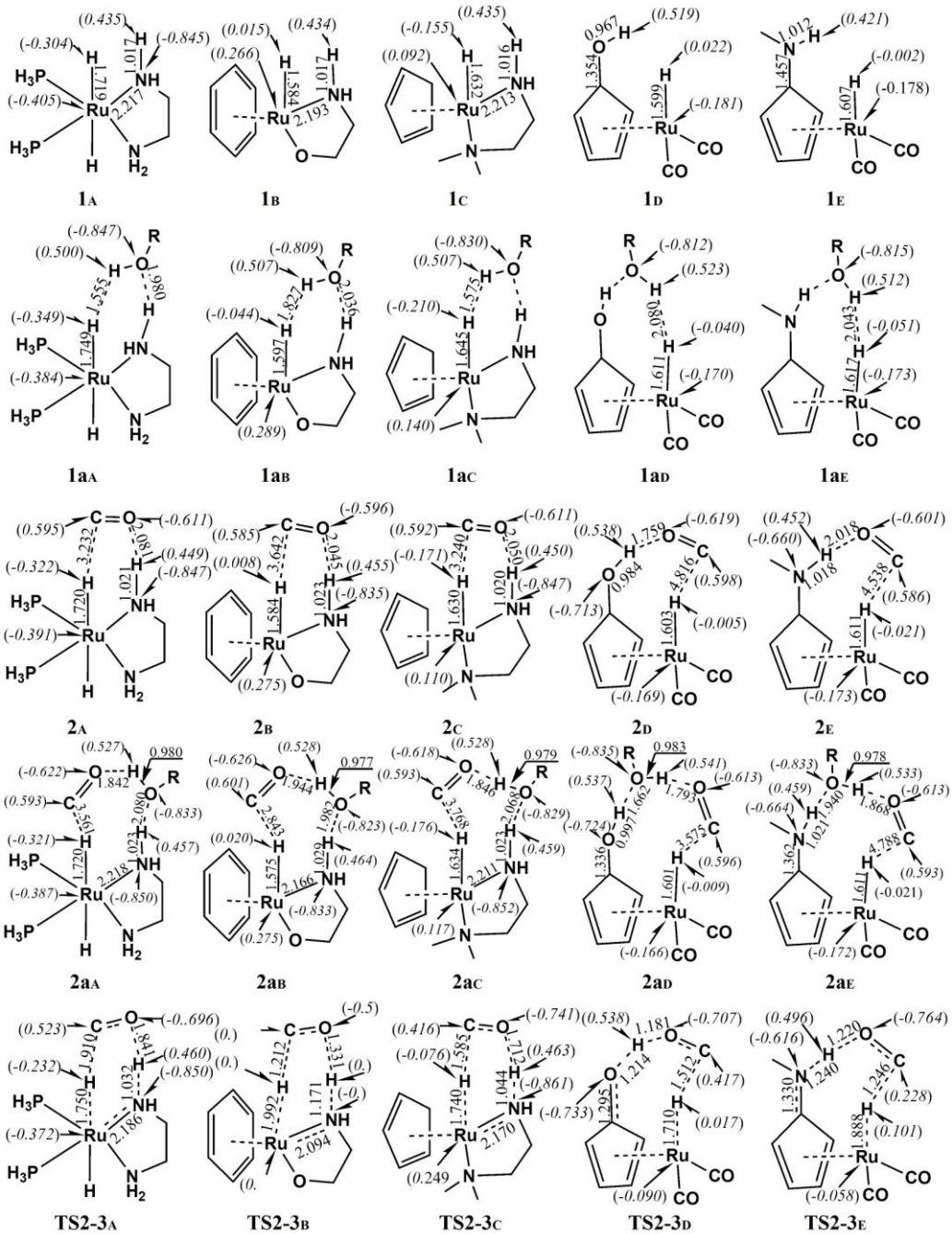


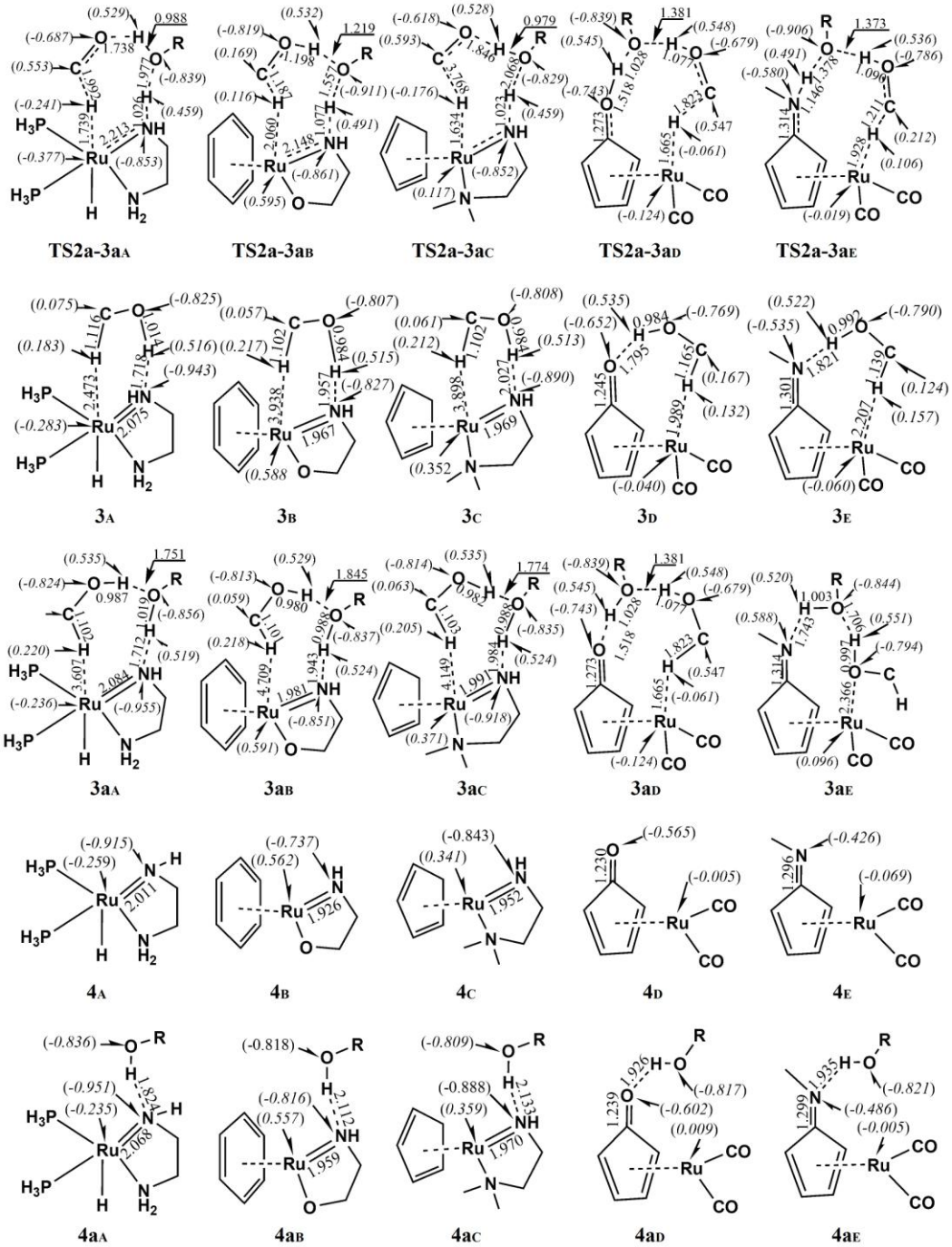
E (full model)

		C^1-N^1(O^1)	H^1-N^1(O^1)	Ru^1-H^2	Ru^1-C^2	Ru^1-C^3	C^2-O^3	C^3-O^2	∠C^1-N^1(O^1)-H^1	∠C^2-Ru^1-H^2
D	S	1.354 Å	0.967 Å	1.600 Å	1.888 Å	1.889 Å	1.157 Å	1.156 Å	110.36 °	85.30 °
	F	1.355 Å	0.969 Å	1.601 Å	1.884 Å	1.889 Å	1.158 Å	1.157 Å	109.40 °	84.66 °
E	S	1.376 Å	1.012 Å	1.607 Å	1.889 Å	1.888 Å	1.158 Å	1.158 Å	113.15 °	85.45 °
	F	1.385 Å	1.014 Å	1.608 Å	1.887 Å	1.886 Å	1.158 Å	1.158 Å	110.51 °	84.36 °

Fig. S2 Structural geometries of the intermediates and transition states of catalytic cycles of **A-E** systems.

(plain text : distance, Å; italic text in parentheses: NPA charge)




TS2a-3aA
TS2a-3aB
TS2a-3aC
TS2a-3aD
TS2a-3aE
3A
3B
3C
3D
3E
3aA
3aB
3aC
3aD
3aE
4A
4B
4C
4D
4E
4aA
4aB
4aC
4aD
4aE

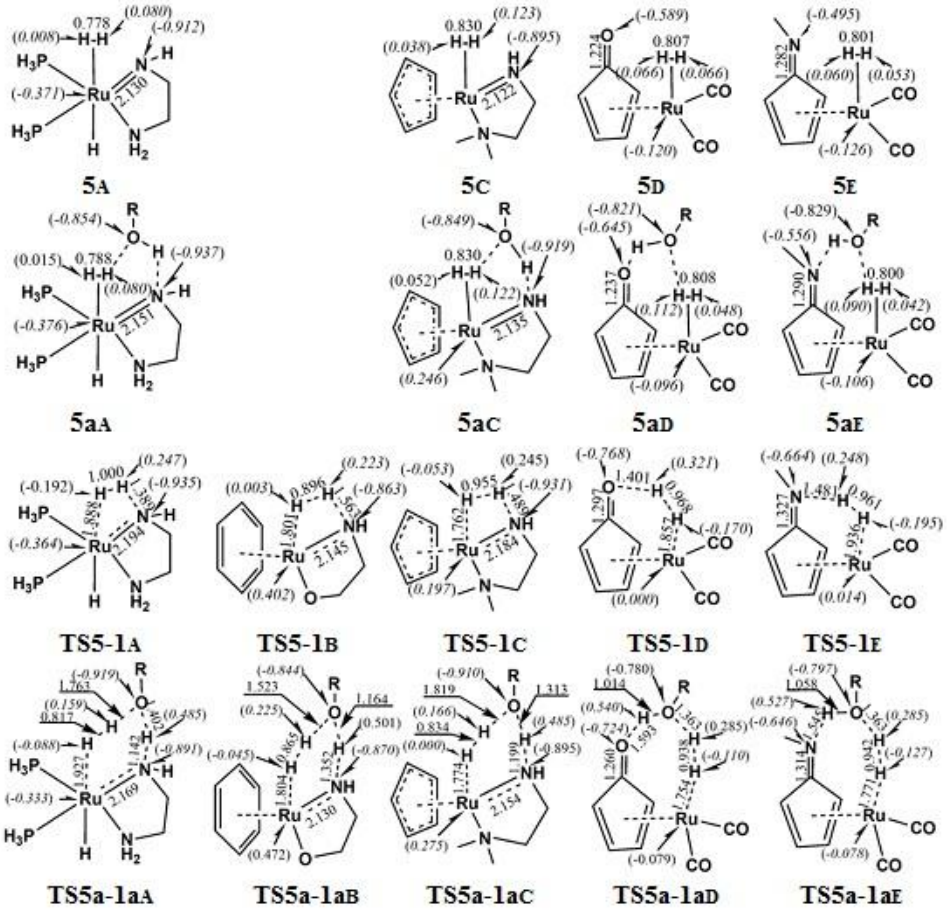
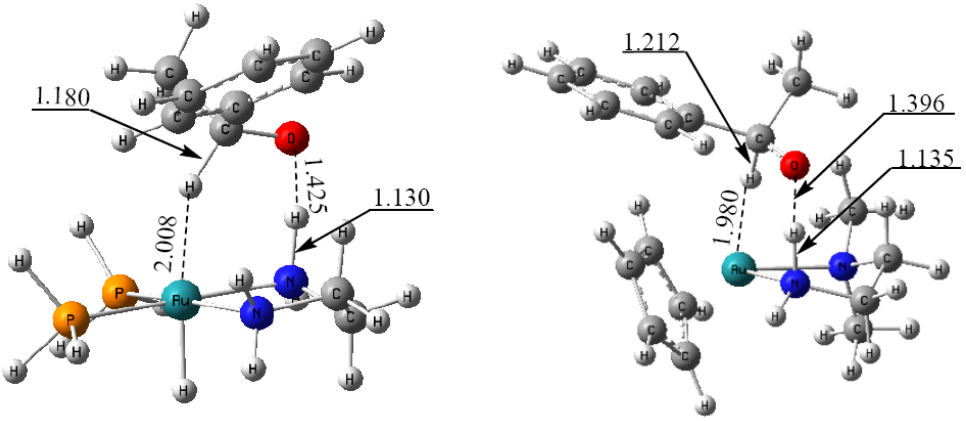
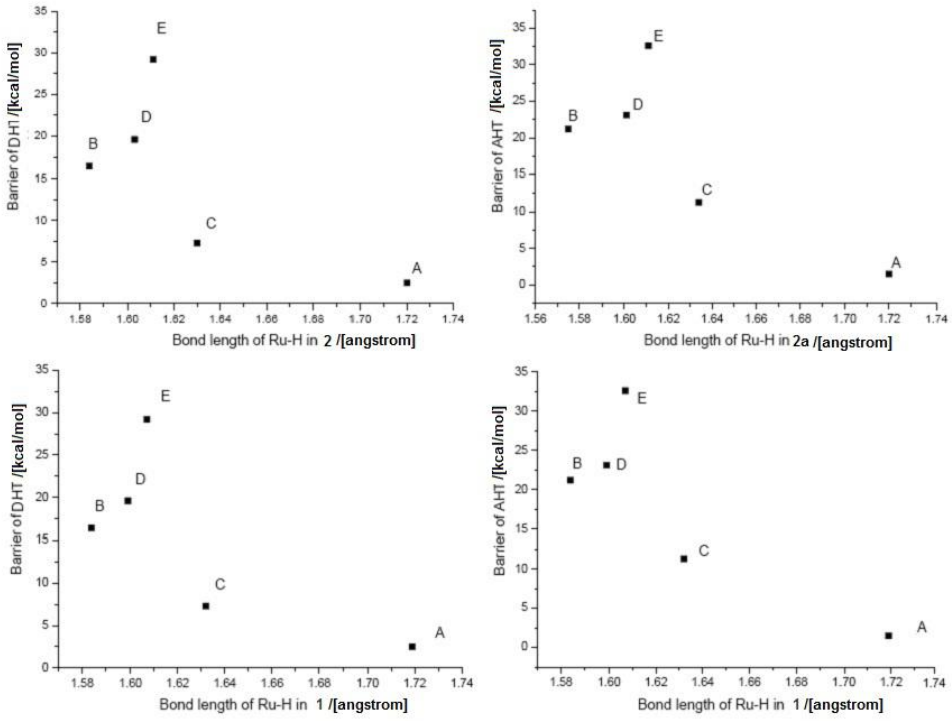

5A
5C
5D
5E
5aA
5aC
5aD
5aE
TS5-1A
TS5-1B
TS5-1C
TS5-1D
TS5-1E
TS5a-1aA
TS5a-1aB
TS5a-1aC
TS5a-1aD
TS5a-1aE

Figure S3 The structures of intermediates in which only the hydride H^3 transfers to C^5 but proton H^4 does not, for **A** and **C** systems.



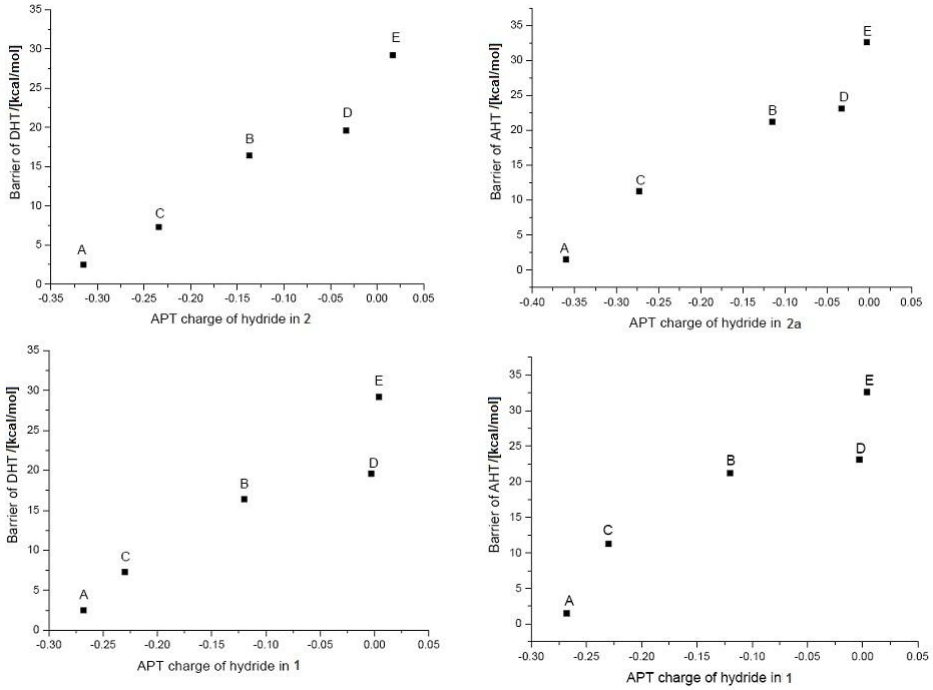
For A and C, the hydrogen transfers proceed via a stepwise mechanism (ref 46) in which hydride H^3 transferring to C^5 in carbonyl precedes proton H^4 transferring to O^6 in carbonyl. As shown in the figure above, the C-H distances are 1.180 and 1.212 Å, and the N-H distances are 1.130 and 1.135 Å, for A and C respectively. These intermediate are formed after hydride transferring to carbonyl. These intermediates can change to complexes **3** via a transition state for proton transfer.

Figure S4 The correlations between barriers of HT (hydrogen transfer) step and Ru-H bond length in **1**, **2** and **2a**.



The alcohol in complexes **2** and **2a** do not change the Ru-H bond length notably. And the correlations above imply that longer Ru-H bond in **1** will lead to lower energy barrier of hydrogen transfer generally.

Figure S5 The correlations between barriers of HT (hydrogen transfer) and charges on the hydride in **1**, **2** and **2a**. (barrier unit:kcal/mol)



The alcohol in complex **2** and **2a** increases the negative charge on hydride slightly; The correlations shown above give the similar tendency: The more negative the charge hydride carries, the lower the energy barrier of the hydrogen transfer is.

Table S1 Energy barriers of the whole catalytic reaction for all systems. (unit: kcal/mol)

	A	B	C	D	E
Electronic energy barrier					
DHT	2.5	16.4	7.3	19.6	29.2
AHT	1.5	21.2	11.2	23.1	32.6
DDA	11.4	17.5	6.4	31.7	31.1
DDH	12.2	12.5	12.9	8.5	4.8
ADH	12.0	15.8	15.7	14.2	17.8
ADA	6.7	13.3	5.5	4.6	7.5
Enthalpy barrier					
DHT	1.7	14.5	7.7	15.6	24.8
AHT	0.9	17.7	9.9	19.9	26.5
DDH	9.7	8.7	9.6	3.7	1.2
ADH	9.4	11.2	13.0	8.7	10.6
DDA	9.9	18.4	5.2	29.2	28.9
ADA	4.8	12.4	2.7	3.0	5.9
Free energy barrier					
DHT	5.5	17.8	6.4	20.4	30.5
AHT	6.4	21.5	13.8	26.4	34.7
DDH	12.1	13.4	12.5	5.3	3.1
ADH	12.3	16.1	16.6	10.3	13.7
DDA	11.0	27.6	5.9	29.9	30.6
ADA	6.4	23.2	3.5	5.8	7.6
Electronic energy barrier with solvent effect (ethanol)					
DHT	3.8	16.0	6.0	19.5	26.1
AHT	3.1	18.5	9.9	22.8	30.6
DDH	11.0	10.6	11.0	10.0	5.0
ADH	9.9	14.1	13.2	18.4	15.7
DDA	12.2	18.4	8.9	32.7	31.8
ADA	4.0	14.1	4.8	5.6	7.4
Electronic energy barrier with solvent effect (benzene)					
DHT	2.7	16.2	6.9	19.8	27.4
AHT	1.9	20.3	10.9	23.0	30.5
DDH	11.9	11.8	12,1	8.9	5.5
ADH	11.5	15.2	14.8	14.6	15.8
DDA	11.5	17.6	6.9	32.1	31.3
ADA	5.4	12.9	5.1	4.8	7.4

Table S2 Absolute electronic energies of all structures for A-E systems. (unit: a.u)

	A	B	C	D	E
1	-971.9573	-536.5528	-557.1923	-589.9804	-609.4318
2	-1356.8838	-921.4766	-942.1169	-974.9127	-994.3583
TS2-3	-1356.8798	-921.4505	-942.1053	-974.8814	-994.3118
3	-1356.8992	-921.4704	-942.1259	-974.8949	-994.3195
4	-970.7641	-535.3397	-555.9952	-588.7601	-608.1907
5	-971.9409	-	-557.1600	-589.9543	-609.3779
TS5-1	-971.9228	-536.4903	-557.1498	-589.9038	-609.3284
1a	-1166.3544	-730.9400	-751.5865	-784.3749	-803.8205
2a	-1551.2739	-1115.8674	-1136.5075	-1169.3053	-1188.7481
TS2a-3a	-1551.2714	-1115.8336	-1136.4895	-1169.2685	-1188.6962
3a	-1551.2906	-1115.8588	-1136.5146	-1169.291	-1188.7246
4a	-1165.1554	-729.7274	-750.3812	-783.1485	-802.5799
5a	-1166.3397	-	-751.5578	-784.3438	-803.7683
TS5a-1a	-1166.3290	-730.8847	-751.5490	-784.3364	-803.7564

Cartesian coordinates of all stationary points optimized at B3LYP/BSI level.

1_A

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.179141	-0.000116	0.001713
P	-1.733049	1.639730	0.032491
N	1.530424	1.410512	0.069415
P	-1.733514	-1.639460	-0.034409
N	1.530521	-1.410689	-0.069426
C	2.759754	-0.689367	0.324209
C	2.758738	0.689517	-0.327654
H	1.375160	-2.206450	0.543065
H	1.598499	1.749619	1.025424
H	-2.645541	1.837113	1.107781
H	-1.269306	2.989266	-0.002374
H	-2.660398	-1.815316	-1.100972
H	-2.688124	-1.820116	1.005885
H	2.737352	-0.584099	1.413861
H	3.672900	-1.235049	0.047721
H	3.672513	1.235370	-0.053584
H	2.733391	0.584331	-1.417248
H	-0.092201	0.066719	-1.714579
H	-0.089236	-0.066828	1.717356
H	-2.701456	1.799941	-0.998232
H	-1.269846	-2.989447	-0.032030
H	1.373203	2.206420	-0.542434
H	1.596158	-1.750062	-1.025509

2_A

	Coordinates (Angstroms)		
	X	Y	Z
Ru	1.962146	0.140388	0.153706
P	2.912038	-1.597321	-0.933552

N	1.045289	0.960217	-1.689402
P	2.833104	-0.452772	2.155259
N	1.015229	1.982088	0.942249
C	0.070343	2.508139	-0.069701
C	0.700888	2.379354	-1.451359
H	0.533077	1.805356	1.818931
H	0.201990	0.438991	-1.934938
H	2.462983	-2.948875	-0.850702
H	2.920282	-1.548641	-2.359368
H	4.228285	-0.653595	2.354964
H	2.427680	-1.609155	2.882083
H	-0.834924	1.895955	-0.022272
H	-0.206675	3.553532	0.126140
H	0.011950	2.768477	-2.213283
H	1.630279	2.957277	-1.491246
H	3.341391	1.097375	-0.209633
H	0.490665	-0.683325	0.490264
H	4.292870	-1.911496	-0.794170
H	2.666780	0.453406	3.245848
H	1.695003	0.891523	-2.468056
H	1.764507	2.646288	1.118447
C	-2.197728	-0.934488	-1.285330
O	-1.798288	-0.110086	-2.107737
C	-1.588875	-2.315527	-1.226052
H	-2.331162	-3.095751	-1.035713
H	-1.071288	-2.513268	-2.166407
H	-0.843979	-2.315992	-0.418467
C	-3.279854	-0.561283	-0.318773
C	-4.017756	0.612616	-0.550518
C	-3.567788	-1.337312	0.815997
C	-5.026557	0.998901	0.330062
H	-3.788454	1.203595	-1.431375
C	-4.569653	-0.942591	1.705196
H	-2.997958	-2.237551	1.019603
C	-5.302942	0.222444	1.461916
H	-5.598645	1.902022	0.137102
H	-4.776875	-1.542992	2.586225
H	-6.087146	0.524222	2.150664

TS2-3$_A$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.520975	-0.041146	-0.316503
P	-2.876984	-0.663219	1.387055
N	-1.277541	1.993741	0.445324
P	-1.644544	-2.065693	-1.339718
N	-0.320621	0.873330	-1.943690
C	0.169534	2.204998	-1.504792
C	-0.905798	2.890999	-0.671086
H	0.465228	0.284866	-2.208379
H	-0.506536	1.954818	1.130415
H	-2.453808	-1.441059	2.504203
H	-3.481388	0.371005	2.158118
H	-2.884454	-2.736298	-1.527157
H	-0.927692	-3.221324	-0.913145
H	1.055021	2.039429	-0.886292
H	0.455664	2.836582	-2.356389
H	-0.528800	3.858021	-0.310348
H	-1.801176	3.069351	-1.275078
H	-2.901842	0.447127	-1.153284
H	-0.022686	-0.416852	0.505698
H	-4.073378	-1.392749	1.150337
H	-1.230342	-2.148377	-2.701608
H	-2.108360	2.348356	0.912155
H	-0.932856	0.960362	-2.750592
C	1.337931	0.238921	1.674513
O	1.111783	1.456125	1.852629
C	0.939199	-0.751814	2.759344
H	1.719808	-0.728704	3.533594
H	-0.001432	-0.432543	3.210485
H	0.838637	-1.776433	2.399619
C	2.451593	-0.160941	0.727970
C	3.360211	0.828889	0.321747
C	2.651046	-1.479066	0.285004
C	4.437604	0.513625	-0.511669
H	3.213262	1.841180	0.684983
C	3.725151	-1.795828	-0.547304
H	1.946493	-2.254031	0.568501
C	4.623610	-0.799837	-0.950618
H	5.135871	1.291645	-0.809238
H	3.861439	-2.819585	-0.885604
H	5.461522	-1.048900	-1.596019

3_A

	Coordinates (Angstroms)		
	X	Y	Z

Ru	1.601356	0.036181	-0.334531
P	2.994676	0.028642	1.469891
N	1.092353	-1.950409	-0.019914
P	1.790328	2.310390	-0.743554
N	0.375621	-0.363783	-2.127980
C	-0.319955	-1.675051	-1.961789
C	0.620325	-2.625256	-1.233438
H	-0.298229	0.365524	-2.354107
H	-0.197749	-1.768071	1.099452
H	2.670947	0.632010	2.717151
H	3.365420	-1.235787	2.002550
H	3.048983	2.971190	-0.801616
H	1.158920	3.316854	0.046233
H	-1.206887	-1.492268	-1.350051
H	-0.641679	-2.080320	-2.929753
H	0.069246	-3.550518	-0.998575
H	1.447480	-2.909281	-1.908778
H	2.900813	-0.103324	-1.214305
H	-0.333174	0.346903	1.174504
H	4.304860	0.564526	1.375079
H	1.318597	2.819896	-1.989034
H	1.778165	-2.546036	0.442045
H	1.034602	-0.411402	-2.902800
C	-1.223329	-0.166019	1.610869
O	-0.982593	-1.548461	1.702018
C	-1.429929	0.405078	3.022450
H	-2.284697	-0.088878	3.496473
H	-0.541346	0.214245	3.632499
H	-1.622623	1.483195	2.998141
C	-2.412844	0.157784	0.704816
C	-2.543902	1.426621	0.119826
C	-3.408986	-0.797788	0.463866
C	-3.643647	1.736824	-0.685871
H	-1.778528	2.180079	0.297092
C	-4.511997	-0.490625	-0.339734
H	-3.297498	-1.783181	0.905108
C	-4.634165	0.776485	-0.918370
H	-3.727952	2.725329	-1.130368

H	-5.276557	-1.243185	-0.515371
H	-5.490343	1.013799	-1.543898

$2a_A$

	Coordinates (Angstroms)		
	X	Y	Z

Ru	2.173560	-0.963492	0.098161
P	3.213693	-0.353885	-1.813034
P	2.327646	-3.174101	-0.353889
H	3.684065	-0.991454	0.907261
H	4.457577	-0.918924	-2.211929
H	2.618152	-0.420534	-3.106484
H	3.630680	1.005057	-1.925745
H	1.621646	-3.820186	-1.410389
H	1.910863	-4.090145	0.659117
H	3.570128	-3.817310	-0.616866
N	1.986326	1.129708	0.806696
N	1.214121	-1.277029	2.072260
C	1.719967	1.107490	2.261437
C	0.693746	0.021410	2.559981
H	2.861999	1.615205	0.631460
H	0.464981	-1.961143	2.016821
H	1.928682	-1.638421	2.698821
H	2.661287	0.876609	2.771871
H	1.351644	2.076846	2.623042
H	-0.231086	0.229601	2.013541
H	0.463878	-0.001871	3.634544
O	-0.262707	3.050377	0.007453
C	-0.489242	4.461563	0.109216
C	-1.227731	4.990349	-1.123664
C	0.871221	5.125018	0.298501
H	-1.105669	4.659200	1.001471
H	-0.631161	4.819623	-2.027137
H	-2.191884	4.485440	-1.246962
H	-1.419100	6.066005	-1.031744
H	1.372508	4.733079	1.189490
H	1.511390	4.934128	-0.570476
H	0.761510	6.208394	0.415043
H	1.246435	1.658079	0.337571
H	-1.451172	1.317969	-2.322985

C	-1.782238	0.336491	-1.978769
C	-2.681008	0.503655	-0.785272
H	-0.884154	-0.223029	-1.652302
H	-2.259842	-0.206998	-2.797719
H	0.596643	-0.873011	-0.582551
O	-2.629657	1.528566	-0.096361
H	-1.121735	2.586735	-0.074451
C	-3.615862	-0.596512	-0.392822
C	-3.537494	-1.878731	-0.962094
C	-4.586409	-0.341858	0.592444
C	-4.413418	-2.886392	-0.552482
H	-2.782774	-2.099278	-1.709246
C	-5.468163	-1.344388	0.990590
H	-4.632186	0.650277	1.029394
C	-5.382503	-2.619960	0.419009
H	-4.339437	-3.877172	-0.991271
H	-6.221391	-1.135823	1.745035
H	-6.068622	-3.402633	0.730667

TS2a-3a$_A$

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.487372	-1.680628	0.131323
P	0.173130	-2.776535	-1.736534
P	-2.690532	-1.878230	-0.366139
H	-0.584444	-3.157937	0.951470
H	-0.466662	-3.970153	-2.171754
H	0.234054	-2.174292	-3.026528
H	1.497603	-3.299941	-1.765144
H	-3.372185	-1.072003	-1.324497
H	-3.634271	-1.665415	0.680082
H	-3.236420	-3.114266	-0.808060
N	1.577245	-1.529971	0.913284
N	-0.856476	-0.630468	2.044102
C	1.504605	-1.206268	2.356173
C	0.441908	-0.135179	2.567292
H	2.048094	-2.422381	0.789546
H	-1.495584	0.151031	1.911358
H	-1.285768	-1.282168	2.696184
H	1.229758	-2.119833	2.894049

H	2.470164	-0.852608	2.742897
H	0.701231	0.759341	1.993542
H	0.378310	0.136281	3.630198
O	3.190234	0.720411	-0.228344
C	4.396374	1.430828	0.067477
C	4.694431	2.474524	-1.013059
C	5.511949	0.398203	0.199488
H	4.279755	1.950446	1.033279
H	4.829683	1.986937	-1.985296
H	3.869611	3.189855	-1.098973
H	5.606340	3.034844	-0.774631
H	5.276914	-0.327583	0.985108
H	5.637966	-0.145792	-0.743574
H	6.462335	0.881327	0.450716
H	2.139288	-0.818079	0.432738
H	1.236809	1.172547	-2.399851
C	0.247480	1.620851	-2.298867
C	-0.044186	1.854244	-0.826765
H	-0.484392	0.978069	-2.787395
H	0.253728	2.598282	-2.803511
H	-0.330547	-0.101391	-0.579929
O	0.894895	2.149583	-0.056920
H	2.424827	1.344733	-0.237002
C	-1.450802	2.182792	-0.395695
C	-2.569141	1.998809	-1.225907
C	-1.643044	2.763120	0.870508
C	-3.845024	2.365966	-0.794130
H	-2.450565	1.555971	-2.208466
C	-2.919731	3.123355	1.306110
H	-0.770881	2.943882	1.490463
C	-4.027638	2.924280	0.475516
H	-4.698550	2.215234	-1.449396
H	-3.049007	3.574307	2.286593
H	-5.021313	3.209818	0.809239

$3a_A$

Coordinates (Angstroms)

	X	Y	Z
Ru	0.977520	-1.583666	0.115981
P	2.753578	-1.974933	-1.254504

P	-0.539681	-2.760052	-1.187916
H	1.286793	-2.975606	0.775279
H	3.069112	-3.288477	-1.689886
H	2.907449	-1.350798	-2.524392
H	4.049019	-1.647034	-0.767689
H	-1.104292	-2.257127	-2.397012
H	-1.785406	-3.148583	-0.619231
H	-0.225869	-4.042053	-1.718790
N	2.104672	-0.302780	1.311731
N	-0.475328	-1.149055	1.718049
C	1.571551	-0.209341	2.677798
C	0.059706	-0.056334	2.585679
H	3.101891	-0.507653	1.368395
H	-1.406968	-0.899121	1.387020
H	-0.569740	-2.010706	2.252007
H	1.813186	-1.101798	3.281901
H	1.978502	0.660367	3.220239
H	-0.196176	0.886472	2.095503
H	-0.410354	-0.074020	3.577604
O	1.754072	2.006760	-0.095609
C	2.776201	2.989077	0.084139
C	2.285472	4.298915	-0.528108
C	4.094467	2.520164	-0.541174
H	2.936408	3.146143	1.164089
H	2.106786	4.171425	-1.602210
H	1.349181	4.619073	-0.060367
H	3.028288	5.093170	-0.394520
H	4.426719	1.578495	-0.091193
H	3.965880	2.359006	-1.617729
H	4.886207	3.264361	-0.392912
H	1.950255	1.165141	0.445061
H	-1.056527	3.397546	-2.209889
C	-1.971042	2.904898	-1.863745
C	-1.616837	1.788083	-0.866003
H	-2.505262	2.510258	-2.735336
H	-2.605149	3.651977	-1.375173
H	-0.969992	1.058514	-1.378827
O	-0.930180	2.322851	0.256576
H	0.040207	2.320604	0.078297
C	-2.862113	1.049051	-0.392587
C	-3.505262	0.133393	-1.240195
C	-3.406544	1.282241	0.878393
C	-4.664414	-0.531706	-0.832487
H	-3.094293	-0.063754	-2.228210

C	-4.567541	0.616986	1.289289
H	-2.909518	1.986557	1.536942
C	-5.201229	-0.291671	0.437014
H	-5.146034	-1.238298	-1.503214
H	-4.978180	0.812805	2.276556
H	-6.102507	-0.807398	0.756556

4_A

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.158995	-0.011563	0.087754
P	-1.658189	1.725168	-0.186789
N	1.603697	1.289910	0.349946
P	-1.698853	-1.680035	-0.007137
N	1.336572	-1.294064	-0.313266
C	2.693775	-0.855183	-0.021464
C	2.768528	0.638837	-0.313572
H	1.259113	-2.306019	-0.243562
H	1.748032	1.325155	1.358157
H	-2.729206	2.048080	0.698488
H	-1.134419	3.052991	-0.227278
H	-2.725934	-1.760886	-0.990783
H	-2.536702	-1.965697	1.102534
H	2.989852	-1.028322	1.032893
H	3.441092	-1.373747	-0.643907
H	3.720044	1.075937	0.019089
H	2.656342	0.803956	-1.389554
H	-0.531644	0.180116	1.618182
H	-2.440318	1.862376	-1.371306
H	-1.214407	-3.005511	-0.193670
H	1.493867	2.250495	0.031883

5_A

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.158127	-0.005244	0.086433

P	-1.785783	-1.661211	-0.128329
N	1.554032	-1.405816	-0.066589
P	-1.615162	1.740968	-0.047362
N	1.476813	1.359095	0.133477
C	2.654887	0.727130	-0.443704
C	2.810004	-0.643401	0.198338
H	1.288397	2.207897	-0.398333
H	1.547593	-1.726137	-1.032789
H	-2.805547	-1.517744	-1.107928
H	-1.380931	-2.961502	-0.551291
H	-2.394873	2.205879	1.048321
H	-2.672444	1.738445	-0.994346
H	2.609901	0.581112	-1.544906
H	3.570674	1.311104	-0.243437
H	3.689909	-1.184504	-0.174843
H	2.897274	-0.526431	1.283331
H	-0.137242	0.053433	-1.508812
H	-2.662675	-2.142484	0.889929
H	-1.073149	3.005110	-0.401714
H	1.502133	-2.235382	0.520878
H	-0.236302	-0.286336	2.063909
H	0.223807	0.336613	1.988323

TS5-1$_A$

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-0.176409	-0.002761	0.025633
P	-1.693734	1.685011	-0.084303
N	1.534303	1.344880	0.291103
P	-1.764715	-1.654164	0.033061
N	1.539478	-1.389469	-0.207499
C	2.807367	-0.697089	0.153837
C	2.721226	0.758066	-0.300343
H	1.451776	-2.261075	0.309795
H	0.900826	0.781097	1.391184
H	-2.434180	2.176125	1.027539
H	-1.224144	2.952565	-0.523161
H	-2.894586	-1.610738	-0.828907
H	-2.491095	-2.041193	1.195338
H	2.896249	-0.733603	1.244124

H	3.678524	-1.200686	-0.284739
H	3.645480	1.272133	0.013409
H	2.694479	0.780440	-1.406777
H	-0.279922	-0.036209	-1.608696
H	0.232154	0.202144	1.857545
H	-2.795736	1.600532	-0.974508
H	-1.369235	-2.976550	-0.324263
H	1.407149	2.320570	0.044602
H	1.532989	-1.620506	-1.197900

$4a_A$

	Coordinates (Angstroms)		
	X	Y	Z

Ru	1.120079	0.031640	-0.134634
H	2.437741	0.447751	-0.888166
H	2.263665	-2.316915	-2.053099
H	0.524266	-3.052000	-1.103229
P	1.070255	-1.795047	-1.489831
H	0.343992	-1.686318	-2.708306
H	2.115639	-1.937800	2.336594
H	3.066682	-0.067104	2.468855
P	2.531775	-0.905285	1.445735
H	3.776114	-1.514936	1.119017
N	-0.405069	0.933323	-1.200466
C	-0.440577	2.391301	-1.058828
H	-0.533733	0.686828	-2.180353
N	1.069509	2.021116	0.817775
C	-0.184660	2.719042	0.406542
H	1.162551	2.021918	1.831639
H	1.880678	2.512258	0.445780
H	0.317980	2.901005	-1.682075
H	-1.419544	2.809297	-1.345171
H	-0.996005	2.313855	1.018209
H	-0.113630	3.801280	0.577276
O	-2.299866	0.080521	0.679401
H	-1.717756	0.313530	-0.096584
C	-3.324242	-0.822843	0.281378
H	-2.876149	-1.663016	-0.278563
C	-4.351423	-0.134091	-0.626723
H	-4.827249	0.698335	-0.095137

H	-3.868002	0.267902	-1.524040
H	-5.132719	-0.835049	-0.946083
C	-3.965287	-1.380880	1.550177
H	-4.406636	-0.567488	2.137793
H	-4.753959	-2.102675	1.309037
H	-3.212852	-1.878246	2.170276

$5a_A$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.141208	-0.094082	-0.003142
H	-1.746624	0.052261	-1.477448
H	-3.629509	-2.167314	-0.395244
H	-3.398924	-1.938146	1.684860
P	-3.125776	-1.190587	0.503548
H	-4.327031	-0.425339	0.563540
H	0.663176	-2.831155	0.078385
H	0.910372	-1.784864	-1.761082
P	-0.080388	-1.976398	-0.770204
H	-0.823376	-2.984920	-1.438604
N	-1.923855	1.938573	0.432252
C	-1.077478	2.926077	-0.300705
H	-2.900432	2.039366	0.166146
H	-1.875467	2.122870	1.433027
N	0.531935	1.073001	-0.684020
C	0.374237	2.447274	-0.216502
H	1.837364	0.258392	0.007825
H	0.507658	1.081079	-1.702880
H	-1.408243	2.921383	-1.343875
H	-1.208984	3.940151	0.105553
H	0.696141	2.502400	0.836819
H	1.014604	3.150235	-0.773563
O	2.482387	-0.321849	0.534000
C	3.813502	0.138416	0.367843
H	3.860748	1.221433	0.584802
C	4.690453	-0.589665	1.385780
H	4.666531	-1.669713	1.198243
H	5.731410	-0.250474	1.328381
H	4.320613	-0.413876	2.401049
C	4.308783	-0.079444	-1.069523

H	4.298887	-1.148436	-1.314109
H	3.660840	0.439528	-1.784401
H	5.331336	0.296877	-1.200439
H	-0.673107	-0.262493	1.868963
H	0.024973	-0.067037	1.561156

TS5a-1a$_A$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.101470	0.035735	-0.083484
P	1.016392	-1.976849	-1.172585
P	2.988096	-0.503565	1.121038
H	2.101184	0.557758	-1.228801
H	2.197207	-2.601438	-1.650847
H	0.432417	-3.122187	-0.578240
H	0.290624	-2.016589	-2.389843
H	2.996583	-1.356676	2.259270
H	3.730708	0.547532	1.730120
H	4.095577	-1.108677	0.472380
N	-0.580422	0.764945	-1.243585
N	0.955782	2.115097	0.662165
C	-0.695364	2.227586	-1.138461
C	-0.386853	2.644461	0.294317
H	-0.542771	0.497701	-2.224261
H	1.108287	2.208693	1.663900
H	1.685159	2.651927	0.197405
H	0.015223	2.713610	-1.821628
H	-1.703746	2.576953	-1.406046
H	-1.113843	2.192029	0.975212
H	-0.436791	3.735490	0.406689
O	-2.173885	-0.662107	0.081063
C	-3.401560	-0.327388	0.642870
C	-3.911635	-1.469231	1.539986
C	-4.445232	0.014643	-0.440329
H	-3.312634	0.575467	1.295455
H	-4.049983	-2.376812	0.939375
H	-3.174556	-1.692438	2.319364
H	-4.865522	-1.219780	2.024340
H	-4.095991	0.848081	-1.062758
H	-4.596867	-0.852061	-1.095701

H	-5.413514	0.297889	-0.005380
H	-1.439709	0.214286	-0.731011
H	-0.653075	-0.548681	0.965990
H	0.021476	-0.492047	1.422635

$\mathbf{1a_A}$

Coordinates (Angstroms)

	X	Y	Z
H	1.647140	-0.190466	-0.432354
O	2.489114	0.119580	0.002421
H	1.160685	1.057719	1.130948
H	4.756749	1.430297	-0.133049
Ru	-1.116834	-0.043792	0.092029
H	-2.400075	0.426093	1.098501
H	-1.837312	-2.597748	1.964335
H	0.025338	-2.965911	1.044567
P	-0.761345	-1.841795	1.423020
H	-0.099520	-1.614553	2.663721
H	-2.136770	-2.213825	-2.131369
H	-3.224037	-0.411582	-2.275981
P	-2.545147	-1.159054	-1.268101
H	-3.705457	-1.819165	-0.777412
N	0.178864	1.272555	1.323356
C	-0.119565	2.681261	0.986686
H	0.004626	1.107585	2.310734
N	-1.347113	1.886517	-0.974692
C	-0.276766	2.806616	-0.524364
H	-1.303494	1.759741	-1.982045
H	-2.265030	2.257296	-0.742082
H	-1.058373	2.952155	1.481639
H	0.665557	3.365159	1.337566
H	0.649212	2.492839	-1.015301
H	-0.482964	3.849976	-0.800738
H	0.209617	-0.399233	-0.987818
C	3.627791	-0.318968	-0.739981
H	3.530541	0.028188	-1.782228
C	3.725896	-1.847812	-0.742629
H	3.835527	-2.222362	0.281679
H	2.823882	-2.292996	-1.175498
H	4.588546	-2.184006	-1.330657

C	4.856294	0.340045	-0.119066
H	4.971630	0.019873	0.922984
H	5.765007	0.067491	-0.667087

$\mathbf{1_B}$

Coordinates (Angstroms)

	X	Y	Z
Ru	0.008431	0.003273	-0.272044
N	-1.713413	1.348662	-0.085745
O	-1.468181	-1.343959	0.188929
C	-2.862168	0.571927	0.473883
C	-2.737195	-0.850891	-0.077732
H	-1.532100	2.185939	0.462682
H	-2.741635	0.550033	1.561334
H	-3.820704	1.050360	0.228217
H	-3.501217	-1.491051	0.396955
H	-2.964298	-0.825790	-1.164841
C	1.614580	0.632301	1.507196
C	1.697231	1.395962	0.284105
C	1.601921	-0.754199	1.441163
C	2.003111	0.767969	-0.950832
C	1.689796	-1.406660	0.157706
C	1.982307	-0.661024	-1.010634
H	1.484753	1.142012	2.456659
H	1.645322	2.479490	0.328204
H	2.178162	1.357268	-1.842949
H	2.123845	-1.169867	-1.957033
H	1.584246	-2.483345	0.094474
H	1.438491	-1.348461	2.333841
H	-0.535885	-0.106109	-1.755986
H	-1.928128	1.654226	-1.031965

$\mathbf{2_B}$

Coordinates (Angstroms)

	X	Y	Z
Ru	-2.004507	-0.102204	-0.124639

N	-1.007640	1.273606	1.244571
O	-2.830242	1.676299	-0.735232
C	-1.654444	2.613329	1.119519
C	-2.068176	2.769097	-0.345418
H	-1.030724	0.953833	2.210034
H	-2.553151	2.608901	1.744605
H	-0.980042	3.409438	1.465412
H	-2.651138	3.699763	-0.463116
H	-1.148652	2.885736	-0.958492
C	-4.131179	-1.306874	0.165107
C	-3.377018	-1.599046	1.293785
C	-3.528196	-1.402267	-1.141185
C	-1.989729	-1.968511	1.137308
C	-2.237952	-1.965243	-1.297741
C	-1.454064	-2.272764	-0.141053
H	-5.142996	-0.927230	0.261343
H	-3.796228	-1.472454	2.287118
H	-1.377326	-2.130855	2.019024
H	-0.448084	-2.662676	-0.239897
H	-1.825767	-2.105222	-2.290377
H	-4.087104	-1.088254	-2.015005
H	-0.787394	0.287147	-1.059867
C	2.684699	0.982208	-0.208853
O	2.013853	1.235407	0.789860
H	-0.019531	1.334234	0.987927
C	2.222900	1.426767	-1.580328
H	2.967424	2.083584	-2.044722
H	2.083124	0.565541	-2.242386
H	1.273796	1.954835	-1.489413
C	3.975014	0.232361	-0.075214
C	4.765082	-0.104788	-1.187191
C	4.405350	-0.146366	1.208858
C	5.959197	-0.808781	-1.018437
H	4.452495	0.175863	-2.187735
C	5.597442	-0.847507	1.376715
H	3.788067	0.120966	2.060113
C	6.377219	-1.180673	0.262436
H	6.561605	-1.066473	-1.884602
H	5.921425	-1.135633	2.372632
H	7.306216	-1.728645	0.392654

TS2-3$_B$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-1.220607	-0.306155	-0.037330
N	-1.311346	1.285119	1.320557
O	-2.385634	0.946426	-1.084783
C	-2.411168	2.211490	0.946534
C	-2.423360	2.259511	-0.577404
H	-1.399764	1.008027	2.296944
H	-3.362299	1.813743	1.322923
H	-2.246850	3.206018	1.383223
H	-3.335237	2.758249	-0.940814
H	-1.561709	2.852695	-0.922311
C	-2.646957	-1.965774	0.158253
C	-1.818629	-1.939040	1.321344
C	-2.044081	-2.101845	-1.132550
C	-0.402501	-2.061281	1.208105
C	-0.643189	-2.159204	-1.254467
C	0.178046	-2.104570	-0.077212
H	-3.719741	-1.842581	0.247453
H	-2.273885	-1.804718	2.297298
H	0.228305	-1.998150	2.087037
H	1.256280	-2.064522	-0.180051
H	-0.180627	-2.169560	-2.234404
H	-2.664028	-2.039656	-2.019834
H	0.330402	0.842698	-0.530307
C	1.233255	1.606360	-0.262875
O	0.919507	2.286575	0.845946
H	-0.275548	1.817331	1.196858
C	1.332123	2.491537	-1.524103
H	2.211655	3.137783	-1.427302
H	1.420165	1.914659	-2.449913
H	0.446163	3.125967	-1.591644
C	2.439144	0.663541	-0.109653
C	2.941021	-0.093299	-1.181132
C	3.068483	0.554038	1.136907
C	4.040066	-0.940335	-1.010014
H	2.473990	-0.024720	-2.160209
C	4.167881	-0.292883	1.312717
H	2.682269	1.157093	1.952219
C	4.657552	-1.046081	0.241294
H	4.417300	-1.513043	-1.853620
H	4.647609	-0.358756	2.286188

H	5.514602	-1.700539	0.375126

3_B

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-1.604936	-0.102823	0.000479
N	-1.236460	1.501146	1.077127
O	-2.244585	1.268824	-1.282555
C	-1.872255	2.733267	0.575179
C	-1.880961	2.595845	-0.938612
H	-1.201052	1.474410	2.094706
H	-2.901955	2.818362	0.961597
H	-1.317452	3.628043	0.894823
H	-2.588668	3.298224	-1.403422
H	-0.874303	2.825123	-1.332521
C	-3.091089	-1.708660	0.030323
C	-2.418746	-1.691380	1.300584
C	-2.355133	-1.935845	-1.168271
C	-1.010778	-1.838315	1.356464
C	-0.950581	-1.991950	-1.118404
C	-0.274887	-1.890973	0.144452
H	-4.162376	-1.549428	-0.014251
H	-2.988969	-1.527734	2.208342
H	-0.488355	-1.757258	2.302873
H	0.808439	-1.865126	0.169591
H	-0.371261	-2.027188	-2.033518
H	-2.864564	-1.899421	-2.124373
H	1.644892	1.844698	-1.073817
C	2.313247	1.772497	-0.200893
O	1.613737	2.155857	0.974491
H	0.688574	1.822322	0.930211
C	3.465373	2.766445	-0.388657
H	4.130400	2.735697	0.480968
H	4.051868	2.527121	-1.281649
H	3.066920	3.781123	-0.484653
C	2.829920	0.336426	-0.129518
C	3.024569	-0.407743	-1.302154
C	3.158105	-0.249863	1.100749
C	3.538550	-1.707331	-1.250999
H	2.767257	0.031776	-2.263971

C	3.670694	-1.549905	1.156706
H	2.996542	0.321847	2.009447
C	3.863483	-2.284244	-0.018616
H	3.682265	-2.269409	-2.170174
H	3.922382	-1.989799	2.118426
H	4.261525	-3.294262	0.024913

$2a_B$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.723266	-0.033151	-0.107344
N	1.674817	2.132060	-0.162528
O	1.538140	0.380907	1.918208
C	2.081947	2.610089	1.188846
C	1.334237	1.733335	2.192423
H	2.253822	2.546285	-0.889397
H	3.162622	2.465218	1.291606
H	1.850975	3.677424	1.318409
H	1.682453	1.967866	3.213660
H	0.262769	2.017541	2.146658
C	3.680457	-1.542106	0.067305
C	3.944759	-0.694117	-0.998735
C	2.387595	-2.173604	0.170059
C	2.906760	-0.443533	-1.970789
C	1.455347	-2.092822	-0.891398
C	1.718514	-1.219136	-1.994111
H	4.404516	-1.671065	0.864865
H	4.889562	-0.163650	-1.064651
H	3.085683	0.270578	-2.768979
H	0.997526	-1.103308	-2.794354
H	0.519784	-2.637047	-0.834946
H	2.150507	-2.764060	1.047701
H	-1.451765	4.733625	-1.327928
C	-2.101788	3.941752	-0.934381
O	-1.203780	2.866189	-0.626873
H	0.706910	2.423125	-0.344076
C	-3.092466	3.527083	-2.025532
H	-3.741185	2.718884	-1.668085
H	-3.728191	4.370802	-2.319053
H	-2.557798	3.170886	-2.911720

C	-2.798439	4.453938	0.329142
H	-3.418762	5.329913	0.106333
H	-3.444948	3.677027	0.753702
H	-2.060169	4.736884	1.086130
H	0.162369	0.159889	-0.186509
H	-1.717409	2.107036	-0.288994
C	-2.354717	-0.361937	1.027897
O	-2.750883	0.588577	0.348907
C	-1.673123	-0.137835	2.352086
H	-1.897254	0.873201	2.696470
H	-1.991256	-0.860363	3.108996
H	-0.579206	-0.224645	2.224522
C	-2.545313	-1.760200	0.519146
C	-2.005263	-2.877664	1.177184
C	-3.282401	-1.954212	-0.661643
C	-2.196587	-4.162145	0.662600
H	-1.424097	-2.750194	2.084244
C	-3.479096	-3.236229	-1.171325
H	-3.691230	-1.083614	-1.163833
C	-2.935049	-4.344293	-0.510499
H	-1.771026	-5.018831	1.177619
H	-4.055384	-3.374419	-2.081911
H	-3.087310	-5.344336	-0.907209

TS2a-3a$_B$

Coordinates (Angstroms)

	X	Y	Z
Ru	0.079446	-1.494726	-0.020922
N	2.142988	-1.189185	0.489790
O	-0.002768	-1.907999	1.921687
C	2.373197	-1.618828	1.895151
C	1.073938	-1.366582	2.655153
H	2.754845	-1.706811	-0.137090
H	2.602185	-2.690218	1.901390
H	3.218397	-1.075213	2.336198
H	1.106164	-1.846675	3.644724
H	0.951512	-0.284683	2.814367
C	-0.301453	-3.441033	-0.955564
C	0.512947	-2.674817	-1.846778
C	-1.570620	-2.920203	-0.544010

C	0.084497	-1.404154	-2.321749
C	-1.977872	-1.640729	-0.971233
C	-1.124397	-0.868198	-1.828895
H	0.047224	-4.395192	-0.578029
H	1.491025	-3.052004	-2.128401
H	0.738839	-0.795450	-2.934008
H	-1.387995	0.158249	-2.057721
H	-2.882648	-1.192710	-0.578069
H	-2.161904	-3.462754	0.185324
H	4.576413	1.477673	-0.224678
C	3.687460	2.080001	-0.486772
O	2.543853	1.321736	-0.160775
H	2.373357	-0.152333	0.312035
C	3.748161	2.367540	-1.996036
H	2.883114	2.967120	-2.303516
H	4.660594	2.914133	-2.266361
H	3.728552	1.429223	-2.562002
C	3.747335	3.378789	0.332866
H	4.661682	3.946630	0.118988
H	2.884535	4.014529	0.102330
H	3.724787	3.152741	1.404457
H	-0.213948	0.453695	0.579534
H	1.455982	1.835198	-0.358013
C	-0.407253	1.624313	0.530559
O	0.309962	2.162221	-0.483103
C	0.012734	2.144745	1.924335
H	1.092103	2.027538	2.046811
H	-0.228920	3.212065	1.978953
H	-0.506676	1.628313	2.737662
C	-1.916736	1.755919	0.318611
C	-2.837261	1.127216	1.173152
C	-2.403973	2.547872	-0.729137
C	-4.212100	1.288458	0.985317
H	-2.477965	0.498511	1.984271
C	-3.781351	2.711373	-0.918759
H	-1.683223	3.033510	-1.378901
C	-4.690637	2.082760	-0.064048
H	-4.910333	0.797126	1.658322
H	-4.142415	3.334144	-1.733379
H	-5.759895	2.211589	-0.208627

$3a_B$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	1.866991	-0.600515	0.091096
N	2.349448	1.288289	0.441885
O	1.790311	-0.641838	2.067385
C	2.699273	1.563044	1.846851
C	1.818217	0.640303	2.673655
H	2.936705	1.810556	-0.205862
H	3.764399	1.343918	2.031897
H	2.527501	2.619147	2.108373
H	2.187803	0.546635	3.705569
H	0.795120	1.054726	2.719337
C	2.851746	-2.436143	-0.582302
C	3.091348	-1.410093	-1.560164
C	1.521233	-2.844652	-0.279588
C	1.997290	-0.755176	-2.177177
C	0.437604	-2.128059	-0.820492
C	0.680993	-1.050309	-1.737943
H	3.689760	-2.902479	-0.076674
H	4.108713	-1.114436	-1.791524
H	2.166932	0.069914	-2.859553
H	-0.151760	-0.452983	-2.090595
H	-0.574226	-2.328068	-0.488151
H	1.349299	-3.587492	0.490730
H	1.106797	4.010941	-1.178575
C	0.066301	3.796995	-0.885932
O	-0.079260	2.372594	-0.757521
H	0.674284	2.003660	-0.235715
C	-0.862401	4.252536	-2.007967
H	-1.904251	4.026598	-1.756735
H	-0.770048	5.331971	-2.169776
H	-0.615645	3.739178	-2.942677
C	-0.228948	4.502338	0.440934
H	-0.088856	5.585622	0.345382
H	-1.262860	4.312352	0.748801
H	0.437969	4.142957	1.232204
H	-2.331745	1.020187	1.474841
H	-1.812504	1.782707	-0.525901
C	-3.085388	0.859822	0.688520
O	-2.781314	1.661904	-0.444856
C	-4.448652	1.320296	1.220994
H	-5.209403	1.204237	0.441745

H	-4.753189	0.731366	2.092220
H	-4.400150	2.376691	1.503171
C	-3.109091	-0.631058	0.356486
C	-2.847746	-1.584533	1.351143
C	-3.449360	-1.075583	-0.928999
C	-2.939083	-2.952305	1.075397
H	-2.562627	-1.256219	2.348412
C	-3.538805	-2.442789	-1.209545
H	-3.636035	-0.337554	-1.703166
C	-3.288438	-3.386964	-0.207729
H	-2.732859	-3.676061	1.859555
H	-3.806316	-2.771594	-2.210542
H	-3.361016	-4.449126	-0.425158

4_B

Coordinates (Angstroms)

	X	Y	Z
Ru	0.022405	-0.048166	-0.032394
N	1.529943	-1.244622	-0.112957
O	1.487371	1.299502	0.182933
C	2.853621	-0.669821	0.164220
C	2.749912	0.801381	-0.213895
H	1.502099	-2.258941	-0.042852
H	3.099036	-0.786718	1.234613
H	3.639642	-1.180223	-0.413004
H	3.544347	1.393288	0.266835
H	2.871571	0.901379	-1.308696
C	-1.615252	0.507761	1.364662
C	-1.679238	-0.902613	1.096977
C	-1.713049	1.438845	0.297331
C	-1.817163	-1.368912	-0.233330
C	-1.751731	0.981104	-1.035503
C	-1.750626	-0.429754	-1.299555
H	-1.472453	0.859045	2.379766
H	-1.603773	-1.608376	1.916971
H	-1.819222	-2.432555	-0.443380
H	-1.724152	-0.780952	-2.325094
H	-1.696662	1.684676	-1.857686
H	-1.593659	2.497062	0.499653

TS5-1_B

Coordinates (Angstroms)

	X	Y	Z
Ru	0.032526	0.011334	-0.301736
N	-1.663651	1.322090	-0.235089
O	-1.446536	-1.329591	0.038860
C	-2.740943	0.627495	0.466509
C	-2.735040	-0.792240	-0.097168
H	-1.425446	2.222421	0.170942
H	-2.579878	0.575341	1.557440
H	-3.707333	1.125509	0.284395
H	-3.448793	-1.438342	0.437330
H	-3.048762	-0.747417	-1.159224
C	1.124834	-0.027780	1.664614
C	1.404784	1.208832	1.002586
C	1.397519	-1.246911	0.988030
C	2.011595	1.228225	-0.279945
C	1.965582	-1.254297	-0.309743
C	2.217318	-0.005425	-0.953072
H	0.653741	-0.035640	2.639796
H	1.148619	2.144425	1.489343
H	2.211243	2.167558	-0.781799
H	2.576007	0.001559	-1.977047
H	2.123456	-2.186720	-0.837171
H	1.085924	-2.183057	1.438369
H	-0.579382	0.113603	-1.992116
H	-1.096601	0.696794	-1.549991

$4a_B$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.030060	0.131232	-0.034336
N	-0.264053	1.125921	-1.117306
O	1.235582	1.913307	0.825568
C	-0.224864	2.588116	-0.949848
C	0.202317	2.822466	0.491121

H	-0.550565	0.843796	-2.052558
H	0.504311	3.034756	-1.647415
H	-1.204942	3.045113	-1.157872
H	0.559182	3.852444	0.642020
H	-0.665792	2.666754	1.157836
C	3.027304	-0.774469	-0.236433
C	2.176574	-1.308753	-1.264730
C	2.691713	-0.952030	1.134702
C	0.970002	-1.962814	-0.915909
C	1.448427	-1.518605	1.477731
C	0.563045	-1.979067	0.444868
H	3.926041	-0.232813	-0.508122
H	2.445002	-1.175308	-2.306903
H	0.286113	-2.302396	-1.685188
H	-0.432339	-2.325149	0.698645
H	1.119208	-1.528162	2.510339
H	3.311858	-0.500973	1.900779
H	-3.999943	0.309105	-1.098326
C	-3.799697	-0.282534	-0.188866
O	-2.469878	-0.805354	-0.253561
H	-1.831715	-0.071630	-0.362216
C	-4.746148	-1.478898	-0.171329
H	-4.564552	-2.091596	0.719131
H	-5.790861	-1.149898	-0.158520
H	-4.588414	-2.104666	-1.055281
C	-3.982292	0.622832	1.033379
H	-4.996917	1.037551	1.066092
H	-3.808107	0.056401	1.955310
H	-3.275771	1.459908	1.010017

TS5a-1a$_B$

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.864852	0.009646	-0.143663
N	0.645526	0.925083	1.046713
O	-0.666231	1.757167	-1.142712
C	0.807422	2.335480	0.632654
C	0.561169	2.375170	-0.872737
H	0.419169	0.881550	2.038826
H	0.067218	2.977268	1.131562

H	1.811813	2.707273	0.890683
H	0.527238	3.413679	-1.238842
H	1.399531	1.868571	-1.390334
C	-3.092186	0.141222	-0.413430
C	-2.784532	0.285610	0.968279
C	-2.673178	-1.002410	-1.137410
C	-2.026613	-0.739805	1.620625
C	-1.888627	-1.989228	-0.468704
C	-1.621340	-1.905277	0.924739
H	-3.579597	0.956363	-0.937281
H	-3.080763	1.178383	1.505412
H	-1.743335	-0.613373	2.660798
H	-1.017530	-2.659290	1.414762
H	-1.482603	-2.819188	-1.037176
H	-2.861320	-1.078883	-2.201181
H	3.485341	0.498976	-0.840111
C	3.561865	-0.412076	-0.218208
O	2.273978	-0.775894	0.257055
H	1.665277	0.092600	0.737857
C	4.490995	-0.107083	0.963579
H	4.593801	-0.994069	1.599301
H	5.487928	0.191756	0.617254
H	4.086627	0.705712	1.577058
C	4.105575	-1.543180	-1.093681
H	5.093205	-1.292267	-1.498524
H	4.193258	-2.464144	-0.505712
H	3.429965	-1.738475	-1.933168
H	0.448956	-0.526952	-1.257366
H	1.085356	-0.666222	-0.688621

$\mathbf{1a_B}$

Coordinates (Angstroms)

	X	Y	Z

Ru	-0.873626	0.028978	-0.109779
N	0.278971	1.241005	1.302582
O	-0.893239	1.835131	-1.077812
C	0.209973	2.668643	0.867701
C	0.140406	2.664819	-0.661131
H	-0.047261	1.140268	2.260722
H	-0.716217	3.093851	1.267240

H	1.062806	3.240415	1.259487
H	-0.035930	3.693608	-1.020735
H	1.125893	2.345688	-1.058563
C	-3.278422	-0.283631	-0.190134
C	-2.899448	-0.598801	1.110617
C	-2.557483	-0.848283	-1.302276
C	-1.769930	-1.470165	1.325712
C	-1.569865	-1.839284	-1.085996
C	-1.176301	-2.174202	0.248220
H	-4.055675	0.450116	-0.374640
H	-3.394023	-0.133196	1.957106
H	-1.430860	-1.666537	2.338060
H	-0.392625	-2.900107	0.429474
H	-1.072692	-2.299708	-1.932026
H	-2.795467	-0.535841	-2.312170
H	4.688886	-0.294533	1.144868
C	4.050991	-0.520963	0.281976
O	2.716163	-0.414986	0.801493
H	1.245581	0.906554	1.287686
C	4.338410	-1.949864	-0.184203
H	3.709016	-2.211663	-1.044205
H	5.385203	-2.058987	-0.489915
H	4.135779	-2.663020	0.620657
C	4.306403	0.517562	-0.812721
H	5.349666	0.482594	-1.146901
H	3.665709	0.332135	-1.683298
H	4.096180	1.526412	-0.444447
H	0.544326	-0.168226	-0.818127
H	2.066651	-0.598032	0.095905

$\mathbf{1}_{C}$

Coordinates (Angstroms)

	X	Y	Z
C	-1.806949	-0.857720	1.274020
C	-1.936318	-1.423581	-0.052421
C	-2.415118	-0.386589	-0.915273
C	-2.520227	0.822760	-0.152914
C	-2.160089	0.505206	1.212953
Ru	-0.389278	0.182767	-0.294370
N	1.663843	-0.743159	0.013277

C	1.926253	-1.827569	-0.960481
C	1.799565	-1.298756	1.378758
C	2.644917	0.351916	-0.201495
C	2.187077	1.653766	0.446995
N	0.852676	2.002561	-0.085831
H	0.402700	2.709155	0.489636
H	2.726617	0.505581	-1.281656
H	2.094961	1.539685	1.531223
H	2.810824	-1.708633	1.543910
H	1.594370	-0.529111	2.123483
H	1.066833	-2.096061	1.509321
H	3.640452	0.065945	0.176538
H	-2.657038	-0.496302	-1.963548
H	-2.909862	1.767449	-0.508004
H	-1.812345	-2.465214	-0.317675
H	-2.159292	1.198046	2.045578
H	-1.487854	-1.389423	2.161797
H	2.944166	-2.236211	-0.835233
H	1.198003	-2.625162	-0.807332
H	1.797255	-1.438917	-1.970090
H	2.935837	2.437240	0.259936
H	0.924596	2.378081	-1.027390
H	0.087701	0.289679	-1.851186

$\mathbf{2}_{C}$

Coordinates (Angstroms)

	X	Y	Z
C	2.584410	2.469413	-0.443971
C	2.276145	2.331997	0.964010
C	0.855203	2.375317	1.108023
C	0.271268	2.469755	-0.201518
C	1.361375	2.533865	-1.146661
Ru	1.336212	0.521620	0.022442
N	2.815889	-1.179498	0.313386
C	2.981453	-1.520852	1.743902
C	4.146062	-0.835846	-0.237648
C	2.240997	-2.347343	-0.406515
C	1.650890	-1.938264	-1.750981
N	0.628628	-0.897337	-1.513590
H	0.415628	-0.405260	-2.376969

H	1.437758	-2.749852	0.216833
H	2.421704	-1.519011	-2.405126
H	4.855310	-1.672665	-0.115907
H	4.064901	-0.583796	-1.295141
H	4.531516	0.038004	0.289275
H	3.000112	-3.136011	-0.538923
H	0.312766	2.352712	2.043375
H	-0.780172	2.581855	-0.428213
H	2.994233	2.307650	1.773811
H	1.256028	2.621384	-2.221782
H	3.573580	2.510148	-0.881559
H	3.662519	-2.380418	1.871131
H	3.390927	-0.656939	2.270062
H	2.005284	-1.748411	2.170575
H	1.234780	-2.824789	-2.250113
H	-0.238843	-1.330635	-1.194901
H	-3.558615	-0.002906	2.225137
C	-3.941930	0.119847	1.217787
C	-4.885203	1.117075	0.962501
C	-3.474024	-0.699395	0.176799
C	-5.380863	1.296761	-0.332015
H	-5.231233	1.753384	1.771801
C	-3.974970	-0.506380	-1.122460
C	-4.925370	0.480681	-1.374503
H	-6.118711	2.069552	-0.528760
H	-3.608260	-1.145728	-1.918879
H	-5.311661	0.617297	-2.380567
C	-2.451000	-1.767784	0.402721
O	-1.913596	-2.324724	-0.555248
C	-2.072854	-2.151161	1.816452
H	-1.375677	-1.397794	2.203743
H	-2.938023	-2.208564	2.483248
H	-1.560185	-3.114262	1.792387
H	0.398626	-0.356722	1.025890

TS1-2$_C$

Coordinates (Angstroms)

	X	Y	Z
C	1.628808	2.659243	-0.603507
C	1.500225	2.514921	0.821138

C	0.135191	2.269831	1.148265
C	-0.604705	2.223099	-0.091148
C	0.317634	2.454150	-1.155595
Ru	0.867078	0.572984	-0.109374
N	2.572891	-0.790780	0.535180
C	2.486612	-1.166846	1.963647
C	3.878321	-0.128707	0.308889
C	2.458989	-2.010682	-0.312161
C	2.152531	-1.648518	-1.760112
N	0.931128	-0.814926	-1.776137
H	0.824404	-0.360156	-2.679057
H	1.627247	-2.605776	0.072575
H	2.974261	-1.085547	-2.214121
H	4.710417	-0.806187	0.562219
H	3.970023	0.183887	-0.730854
H	3.942937	0.760629	0.937020
H	3.377911	-2.615121	-0.245922
H	-0.275067	2.164951	2.142831
H	-1.668177	2.060537	-0.192256
H	2.306796	2.606543	1.538330
H	0.062054	2.488335	-2.207571
H	2.526456	2.917260	-1.148597
H	3.296641	-1.862353	2.240016
H	2.566631	-0.266372	2.575578
H	1.522850	-1.633428	2.159737
H	2.021924	-2.572683	-2.339323
H	0.106687	-1.436201	-1.623719
H	-2.520832	-0.141516	2.206171
C	-3.042011	-0.124460	1.254171
C	-4.193010	0.655562	1.123297
C	-2.545142	-0.859748	0.166492
C	-4.869029	0.713833	-0.100427
H	-4.561556	1.220066	1.975871
C	-3.235324	-0.802363	-1.052451
C	-4.384760	-0.019616	-1.187856
H	-5.764720	1.320493	-0.202101
H	-2.859212	-1.392909	-1.881365
H	-4.907963	0.010598	-2.140209
C	-1.324081	-1.766646	0.267031
O	-0.991416	-2.430302	-0.765289
C	-1.118424	-2.449723	1.624806
H	-1.079866	-1.755547	2.467071
H	-1.955082	-3.142867	1.782821
H	-0.199391	-3.038904	1.595232

H	-0.244555	-0.626664	0.484241

$\mathbf{3}_{C}$

	Coordinates (Angstroms)		
	X	Y	Z

C	-2.152632	-2.629196	-0.316413
C	-2.229492	-2.277648	1.070638
C	-0.920679	-1.951591	1.522496
C	-0.008789	-2.145742	0.414417
C	-0.761353	-2.589314	-0.711469
Ru	-1.412277	-0.574514	-0.170344
N	-2.830254	1.156082	0.194696
C	-3.134349	1.376143	1.622976
C	-4.092221	0.893102	-0.534643
C	-2.143235	2.355701	-0.369924
C	-1.462139	2.002404	-1.686571
N	-0.762084	0.733531	-1.490084
H	-0.148884	0.516028	-2.271946
H	-1.374720	2.654191	0.348232
H	-2.198068	1.944996	-2.507430
H	-4.786528	1.744001	-0.435825
H	-3.883533	0.721618	-1.591294
H	-4.564042	-0.002322	-0.126158
H	-2.857675	3.186859	-0.484577
H	-0.648306	-1.639350	2.521472
H	1.062762	-1.998204	0.444958
H	-3.136801	-2.221578	1.657799
H	-0.367301	-2.847489	-1.685063
H	-2.981043	-2.938816	-0.939626
H	-3.792387	2.250340	1.757996
H	-3.631801	0.492512	2.027536
H	-2.204912	1.537455	2.171524
H	-0.770480	2.818590	-1.945036
H	0.747507	1.464493	-0.352147
H	3.316054	-0.748901	2.062776
C	3.672299	-0.585864	1.047170
C	4.590728	-1.478001	0.486046
C	3.200925	0.515682	0.318937
C	5.047474	-1.281694	-0.820815
H	4.943229	-2.327492	1.065133

C	3.663769	0.703532	-0.990520
C	4.579341	-0.188435	-1.556662
H	5.757458	-1.975718	-1.262059
H	3.292200	1.549181	-1.561372
H	4.927317	-0.030257	-2.574207
C	2.236434	1.507761	0.963246
O	1.372620	2.126979	0.019078
C	2.988348	2.635192	1.678746
H	3.669062	2.233782	2.436139
H	3.575100	3.210739	0.955140
H	2.275298	3.310315	2.162854
H	1.639519	0.958329	1.709468

$2a_C$

	Coordinates (Angstroms)		
	X	Y	Z

Ru	-1.617694	-0.974275	-0.196307
H	-0.716291	-0.369596	1.024897
N	-3.354043	-0.215587	1.050510
N	-1.706112	1.130682	-0.867913
C	-2.958318	1.765073	-0.401315
C	-3.265259	1.268180	1.006152
H	-0.904458	1.667857	-0.526956
O	0.465743	3.150106	-0.075982
H	1.290601	2.656484	0.111111
C	0.807757	4.380243	-0.728151
C	-2.284251	-2.553464	-1.800327
C	-2.140185	-3.145071	-0.497738
C	-0.779739	-3.031516	-0.074118
C	-0.069910	-2.294992	-1.090877
C	-1.014055	-1.987193	-2.125862
C	-3.262696	-0.669791	2.455545
C	-4.646302	-0.676256	0.495409
H	-1.657497	1.162444	-1.882755
H	-2.446312	1.563491	1.667670
H	-3.763498	1.496794	-1.092467
H	-5.494209	-0.280051	1.080006
H	-4.744225	-0.362834	-0.543690
H	-4.673477	-1.766374	0.521271
H	-4.195248	1.725150	1.383976

H	-0.357081	-3.453464	0.827276
H	0.988029	-2.073620	-1.108261
H	-2.919627	-3.661600	0.049893
H	-0.781464	-1.443607	-3.034497
H	-3.173496	-2.546114	-2.415698
H	-4.092346	-0.262776	3.059434
H	-3.302957	-1.760180	2.479603
H	-2.306753	-0.353630	2.871461
H	-2.884714	2.861220	-0.388828
H	1.380919	4.151379	-1.641103
C	1.667332	5.260842	0.182947
H	2.584792	4.738337	0.473249
H	1.952102	6.188552	-0.327437
H	1.115152	5.519758	1.093683
C	-0.498126	5.060432	-1.127287
H	-0.301226	6.003192	-1.648622
H	-1.083646	4.417500	-1.792742
H	-1.100198	5.277077	-0.237236
C	3.886983	-1.707240	1.140090
C	3.871080	-0.451515	0.509595
C	4.782754	-2.694364	0.724247
H	3.192525	-1.925602	1.944034
C	4.769704	-0.202920	-0.543393
C	5.677596	-2.433772	-0.317138
H	4.780505	-3.665100	1.211199
C	5.670133	-1.184650	-0.950072
H	4.742482	0.767482	-1.027683
H	6.376966	-3.201279	-0.636698
H	6.363944	-0.981529	-1.760763
C	2.915364	0.628027	0.906141
O	2.835466	1.651733	0.220788
C	2.030819	0.454212	2.114029
H	1.710885	1.437824	2.463841
H	1.126399	-0.097896	1.808782
H	2.519301	-0.087133	2.927650

TS2a-3a$_C$

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.415399	-1.202397	-0.482631

H	0.241161	0.277631	0.457398
N	0.183603	-2.432489	1.424026
N	-1.781707	-1.354350	-0.348585
C	-2.198644	-2.295680	0.717264
C	-1.215477	-2.206251	1.878677
H	-2.231800	-0.439119	-0.194974
O	-3.214939	1.138757	0.159481
H	-2.356532	1.659713	0.101677
C	-4.210239	1.764056	-0.652723
C	1.158832	-2.475695	-2.209011
C	2.262428	-2.115859	-1.361097
C	2.405274	-0.697674	-1.348055
C	1.356630	-0.150264	-2.176694
C	0.593972	-1.241335	-2.688371
C	1.124886	-2.017746	2.486320
C	0.411747	-3.869009	1.144720
H	-2.131956	-1.680317	-1.245757
H	-1.259191	-1.201521	2.305487
H	-2.218039	-3.308959	0.304573
H	0.238662	-4.477206	2.047857
H	-0.245483	-4.212484	0.346536
H	1.442315	-4.008060	0.816432
H	-1.486751	-2.924467	2.669885
H	3.166609	-0.132532	-0.829667
H	1.181934	0.897808	-2.372549
H	2.902965	-2.812244	-0.833332
H	-0.260081	-1.150375	-3.348619
H	0.846882	-3.476519	-2.475153
H	0.970249	-2.605102	3.406809
H	2.147722	-2.165961	2.135283
H	0.982944	-0.960662	2.704110
H	-3.208758	-2.068926	1.081992
H	-3.852766	1.799561	-1.696073
C	-4.472013	3.198619	-0.183728
H	-3.549333	3.787068	-0.212830
H	-5.213012	3.690757	-0.825202
H	-4.847442	3.198922	0.846221
C	-5.467247	0.899349	-0.596621
H	-6.259521	1.320192	-1.225510
H	-5.256460	-0.117264	-0.946573
H	-5.838012	0.836938	0.433010
C	2.516355	1.887118	1.388197
C	1.453791	2.254881	0.548768
C	3.798999	2.401125	1.186443

H	2.352963	1.182623	2.197556
C	1.706892	3.154813	-0.495701
C	4.042533	3.293564	0.136250
H	4.609113	2.105132	1.848037
C	2.990137	3.668192	-0.703606
H	0.874856	3.446961	-1.127889
H	5.040517	3.693439	-0.021238
H	3.166535	4.365139	-1.518861
C	0.019714	1.776487	0.755567
O	-0.854363	2.230826	-0.051460
C	-0.420600	1.620763	2.219172
H	-1.411585	1.163283	2.259568
H	0.274826	1.047195	2.834978
H	-0.497762	2.629309	2.645699

$\mathbf{3a_C}$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.817202	-0.751463	-0.427143
H	1.684103	-0.276736	1.746747
N	-2.601226	-0.198421	1.629928
N	-2.364711	1.138454	-0.731742
C	-3.066222	1.859165	0.333685
C	-2.589366	1.292072	1.665377
H	-0.536214	1.906478	-0.668948
O	0.400578	2.210116	-0.590842
H	1.604043	1.670957	0.595533
C	0.673215	3.453438	-1.258143
C	-2.363579	-2.779034	-1.048090
C	-1.165502	-2.912027	-0.275013
C	-0.148671	-2.137886	-0.902327
C	-0.693101	-1.570406	-2.118674
C	-2.057586	-1.973175	-2.211248
C	-1.787840	-0.731838	2.742642
C	-3.985977	-0.712320	1.757395
H	-2.607551	1.511371	-1.646217
H	-1.551334	1.596578	1.827119
H	-4.162067	1.771427	0.244046
H	-4.425143	-0.416180	2.724374
H	-4.606733	-0.324751	0.948768

H	-3.970432	-1.801572	1.688785
H	-3.193586	1.662787	2.508962
H	0.865920	-2.009955	-0.550155
H	-0.146685	-0.966001	-2.829106
H	-1.064441	-3.461292	0.651674
H	-2.747997	-1.724005	-3.005677
H	-3.313719	-3.250820	-0.837726
H	-2.177236	-0.391044	3.716000
H	-1.810069	-1.822898	2.717168
H	-0.754825	-0.398399	2.632877
H	-2.845743	2.940293	0.321633
H	1.570955	3.278217	-1.867699
C	0.997537	4.536930	-0.222105
H	1.806695	4.206483	0.437965
H	1.309781	5.464939	-0.715108
H	0.116856	4.753963	0.395965
C	-0.466765	3.861232	-2.191519
H	-0.205864	4.781689	-2.725210
H	-0.664159	3.082662	-2.936369
H	-1.388963	4.049361	-1.628587
C	3.506819	-1.852146	0.594300
C	3.499704	-0.450823	0.629234
C	4.350499	-2.545775	-0.277861
H	2.846624	-2.408385	1.257132
C	4.356227	0.246871	-0.233144
C	5.205238	-1.841394	-1.130735
H	4.339784	-3.632238	-0.291636
C	5.201776	-0.443343	-1.107112
H	4.345540	1.331832	-0.213333
H	5.860363	-2.376933	-1.811916
H	5.862509	0.111509	-1.767815
C	2.621173	0.294007	1.634363
O	2.342445	1.621273	1.240803
C	3.299736	0.370180	3.009382
H	2.626706	0.843364	3.731636
H	3.571949	-0.626017	3.372391
H	4.211305	0.973982	2.941607

$\mathbf{4}_{\mathbf{C}}$

Coordinates (Angstroms)

X	Y	Z

Ru	0.382619	-0.246105	-0.026075
N	-1.668011	0.716760	-0.008250
C	2.045414	0.809484	-1.078332
C	1.864517	1.461574	0.176093
C	2.046398	0.498576	1.217201
C	2.410091	-0.760187	0.602128
C	2.392688	-0.569533	-0.811417
C	-2.041159	1.012925	1.393826
C	-2.572700	-0.317874	-0.584505
C	-2.228009	-1.693199	-0.021704
N	-0.777150	-1.815535	-0.004307
H	-0.475070	-2.780450	0.094766
H	-2.393506	-0.324865	-1.663453
H	-2.672113	-1.822113	0.982798
H	-3.066356	1.415774	1.451798
H	-1.973731	0.106204	1.995514
H	-1.343412	1.747078	1.800458
H	-3.627500	-0.049809	-0.404380
H	2.618474	-1.317881	-1.559577
H	2.660664	-1.673859	1.124334
H	1.974599	1.268463	-2.054976
H	1.985450	0.691721	2.279935
H	1.582909	2.496896	0.317568
C	-1.749747	1.957769	-0.802718
H	-2.776177	2.361226	-0.805690
H	-1.077411	2.705259	-0.376816
H	-1.438700	1.753142	-1.828568
H	-2.702175	-2.453943	-0.661937

5_C

	Coordinates (Angstroms)		
	X	Y	Z

C	-1.671064	-1.337455	0.804001
C	-1.570028	-0.072519	1.500320
C	-2.204350	0.913171	0.669336
C	-2.630890	0.278790	-0.531080
C	-2.327420	-1.130518	-0.429804
Ru	-0.391272	0.146775	-0.371708
N	1.687102	-0.664233	0.008706

C	2.614275	0.510199	-0.083736
C	2.097490	-1.705431	-0.960432
C	1.761145	-1.252009	1.368093
C	1.943323	1.737454	0.511118
N	0.720047	1.949731	-0.244474
H	0.160438	2.655538	0.232297
H	2.790885	0.700644	-1.146387
H	1.807711	1.587518	1.603021
H	2.784974	-1.595192	1.585415
H	1.468139	-0.510889	2.110755
H	1.082066	-2.103454	1.433173
H	3.574240	0.265075	0.396603
H	-3.137936	0.760699	-1.356143
H	-2.314492	1.964612	0.899886
H	-2.552148	-1.885173	-1.171167
H	-1.207587	0.077993	2.508221
H	-1.314430	-2.291166	1.171387
H	3.114500	-2.067823	-0.739783
H	1.399005	-2.543330	-0.910263
H	2.079013	-1.294512	-1.970871
H	2.637629	2.590820	0.408129
H	0.047671	-0.113986	-2.089837
H	-0.128643	0.695951	-2.045821

TS5-1$_C$

Coordinates (Angstroms)

	X	Y	Z
C	-1.772527	-1.430521	0.468384
C	-1.694611	-0.383352	1.459517
C	-2.210281	0.805254	0.850954
C	-2.593728	0.507360	-0.491898
C	-2.333283	-0.895691	-0.719603
Ru	-0.395813	0.194091	-0.296100
N	1.651469	-0.720652	-0.008326
C	2.650611	0.389401	-0.116959
C	1.948209	-1.757718	-1.022937
C	1.738856	-1.340856	1.334733
C	2.103392	1.671011	0.501528
N	0.859255	1.977415	-0.176457
H	0.364115	2.765435	0.225836

H	2.824226	0.566701	-1.182681
H	1.990897	1.537455	1.594356
H	2.737799	-1.777317	1.496755
H	1.545481	-0.592411	2.102722
H	0.988633	-2.128436	1.419246
H	3.603757	0.082849	0.340107
H	-3.040563	1.195589	-1.195912
H	-2.283101	1.775850	1.325021
H	-2.527619	-1.439280	-1.633899
H	-1.379436	-0.492306	2.487995
H	-1.474226	-2.461460	0.611386
H	2.960751	-2.170048	-0.881153
H	1.218723	-2.565215	-0.937134
H	1.868005	-1.324270	-2.020442
H	2.859916	2.462673	0.359946
H	0.114580	0.553207	-1.943896
H	0.448942	1.284325	-1.428699

$\mathbf{4a_C}$

Coordinates (Angstroms)

	X	Y	Z
C	-2.454620	-1.640415	0.665119
C	-2.386988	-1.792291	-0.758690
C	-1.094157	-2.351105	-1.088298
C	-0.358952	-2.468438	0.128204
C	-1.202751	-2.029144	1.218267
Ru	-0.818756	-0.362030	-0.222932
N	-1.288794	1.744643	0.461105
C	-0.081790	2.553252	0.116736
C	-1.562160	1.840130	1.909510
C	-2.469320	2.230164	-0.289211
C	0.454172	2.141656	-1.249479
N	0.464598	0.679762	-1.293909
H	0.963750	0.332662	-2.109039
H	0.679909	2.333245	0.869476
H	-0.157559	2.575438	-2.060016
H	-2.697522	3.276563	-0.026512
H	-2.283031	2.162048	-1.361563
H	-3.331038	1.604923	-0.048604
H	-0.318402	3.628715	0.159538

H	0.650220	-2.844706	0.230606
H	-0.753520	-2.630100	-2.076235
H	-0.931369	-2.017959	2.264878
H	-3.188932	-1.591104	-1.456552
H	-3.298285	-1.246046	1.216476
H	-1.753970	2.884041	2.207832
H	-2.438436	1.235815	2.152513
H	-0.705385	1.458097	2.466844
H	1.464198	2.564075	-1.360987
H	2.050299	0.450807	0.114934
O	2.750022	0.771910	0.722175
C	3.942965	0.004413	0.564498
H	4.647338	0.447022	1.280457
C	3.721689	-1.463599	0.944491
H	3.027468	-1.943373	0.243683
H	4.664459	-2.022978	0.922181
H	3.297134	-1.536473	1.950459
C	4.524813	0.155706	-0.845717
H	4.670529	1.213366	-1.086798
H	5.490991	-0.355507	-0.931563
H	3.848211	-0.277348	-1.593349

$5a_C$

Coordinates (Angstroms)

	X	Y	Z
Ru	0.907727	-0.379243	-0.152805
N	0.889131	1.871556	-0.361600
C	-0.337946	2.350512	0.355507
C	-0.574837	1.505636	1.596985
N	-0.712883	0.122737	1.143689
C	0.847392	2.328544	-1.770927
C	2.099202	2.447878	0.270962
C	2.522025	-1.779546	-1.026648
C	1.577572	-2.524451	-0.225367
C	1.665807	-2.049215	1.111980
C	2.616556	-0.971452	1.152000
C	3.149148	-0.832949	-0.184247
H	2.709763	-1.919763	-2.082403
H	0.944626	-3.329397	-0.573091
H	1.092981	-2.422410	1.950863

H	2.960242	-0.453841	2.037104
H	3.908395	-0.125876	-0.492036
H	2.985334	2.096819	-0.259354
H	2.164442	2.130093	1.310869
H	2.070639	3.547843	0.229617
H	1.726735	1.954606	-2.299488
H	-0.049182	1.940571	-2.255977
H	0.834843	3.428602	-1.823954
H	-1.187424	2.212649	-0.319212
H	-0.240504	3.422933	0.583107
H	-1.495737	1.866184	2.086996
H	0.244728	1.658005	2.323049
H	-0.684098	-0.492703	1.955061
H	-0.563448	-0.608779	-1.148765
H	0.005656	-0.313849	-1.676581
H	-2.130626	0.022645	0.205802
O	-2.867782	0.065206	-0.488347
C	-3.964612	-0.744772	-0.097697
H	-3.599516	-1.746307	0.194666
C	-4.707334	-0.139428	1.102341
H	-5.544491	-0.775487	1.416919
H	-4.030868	-0.021476	1.956309
H	-5.101184	0.850001	0.841156
C	-4.880906	-0.906213	-1.309975
H	-4.330456	-1.349126	-2.146252
H	-5.739284	-1.547238	-1.077369
H	-5.255422	0.073042	-1.630959

TS5a-1a$_C$

	Coordinates (Angstroms)		
	X	Y	Z

N	0.638863	0.278581	-1.394074
H	1.668871	0.158453	-0.792161
O	2.560143	0.208150	0.170188
H	0.973347	-0.314776	0.889315
H	0.350531	-0.437931	1.430862
C	3.592243	-0.735274	0.179255
H	3.184129	-1.763600	0.059227
H	-2.000777	-2.153566	2.181615
H	-0.556713	-3.343851	0.208616

H	-1.307245	-2.251773	-2.133214
H	-3.259821	-0.438124	-1.645170
H	-3.636180	-0.355541	1.050697
H	0.612757	-0.275539	-2.246589
H	-0.409597	1.873674	-2.346438
H	1.341901	2.115384	-2.221897
H	0.175955	3.509249	-0.499624
H	1.223159	2.250458	0.212306
Ru	-0.792361	-0.381658	0.074726
C	-2.065867	-1.931985	1.125092
C	-1.290059	-2.560537	0.077942
C	-1.701814	-1.989803	-1.159645
C	-2.703053	-0.993030	-0.902571
C	-2.927081	-0.981150	0.524301
C	0.463389	1.705576	-1.700929
C	0.313016	2.425466	-0.368397
N	-0.836058	1.856202	0.406651
C	-2.111989	2.424447	-0.088208
C	-0.687288	2.219545	1.836364
H	-2.122047	3.518841	0.033813
H	-2.246950	2.181701	-1.142326
H	-2.943201	1.999032	0.476244
H	-0.700562	3.313426	1.963389
H	-1.509073	1.782761	2.407549
H	0.256872	1.827942	2.215378
C	4.327934	-0.695488	1.527814
H	5.129461	-1.444141	1.579936
H	4.767201	0.297905	1.681930
H	3.625790	-0.883435	2.347785
C	4.573193	-0.501074	-0.985216
H	5.378244	-1.248027	-0.999201
H	4.047889	-0.549915	-1.946663
H	5.023423	0.495485	-0.897665

$\mathbf{1a_C}$

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.780422	-0.389841	-0.018943
H	0.559451	-0.201672	0.916685
N	-1.171925	1.777034	0.555978

N	0.337866	0.670054	-1.613038
C	-0.042633	2.099066	-1.638583
C	-0.181070	2.588225	-0.202001
H	1.337201	0.574573	-1.412473
O	2.833238	0.380123	-0.066834
H	2.025371	0.048405	0.398261
C	3.898987	-0.563902	0.091520
C	-2.884348	-1.373499	-0.292715
C	-2.330744	-1.635924	1.018668
C	-1.127606	-2.385995	0.837239
C	-0.899630	-2.547465	-0.570743
C	-2.008141	-1.922530	-1.254743
C	-0.978763	2.005051	2.006371
C	-2.551000	2.179935	0.200288
H	0.163942	0.237113	-2.515808
H	0.784758	2.478386	0.298853
H	-0.990583	2.193297	-2.177250
H	-2.730002	3.240886	0.443641
H	-2.729514	2.019268	-0.863253
H	-3.255349	1.562392	0.759287
H	-0.456659	3.655364	-0.181591
H	-0.497408	-2.770323	1.627663
H	-0.105528	-3.120638	-1.029274
H	-2.794999	-1.401391	1.967338
H	-2.143819	-1.881425	-2.328905
H	-3.808947	-0.850788	-0.501617
H	-1.123163	3.068508	2.262887
H	-1.699405	1.401379	2.560293
H	0.023836	1.685326	2.288217
H	0.699553	2.718017	-2.161974
H	3.561106	-1.547613	-0.273102
C	4.293656	-0.696584	1.564977
H	3.439051	-1.021287	2.168240
H	5.096333	-1.433076	1.689825
H	4.641722	0.267263	1.953695
C	5.056386	-0.087379	-0.780645
H	5.898345	-0.785884	-0.724378
H	4.744501	-0.006313	-1.826995
H	5.400730	0.898644	-0.448477

$\mathbf{1}_{\mathbf{D}}$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.345068	-0.000943	-0.101822
C	2.035207	0.021232	-0.392014
C	1.631777	1.139470	0.389195
C	1.628495	-1.172652	0.275727
C	1.086650	-0.781675	1.559351
C	1.092311	0.628565	1.629610
O	2.717573	0.145849	-1.554557
H	2.708200	-0.689203	-2.041201
H	-0.479835	0.028662	-1.695189
C	-1.673527	-1.340928	-0.169592
C	-1.631006	1.381878	-0.141538
O	-2.467665	-2.180658	-0.217673
O	-2.398688	2.246008	-0.172069
H	1.816533	-2.184408	-0.058086
H	1.817844	2.173773	0.137380
H	0.740497	-1.461034	2.325966
H	0.750546	1.228760	2.461236

2_D

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-2.307777	0.347435	-0.090965
C	-1.379101	-1.864372	0.248275
C	-2.783821	-1.856517	0.499523
C	-1.165765	-1.411360	-1.092775
C	-2.463520	-1.287892	-1.721121
C	-3.451789	-1.561305	-0.748571
O	-0.468586	-2.245393	1.151976
H	0.444602	-2.010640	0.855278
H	-1.298353	0.864800	1.042927
C	-1.755540	1.857613	-1.076608
C	-3.617702	1.332482	0.846551
O	-1.390361	2.771152	-1.688679
O	-4.422049	1.916519	1.440098
H	-0.205055	-1.329610	-1.581746
H	-3.248355	-2.160342	1.426896
H	-2.637053	-1.033253	-2.757636

H	-4.521736	-1.552172	-0.903567
O	2.009611	-1.458736	0.369742
C	2.581735	-0.471292	0.843174
C	3.916100	-0.068674	0.313607
C	4.512679	-0.855219	-0.688948
C	4.593513	1.068154	0.788000
C	5.759332	-0.510836	-1.205012
H	3.982309	-1.731642	-1.045798
C	5.841930	1.412881	0.267944
H	4.150989	1.688527	1.559969
C	6.425956	0.624358	-0.727731
H	6.213845	-1.123616	-1.977866
H	6.356968	2.294271	0.638061
H	7.398044	0.893002	-1.131377
C	1.940856	0.330577	1.953665
H	2.594243	0.363121	2.832645
H	1.769996	1.363600	1.631508
H	0.983644	-0.113117	2.228212

TS2-3_D

	Coordinates (Angstroms)		
	X	Y	Z

Ru	1.220794	-0.569573	-0.060659
C	2.156886	1.647581	-0.277069
C	2.922573	0.820738	0.634903
C	2.124591	0.934756	-1.541813
C	2.991367	-0.204115	-1.440822
C	3.484500	-0.273796	-0.104347
O	1.531031	2.738854	0.028928
H	0.322580	2.653058	-0.052140
H	-0.208802	0.256674	0.382915
C	0.161082	-1.674310	-1.191445
C	1.034926	-1.749128	1.417043
O	-0.457932	-2.328968	-1.913864
O	0.954097	-2.450144	2.333604
H	1.622103	1.285104	-2.432889
H	3.131097	1.076371	1.664700
H	3.245213	-0.884187	-2.243003
H	4.177658	-1.012572	0.274746
O	-0.820994	2.367472	-0.122731

C	-1.173165	1.388794	0.654662
C	-2.424887	0.660329	0.247862
C	-3.047089	0.996654	-0.965099
C	-3.001718	-0.331539	1.058308
C	-4.224204	0.357497	-1.355871
H	-2.601096	1.767804	-1.582908
C	-4.178614	-0.969452	0.665434
H	-2.532098	-0.619375	1.993063
C	-4.793654	-0.627619	-0.543226
H	-4.698213	0.630111	-2.294464
H	-4.613203	-1.735509	1.301058
H	-5.709228	-1.126090	-0.848495
C	-0.876652	1.565056	2.139937
H	-1.623296	2.260640	2.543769
H	-0.924801	0.631728	2.701554
H	0.111872	2.011051	2.262878

3_D

Coordinates (Angstroms)

	X	Y	Z
Ru	1.281733	-0.530596	-0.065488
C	2.212938	1.786207	-0.153686
C	2.854047	0.881194	0.824453
C	2.255069	1.033517	-1.427695
C	3.103533	-0.094411	-1.267217
C	3.472191	-0.190669	0.124281
O	1.612504	2.851572	0.082279
C	0.396371	-1.653958	-1.346555
C	1.093957	-1.820676	1.335575
O	-0.059705	-2.326277	-2.164230
O	1.065807	-2.597676	2.189374
H	1.830448	1.390921	-2.356237
H	2.967588	1.108632	1.875854
H	3.446147	-0.760279	-2.048610
H	4.136013	-0.936741	0.541256
O	-1.037589	2.322248	-0.355155
C	-1.227312	1.255401	0.516195
H	-0.157469	2.731096	-0.193048
H	-0.395180	0.460290	0.336371
C	-2.531717	0.548082	0.191925

C	-3.434816	1.097978	-0.726662
C	-2.860295	-0.657825	0.829484
C	-4.647493	0.454714	-0.995731
H	-3.179959	2.026863	-1.223374
C	-4.069561	-1.299899	0.560127
H	-2.166069	-1.105597	1.536436
C	-4.970015	-0.743362	-0.354898
H	-5.339222	0.893396	-1.709666
H	-4.307152	-2.234466	1.060558
H	-5.911308	-1.242476	-0.566872
C	-1.103028	1.677353	1.986451
H	-1.902280	2.388223	2.219560
H	-1.190267	0.819450	2.659028
H	-0.138894	2.166080	2.155805

$2a_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	-2.019993	-1.306665	0.115369
C	-2.469127	0.966305	-0.616031
C	-3.339708	0.035760	-1.260167
C	-2.640923	0.826467	0.798807
C	-3.754272	-0.072458	1.014372
C	-4.181570	-0.555458	-0.243634
O	-1.659657	1.801692	-1.273869
H	-1.063378	2.296142	-0.646681
H	-0.525106	-1.101261	-0.420917
C	-1.217359	-2.046593	1.654181
C	-1.974337	-2.953589	-0.803623
O	-0.720842	-2.475621	2.608607
O	-1.948602	-3.950729	-1.393201
H	-2.120120	1.403846	1.549680
H	-3.439185	-0.080338	-2.330164
H	-4.181224	-0.324028	1.975484
H	-4.995133	-1.244833	-0.421937
H	-0.834076	6.168423	0.932372
C	-0.995905	5.095446	0.786586
C	0.326302	4.391293	0.504849
H	-1.464109	4.691081	1.689133
H	-1.689438	4.964959	-0.052010

C	1.023350	4.918995	-0.750771
H	0.993165	4.523499	1.369119
H	1.959787	4.381572	-0.933852
H	0.377951	4.799290	-1.628384
H	1.261218	5.983189	-0.640241
O	0.043015	2.982104	0.385845
H	0.881580	2.471523	0.331271
C	2.645992	0.545446	-0.549265
O	2.352623	1.451338	0.235625
C	1.856036	0.338394	-1.821652
H	1.418102	-0.664877	-1.844653
H	1.048382	1.067826	-1.883314
H	2.507002	0.438975	-2.697696
C	3.799354	-0.352174	-0.243954
C	4.177853	-1.399780	-1.101416
C	4.526707	-0.139259	0.941029
C	5.264033	-2.215793	-0.781033
H	3.628210	-1.585523	-2.017985
C	5.609889	-0.954505	1.259407
H	4.222834	0.668845	1.597779
C	5.980915	-1.994414	0.398354
H	5.547944	-3.023939	-1.448492
H	6.164738	-0.784490	2.177414
H	6.824897	-2.631408	0.647551

TS2a-3a$_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.252085	1.647486	0.179500
C	2.064797	1.335335	-0.736195
C	1.294414	2.401751	-1.368202
C	1.990002	1.620740	0.697115
C	1.462200	2.946328	0.875815
C	1.030928	3.425302	-0.394318
O	2.595405	0.336652	-1.320214
H	2.785600	-1.033302	-0.695345
H	-0.521404	0.064746	-0.259909
C	-1.068230	1.246546	1.842762
C	-1.897514	2.109517	-0.637741
O	-1.531336	0.989862	2.873290

O	-2.884408	2.394411	-1.175577
H	2.446734	1.017689	1.469739
H	1.136927	2.483574	-2.435285
H	1.416585	3.493846	1.807808
H	0.599087	4.397739	-0.589692
H	4.690677	-2.281616	2.301975
C	3.930350	-1.792122	1.683141
C	3.732724	-2.558860	0.373916
H	2.998126	-1.751447	2.255632
H	4.264359	-0.767285	1.485995
C	4.995600	-2.602375	-0.485054
H	3.418729	-3.584491	0.603986
H	4.815225	-3.167844	-1.403970
H	5.309051	-1.589207	-0.760902
H	5.816969	-3.078530	0.061764
O	2.647432	-2.007425	-0.397568
H	1.311616	-2.156949	-0.078900
C	-0.559550	-1.709801	-0.676058
O	0.266375	-2.238788	0.167414
C	-0.078253	-1.452622	-2.078125
H	-0.781505	-0.853379	-2.652772
H	0.892771	-0.948128	-2.073302
H	0.043490	-2.428862	-2.568551
C	-1.993502	-1.882057	-0.347684
C	-3.011500	-1.520042	-1.249311
C	-2.350046	-2.452150	0.890017
C	-4.350281	-1.725621	-0.921524
H	-2.768584	-1.065280	-2.202432
C	-3.689338	-2.654037	1.213964
H	-1.568657	-2.729701	1.587636
C	-4.694029	-2.291643	0.310213
H	-5.125190	-1.436966	-1.625085
H	-3.950768	-3.091016	2.173071
H	-5.738475	-2.445804	0.565390

$3a_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	2.172077	-0.289669	0.018244
C	-0.091761	-1.285733	-0.793519

C	1.044478	-1.298152	-1.735959
C	0.479586	-1.812383	0.465318
C	1.717694	-2.447798	0.164423
C	2.068301	-2.129766	-1.196049
O	-1.238777	-0.849720	-0.995824
H	-2.555590	-1.107359	0.136810
H	-3.286083	1.563856	-1.129460
C	3.041637	-0.193347	1.716226
C	3.685139	0.422154	-0.903300
O	3.568745	-0.236872	2.743918
O	4.609348	0.761739	-1.509030
H	-0.073446	-1.900773	1.391059
H	0.987748	-0.941082	-2.755466
H	2.287746	-3.092152	0.821141
H	2.938631	-2.503421	-1.719692
H	-4.555334	-4.211879	0.323340
C	-3.763323	-3.479733	0.518810
C	-4.303684	-2.050831	0.419150
H	-3.359674	-3.666155	1.518991
H	-2.963493	-3.643459	-0.213617
C	-4.876524	-1.734820	-0.965400
H	-5.092930	-1.919314	1.169299
H	-5.267835	-0.712997	-0.994800
H	-4.102206	-1.830094	-1.735817
H	-5.693067	-2.422327	-1.214787
O	-3.292712	-1.102626	0.793439
H	-3.659167	0.639694	0.905728
C	-3.058742	2.141731	-0.219003
O	-3.770737	1.617371	0.884294
C	-3.541960	3.584014	-0.422400
H	-3.043273	4.058863	-1.273080
H	-4.621459	3.582457	-0.599612
H	-3.339794	4.175361	0.476584
C	-1.544070	2.095104	-0.025041
C	-0.687882	2.309306	-1.120539
C	-0.987019	1.883514	1.244165
C	0.690866	2.339640	-0.953054
H	-1.112442	2.452417	-2.110847
C	0.394140	1.904047	1.422597
H	-1.652663	1.712458	2.083248
C	1.256232	2.132326	0.326984
H	1.338505	2.549021	-1.799492
H	0.812248	1.784369	2.417900
H	2.296613	2.383173	0.505033

4_D

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.307363	-0.000025	-0.191704
C	-2.189382	0.000071	-0.379944
C	-1.592596	-1.172176	0.321660
C	-1.592558	1.171803	0.322427
C	-0.947876	0.724806	1.496540
C	-0.947933	-0.725997	1.496071
O	-2.866371	0.000400	-1.407107
C	1.626226	1.393300	-0.206782
C	1.626747	-1.392860	-0.207066
O	2.383958	2.260172	-0.126346
O	2.384868	-2.259405	-0.126728
H	-1.779021	2.200187	0.043107
H	-1.779075	-2.200366	0.041632
H	-0.540610	1.341232	2.287572
H	-0.540675	-1.342971	2.286681

5_D

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-0.319193	-0.000094	-0.221422
C	2.289615	-0.000207	-0.269412
C	1.567423	1.163841	0.331582
C	1.567239	-1.163554	0.332637
C	0.880958	-0.718200	1.500518
C	0.881120	0.719675	1.499864
O	3.162298	-0.000638	-1.128155
C	-1.655388	-1.391318	-0.137921
C	-1.655337	1.391250	-0.138398
O	-2.420041	-2.247510	-0.035991
O	-2.420055	2.247373	-0.036394
H	1.780710	-2.195225	0.084719
H	1.780896	2.195250	0.082581

H	0.452872	-1.339811	2.276492
H	0.452954	1.342066	2.275174
H	-0.127176	0.402964	-2.042633
H	-0.127157	-0.403828	-2.042665

TS5-1$_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	0.267686	-0.000073	-0.128092
C	-2.024884	0.000065	-0.404945
C	-1.604919	-1.167298	0.367824
C	-1.605191	1.166400	0.369340
C	-1.016781	0.713845	1.600668
C	-1.016717	-0.716273	1.599756
O	-2.349274	0.000863	-1.660508
C	1.587400	1.400675	-0.128181
C	1.588507	-1.399747	-0.128776
O	2.338051	2.274300	-0.109205
O	2.340057	-2.272614	-0.110323
H	-1.776811	2.189805	0.067181
H	-1.776505	-2.190313	0.064330
H	-0.654057	1.339229	2.405647
H	-0.653991	-1.342628	2.403982
H	-0.011870	0.000334	-1.963708
H	-0.980127	0.000386	-1.955214

4a$_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	0.641814	-0.282247	-0.011037
C	0.398628	2.168576	-0.043178
C	0.831501	1.612045	1.255249
C	1.378966	1.633718	-1.010272
C	2.445797	1.009033	-0.298488
C	2.108182	0.996240	1.097447
O	-0.688166	2.732635	-0.302108

H	-1.559150	1.136642	-0.594973
C	1.034922	-1.572659	-1.367285
C	0.440312	-1.633248	1.324460
O	1.339411	-2.312898	-2.200093
O	0.383169	-2.414694	2.175193
H	1.343854	1.824083	-2.074597
H	0.318820	1.789717	2.191115
H	3.370479	0.636555	-0.719568
H	2.739930	0.612480	1.887920
H	-4.814481	-0.595614	-0.757452
C	-3.890994	-0.101227	-1.078126
C	-2.751954	-0.428399	-0.114496
H	-3.648560	-0.439052	-2.089691
H	-4.077659	0.978594	-1.108024
C	-3.023340	0.034282	1.314730
H	-2.564763	-1.506732	-0.126505
H	-2.180870	-0.206028	1.969451
H	-3.188822	1.117198	1.347805
H	-3.916839	-0.460178	1.710908
O	-1.521148	0.147586	-0.626867

$5a_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.197374	-0.191786	0.071087
C	-0.378476	1.819019	-0.167353
C	0.835845	1.991326	0.669699
C	0.153066	1.190460	-1.405272
C	1.568232	1.382144	-1.446904
C	1.988255	1.872474	-0.164740
O	-1.559139	2.007152	0.149878
H	-2.506367	0.382538	-0.099515
H	-0.049738	-0.998592	1.196751
C	1.584583	-1.689478	-1.077181
C	2.495649	-0.750199	1.387564
O	1.826018	-2.537920	-1.818159
O	3.297594	-1.022567	2.168978
H	-0.467220	0.869978	-2.231789
H	0.821532	2.384022	1.677750
H	2.217320	1.218484	-2.297268

H	3.005654	2.128817	0.101508
H	-5.984911	-0.650136	-0.627410
C	-4.958892	-0.324196	-0.834837
C	-3.977254	-0.922834	0.176764
H	-4.695447	-0.633740	-1.851030
H	-4.937133	0.771800	-0.792839
C	-4.302691	-0.516659	1.617208
H	-4.013500	-2.016752	0.099204
H	-3.587990	-0.967032	2.313430
H	-4.251779	0.572813	1.732332
H	-5.311128	-0.841536	1.898993
O	-2.626639	-0.586583	-0.161822
H	-0.476352	-0.975082	0.511356

TS5a-1a$_D$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.044983	-0.193463	0.007285
C	-0.343828	1.892278	-0.001716
C	0.651491	1.807176	1.074044
C	0.421610	1.621688	-1.229493
C	1.822104	1.685602	-0.925034
C	1.963111	1.792666	0.492885
O	-1.594526	1.991527	0.117312
H	-2.241002	0.630133	-0.398756
H	-0.381658	-1.169286	0.306393
C	1.621168	-1.396830	-1.364540
C	1.888626	-1.205942	1.397723
O	1.981832	-2.076099	-2.225521
O	2.408759	-1.770727	2.259774
H	-0.010835	1.593237	-2.220770
H	0.420499	1.931707	2.123353
H	2.635207	1.679793	-1.638882
H	2.901488	1.877952	1.024920
H	-5.629545	-0.996096	-0.357824
C	-4.734159	-0.504834	-0.754150
C	-3.500548	-0.936817	0.034125
H	-4.629425	-0.771508	-1.809701
H	-4.879958	0.578860	-0.682267
C	-3.569931	-0.568446	1.515469

H	-3.359656	-2.018736	-0.072485
H	-2.674094	-0.903240	2.046997
H	-3.658995	0.515519	1.642841
H	-4.440578	-1.044523	1.979297
O	-2.324874	-0.360651	-0.598133
H	-1.118096	-0.783094	-0.126975

$\mathbf{1a_D}$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.193252	-0.198031	-0.002151
C	-0.153183	1.782044	0.224931
C	1.071035	1.936146	0.939252
C	0.162451	1.526171	-1.150331
C	1.592280	1.670708	-1.298835
C	2.149237	1.923150	-0.023335
O	-1.365396	1.878076	0.790974
H	-2.002179	1.296496	0.308957
H	-0.048438	-1.048483	0.573549
C	1.393773	-1.570970	-1.283723
C	2.212423	-1.137662	1.286555
O	1.502437	-2.396986	-2.087119
O	2.824802	-1.692865	2.095099
H	-0.558066	1.391284	-1.944789
H	1.147995	2.143395	1.997290
H	2.136151	1.601665	-2.231114
H	3.195548	2.082470	0.196988
H	-5.968316	-0.293282	-0.260231
C	-4.996347	0.173521	-0.448932
C	-3.871021	-0.807421	-0.146416
H	-4.961140	0.490025	-1.495548
H	-4.914918	1.063240	0.185779
C	-3.850786	-1.268895	1.310341
H	-3.971334	-1.682091	-0.804961
H	-3.017841	-1.955878	1.496702
H	-3.745843	-0.413016	1.985960
H	-4.779886	-1.794188	1.557851
O	-2.635868	-0.137346	-0.495333
H	-1.881787	-0.736072	-0.357813

$\mathbf{1}_{E}$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.532863	0.020014	-0.055481
C	-1.848341	-0.418162	0.107733
C	-1.081677	-1.618419	0.271788
C	-1.412375	0.503129	1.115202
C	-0.512513	-0.200029	2.003891
C	-0.312347	-1.498531	1.489108
H	0.231683	0.586749	-1.528526
C	1.582524	1.574735	0.164711
C	1.958681	-0.924108	-0.855434
O	2.200287	2.543858	0.303412
O	2.812276	-1.524392	-1.356902
H	-1.795024	1.501314	1.271148
H	-1.182021	-2.512362	-0.329410
H	-0.072897	0.209510	2.902752
H	0.311807	-2.270235	1.917817
N	-2.830723	-0.214061	-0.834403
H	-2.801631	-0.884869	-1.591182
C	-3.152402	1.140716	-1.264920
H	-2.277512	1.660548	-1.685948
H	-3.941540	1.092755	-2.018433
H	-3.533559	1.722681	-0.420785

$\mathbf{2}_{E}$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-2.107121	-0.514287	0.173504
C	-1.657029	1.833030	-0.334583
C	-1.838477	1.048549	-1.523303
C	-2.844005	1.666783	0.457255
C	-3.818800	0.952443	-0.338866
C	-3.204104	0.577319	-1.553152
H	-0.700566	-0.491673	0.953711
C	-2.773057	-1.422753	1.690424

C	-1.497394	-2.108945	-0.621961
O	-3.178309	-1.956468	2.635157
O	-1.088642	-3.066094	-1.135307
H	-3.034446	2.124189	1.417275
H	-1.123195	0.973714	-2.330515
H	-4.838977	0.747365	-0.045150
H	-3.664645	0.029719	-2.363713
N	-0.555406	2.585828	-0.035688
H	0.272044	2.342084	-0.573043
C	-0.274089	2.941293	1.346611
H	-0.147776	2.051673	1.984464
H	0.642557	3.533723	1.375297
H	-1.083266	3.553615	1.757082
O	2.082854	1.530207	-1.101251
C	2.609210	0.425026	-1.221054
C	3.769892	0.041943	-0.358739
C	4.299495	0.998608	0.525285
C	4.342897	-1.240560	-0.402134
C	5.379183	0.680541	1.345633
H	3.849130	1.985243	0.550118
C	5.422406	-1.559930	0.423647
H	3.947228	-1.997043	-1.071595
C	5.942677	-0.600401	1.296619
H	5.783283	1.426709	2.023588
H	5.855198	-2.555224	0.386333
H	6.783855	-0.849129	1.937491
C	2.087321	-0.562364	-2.245051
H	2.889785	-0.923040	-2.896954
H	1.645424	-1.433531	-1.748150
H	1.321531	-0.075220	-2.849154

TS2-3$_E$

Coordinates (Angstroms)

	X	Y	Z
Ru	1.408034	-0.455270	-0.162856
C	1.391971	1.995386	-0.113747
C	2.279604	1.387933	0.877798
C	1.813146	1.456563	-1.395812
C	3.023772	0.714369	-1.207793
C	3.316878	0.696880	0.195506

H	-0.287171	-0.184212	0.650819
C	0.825290	-1.627050	-1.549984
C	1.764062	-1.914175	1.010126
O	0.516346	-2.302257	-2.434832
O	2.055931	-2.783953	1.712746
H	1.358187	1.677740	-2.350507
H	2.212751	1.562907	1.942891
H	3.644249	0.294627	-1.987777
H	4.176384	0.226009	0.653751
N	0.318598	2.716940	0.188758
H	-0.368782	2.178026	1.051387
C	-0.511515	3.197521	-0.915618
H	-0.928920	2.380473	-1.521372
H	-1.343481	3.768352	-0.498703
H	0.064193	3.860285	-1.572373
O	-1.080104	1.444864	1.748083
C	-1.233923	0.171305	1.373721
C	-2.460255	-0.096628	0.494141
C	-3.465506	0.874964	0.404624
C	-2.633232	-1.311548	-0.185224
C	-4.618279	0.638219	-0.351112
H	-3.330934	1.808447	0.941038
C	-3.781273	-1.549677	-0.942769
H	-1.861146	-2.075264	-0.134168
C	-4.780071	-0.573045	-1.028620
H	-5.391048	1.400469	-0.407327
H	-3.895226	-2.493909	-1.468294
H	-5.673807	-0.756535	-1.618517
C	-1.125936	-0.799714	2.562273
H	-1.148034	-1.846384	2.245755
H	-0.202475	-0.605201	3.113330
H	-1.974188	-0.619567	3.231388

$\mathbf{3}_{\mathbf{E}}$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.588214	-0.292654	0.187012
C	-0.875227	2.112881	-0.137527
C	-1.871326	1.602798	-1.103666
C	-1.453762	1.780992	1.179623

C	-2.805505	1.376613	0.999771
C	-3.063518	1.290501	-0.418358
H	0.408595	-0.562163	-0.760660
C	-1.498525	-1.433214	1.712511
C	-2.241492	-1.708983	-0.919560
O	-1.503025	-2.068190	2.679082
O	-2.724145	-2.518276	-1.588463
H	-0.986923	1.973070	2.135390
H	-1.733304	1.626502	-2.176443
H	-3.538851	1.219035	1.779559
H	-4.010128	1.018346	-0.866243
N	0.293258	2.570573	-0.472177
H	1.060148	1.424672	-1.706260
C	1.191321	3.004458	0.593764
H	1.654923	2.148391	1.103711
H	1.995659	3.600850	0.155972
H	0.681583	3.618321	1.349520
O	1.295258	0.617665	-2.229882
C	1.355197	-0.500466	-1.381551
C	2.525946	-0.447952	-0.402868
C	3.739629	0.137769	-0.791030
C	2.429919	-1.019493	0.872372
C	4.833511	0.146482	0.078643
H	3.813297	0.591583	-1.774648
C	3.522323	-1.013319	1.744392
H	1.491016	-1.467146	1.190961
C	4.729558	-0.429322	1.348937
H	5.767290	0.605427	-0.235158
H	3.428127	-1.457477	2.731616
H	5.579387	-0.419359	2.025674
C	1.391589	-1.752318	-2.260833
H	1.402089	-2.659824	-1.649816
H	0.518819	-1.772175	-2.920014
H	2.294366	-1.739413	-2.880059

$\mathbf{2a_E}$

Coordinates (Angstroms)			
	X	Y	Z

Ru	-2.340940	-1.154296	-0.068437
C	-2.372940	1.166047	0.748920

C	-2.669536	1.070364	-0.654873
C	-3.315638	0.321109	1.429292
C	-4.314762	-0.101036	0.470476
C	-3.919948	0.361633	-0.804595
H	-0.803551	-1.183778	0.414979
C	-2.511593	-2.822370	0.801294
C	-1.748766	-1.954507	-1.668212
O	-2.615386	-3.831445	1.361399
O	-1.366570	-2.420591	-2.660035
H	-3.368615	0.165103	2.497119
H	-2.135220	1.595293	-1.434896
H	-5.204890	-0.670090	0.700386
H	-4.451058	0.209875	-1.734201
N	-1.384206	1.917669	1.305462
H	-0.697544	2.300250	0.653296
C	-0.875049	1.604644	2.629353
H	-0.462206	0.584298	2.682325
H	-0.086059	2.317532	2.877893
H	-1.664089	1.698679	3.383442
C	1.100513	4.330093	-0.752280
C	1.897570	4.881184	0.432964
C	-0.167704	5.129832	-1.029949
H	1.738187	4.354702	-1.649971
H	2.785257	4.268984	0.624622
H	2.229026	5.907230	0.234773
H	1.280453	4.887181	1.338893
H	-0.707711	4.710753	-1.884664
H	-0.832628	5.109696	-0.158907
H	0.075953	6.173893	-1.253035
O	0.702822	2.969113	-0.518339
H	1.501283	2.405516	-0.447739
C	2.938267	0.097225	-0.665799
O	2.921102	1.258322	-0.248522
C	1.903026	-0.375172	-1.660330
H	1.312202	0.475428	-2.001800
H	2.368357	-0.868634	-2.519382
H	1.226171	-1.096022	-1.187201
C	3.981935	-0.852776	-0.177292
C	3.981578	-2.210912	-0.539462
C	4.987986	-0.371387	0.679698
C	4.968278	-3.070419	-0.053051
H	3.210452	-2.605003	-1.192878
C	5.974718	-1.229041	1.159751
H	4.975747	0.677792	0.955349

C	5.966071	-2.580885	0.794586
H	4.956995	-4.119314	-0.333890
H	6.749938	-0.848740	1.818594
H	6.734571	-3.250212	1.170905

TS2a-3a$_E$

Coordinates (Angstroms)

	X	Y	Z
Ru	-0.546815	-1.647531	0.084275
C	1.660809	-1.356953	-1.110476
C	1.731718	-1.998163	0.204831
C	0.647005	-2.093217	-1.847156
C	0.335392	-3.289084	-1.116072
C	1.032047	-3.233698	0.137048
H	-0.564036	0.240309	0.348442
C	-2.320963	-1.674357	-0.629997
C	-1.169229	-1.924771	1.865190
O	-3.363132	-1.758467	-1.116724
O	-1.514487	-2.167576	2.940614
H	0.317654	-1.873612	-2.852746
H	2.361258	-1.648989	1.011520
H	-0.258905	-4.118938	-1.473375
H	1.012418	-3.997611	0.902977
N	2.308716	-0.264108	-1.449162
H	2.736616	0.372572	-0.584252
C	2.091347	0.371987	-2.740891
H	1.070473	0.762406	-2.831857
H	2.782854	1.212063	-2.830013
H	2.285588	-0.326384	-3.563904
C	3.879402	1.991664	0.870903
C	4.316480	2.848805	-0.328424
C	5.051937	1.178530	1.435362
H	3.537811	2.681330	1.663942
H	3.467520	3.419298	-0.720572
H	5.105281	3.557803	-0.047760
H	4.706666	2.212760	-1.134075
H	4.721896	0.587737	2.296446
H	5.438395	0.487239	0.675554
H	5.875600	1.828064	1.756827
O	2.806759	1.135149	0.541179

H	1.555515	1.664710	0.245295
C	-0.441326	1.425459	0.601198
O	0.579619	1.927578	-0.133601
C	-0.185037	1.468445	2.115663
H	0.772343	0.992543	2.342429
H	-0.138285	2.517643	2.427293
H	-0.978463	0.974454	2.681545
C	-1.782230	2.018739	0.183974
C	-2.982188	1.590897	0.772427
C	-1.828843	3.029097	-0.785263
C	-4.201552	2.160928	0.403479
H	-2.971218	0.803261	1.521277
C	-3.049989	3.601385	-1.155546
H	-0.899474	3.361035	-1.233599
C	-4.239913	3.170753	-0.564186
H	-5.120663	1.816013	0.869068
H	-3.068808	4.387144	-1.906063
H	-5.188437	3.615130	-0.852463

$3a_E$

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.189074	-1.492076	-0.267690
C	-1.977879	-1.370985	1.125750
C	-2.065965	-1.931409	-0.236017
C	-0.827363	-2.078370	1.715736
C	-0.522293	-3.221069	0.905221
C	-1.306482	-3.134199	-0.292228
H	1.088187	1.317488	-1.933608
C	2.029741	-1.648475	0.239623
C	0.606438	-1.606936	-2.124542
O	3.106430	-1.872488	0.594702
O	0.811335	-1.766971	-3.253152
H	-0.425161	-1.902827	2.703660
H	-2.776289	-1.597793	-0.980224
H	0.134350	-4.039147	1.170792
H	-1.314180	-3.861576	-1.093297
N	-2.683773	-0.367095	1.558930
H	-2.873682	0.766320	0.270379
C	-2.405926	0.122009	2.903779

H	-1.435507	0.639395	2.962941
H	-3.180705	0.838170	3.192964
H	-2.401035	-0.683954	3.652435
C	-3.538765	2.404930	-0.738679
C	-3.664685	3.293380	0.502896
C	-4.890965	1.859215	-1.206054
H	-3.100705	2.997578	-1.552593
H	-2.683158	3.663743	0.815183
H	-4.310417	4.155771	0.301106
H	-4.101523	2.732430	1.337500
H	-4.762422	1.234606	-2.095393
H	-5.352192	1.248421	-0.421089
H	-5.579780	2.675669	-1.452207
O	-2.615992	1.331923	-0.522257
H	-0.909888	1.107497	-0.412557
C	0.942443	1.712238	-0.918496
O	0.028124	0.844111	-0.216209
C	0.352506	3.124332	-1.019902
H	0.183760	3.543217	-0.022777
H	1.048383	3.779017	-1.553472
H	-0.596768	3.112622	-1.564679
C	2.279796	1.714893	-0.203187
C	3.470875	1.686764	-0.939190
C	2.347318	1.805801	1.194573
C	4.709595	1.756857	-0.294814
H	3.430977	1.603394	-2.023121
C	3.583283	1.869297	1.840808
H	1.427387	1.809918	1.771363
C	4.768498	1.847500	1.098063
H	5.624970	1.729066	-0.879239
H	3.622702	1.931148	2.924934
H	5.729643	1.893599	1.602142

4_E

Coordinates (Angstroms)

	X	Y	Z
Ru	0.517545	0.028057	-0.102584
C	-1.902469	-0.425545	0.067299
C	-1.051271	-1.606580	0.319760
C	-1.395277	0.592068	1.020649

C	-0.483193	-0.027101	1.907406
C	-0.276726	-1.390158	1.474015
C	1.527096	1.640511	-0.019054
C	2.014174	-0.949772	-0.769562
O	2.125310	2.621885	0.117174
O	2.919132	-1.589927	-1.100480
H	-1.757009	1.605333	1.119838
H	-1.128067	-2.525346	-0.245574
H	-0.036229	0.423361	2.783861
H	0.367439	-2.108930	1.962630
N	-2.731068	-0.359403	-0.926662
C	-3.485396	0.855045	-1.164720
H	-3.360138	1.153364	-2.212278
H	-4.553429	0.637497	-1.031420
H	-3.224228	1.709546	-0.525010

5_E

Coordinates (Angstroms)

	X	Y	Z
Ru	0.573725	0.028058	-0.192931
C	-2.025461	-0.401772	0.123652
C	-1.055438	-1.498243	0.385458
C	-1.357477	0.758264	0.790188
C	-0.437658	0.251696	1.760632
C	-0.256538	-1.150472	1.508434
C	1.674708	1.604559	-0.078884
C	2.109620	-1.094356	-0.506850
O	2.304717	2.562959	0.051745
O	3.010520	-1.803885	-0.637739
H	-1.713140	1.779390	0.778170
H	-1.165120	-2.495323	-0.020739
H	0.021501	0.809845	2.566337
H	0.381341	-1.812900	2.078856
N	-3.076189	-0.517854	-0.600797
C	-3.897417	0.651874	-0.855334
H	-3.664485	1.062592	-1.849060
H	-4.950433	0.351993	-0.877856
H	-3.788729	1.462973	-0.119119
H	0.018517	0.609574	-1.914154
H	0.102045	-0.179618	-2.023720

TS5-1$_E$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	0.475911	0.033759	-0.108170
C	-1.831976	-0.595186	0.067258
C	-0.891082	-1.734886	0.045496
C	-1.416995	0.212766	1.206862
C	-0.363154	-0.474413	1.913414
C	-0.089753	-1.699006	1.222713
C	1.238254	1.763073	0.221891
C	2.137247	-0.676594	-0.744366
O	1.650478	2.814028	0.463528
O	3.127789	-1.143830	-1.107894
H	-1.863915	1.150091	1.504638
H	-0.940694	-2.538974	-0.675519
H	0.092202	-0.161814	2.843309
H	0.625568	-2.449459	1.531984
N	-2.545116	-0.252312	-0.998221
C	-3.302029	0.984476	-0.931669
H	-2.645220	1.872116	-1.002454
H	-4.000903	1.022133	-1.771619
H	-3.887512	1.074025	-0.005141
H	-0.352301	0.272274	-1.841770
H	-1.260695	-0.002564	-1.691066

4a$_E$

	Coordinates (Angstroms)		
	X	Y	Z
Ru	-1.611467	0.201249	-0.130069
C	0.310510	-1.165493	0.617412
C	0.252283	0.176226	1.234468
C	-1.018966	-1.754051	0.893134
C	-1.707328	-0.913160	1.802958
C	-0.912054	0.274679	2.017589
C	-3.273415	-0.264309	-0.937999

C	-1.882809	2.063431	-0.473510
O	-4.307330	-0.582407	-1.347878
O	-2.052968	3.199952	-0.592368
H	-1.360745	-2.729270	0.577846
H	1.060246	0.893793	1.164903
H	-2.646711	-1.133742	2.292448
H	-1.182092	1.096224	2.667570
N	1.292808	-1.548761	-0.141631
C	1.262830	-2.847174	-0.788979
H	1.424186	-2.716251	-1.865531
H	2.100513	-3.451015	-0.416596
H	0.336446	-3.417542	-0.643941
C	4.556823	0.337235	0.055828
C	5.259304	1.641223	0.423214
C	5.160071	-0.311584	-1.195201
H	4.660569	-0.366503	0.899989
H	4.810900	2.077774	1.321242
H	6.325044	1.472254	0.612754
H	5.161130	2.365522	-0.393399
H	4.633733	-1.239400	-1.447122
H	5.078826	0.368420	-2.050780
H	6.218323	-0.555291	-1.041847
O	3.176243	0.643207	-0.135588
H	2.663490	-0.186757	-0.249906

$5a_E$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.380401	-0.254677	0.136545
C	0.287306	1.575892	-0.695335
C	-0.030051	0.435229	-1.589157
C	-1.054210	1.984861	-0.207904
C	-2.043956	1.455196	-1.097597
C	-1.399435	0.507822	-1.961879
H	-0.184609	-0.440736	1.605381
C	-2.818338	-0.218523	1.417079
C	-1.732542	-2.096704	-0.306838
O	-3.703584	-0.137051	2.152759
O	-1.957366	-3.178054	-0.639023
H	-1.245917	2.763694	0.517053

H	0.724521	-0.181154	-2.059109
H	-3.084572	1.747627	-1.149289
H	-1.884254	-0.057419	-2.746995
N	1.480754	1.940764	-0.368449
H	2.509899	0.366220	-0.211899
C	1.638562	3.011894	0.603931
H	1.605713	2.614596	1.630300
H	2.618338	3.479217	0.467708
H	0.874130	3.798036	0.521680
C	4.177547	-0.718673	-0.099590
C	4.480847	-2.212306	-0.021987
C	4.854064	0.068284	1.028582
H	4.549950	-0.335089	-1.064797
H	3.984415	-2.746201	-0.838329
H	5.558670	-2.396711	-0.089138
H	4.116579	-2.623914	0.926442
H	4.613970	1.135192	0.958940
H	4.511692	-0.296872	2.003850
H	5.944861	-0.035423	0.981903
O	2.758147	-0.574216	-0.054418
H	0.222668	-0.813872	1.027104

TS5a-1a$_E$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.101138	-0.272508	0.071240
C	0.126077	1.829032	-0.631555
C	-0.414514	0.983163	-1.707677
C	-1.015473	2.028542	0.266529
C	-2.217959	1.608572	-0.402226
C	-1.841289	0.988099	-1.631766
H	0.437820	-0.861672	0.719569
C	-1.937015	-0.733955	1.728968
C	-1.495080	-1.972398	-0.703938
O	-2.454348	-0.956982	2.738009
O	-1.750938	-2.976832	-1.215634
H	-0.989079	2.577217	1.197246
H	0.170848	0.615635	-2.539569
H	-3.231181	1.778917	-0.063844
H	-2.520490	0.583851	-2.370536

N	1.400342	2.106056	-0.472614
H	2.101034	0.736016	-0.613105
C	1.761938	2.890639	0.701089
H	1.631040	2.325591	1.640275
H	2.814305	3.180904	0.629232
H	1.169322	3.812548	0.787306
C	3.569058	-0.692475	-0.113781
C	3.795548	-2.146338	-0.516298
C	3.729017	-0.462447	1.390705
H	4.281610	-0.053584	-0.653814
H	3.668623	-2.270005	-1.595548
H	4.807163	-2.466510	-0.244496
H	3.081180	-2.803452	-0.007751
H	3.544623	0.583444	1.654278
H	3.031841	-1.089029	1.957499
H	4.747332	-0.715919	1.705842
O	2.254955	-0.309916	-0.577145
H	1.142484	-0.658740	0.129015

$\mathbf{1a_E}$

Coordinates (Angstroms)

	X	Y	Z
Ru	-1.202551	-0.378264	-0.004109
C	-0.295628	1.853475	-0.395609
C	-0.304968	1.049021	-1.587798
C	-1.646822	1.900829	0.085980
C	-2.503005	1.298595	-0.913430
C	-1.679896	0.782785	-1.939403
H	0.010001	-0.594744	1.044063
C	-2.302077	-1.077185	1.369734
C	-0.815509	-2.097670	-0.680850
O	-2.971026	-1.477344	2.224848
O	-0.559692	-3.139761	-1.117457
H	-1.986708	2.423337	0.968463
H	0.562983	0.829433	-2.193795
H	-3.582790	1.260175	-0.875355
H	-2.013217	0.270018	-2.831165
N	0.806728	2.444387	0.158605
H	1.678055	1.993543	-0.108029
C	0.775476	2.866171	1.551833

H	0.573826	2.026139	2.235270
H	1.742372	3.304861	1.806120
H	0.008603	3.632514	1.701113
C	3.769559	-0.759008	-0.169050
C	4.005422	-1.523365	1.134388
C	4.970338	0.082116	-0.585498
H	3.543677	-1.479305	-0.970834
H	3.119035	-2.101866	1.418385
H	4.840852	-2.224434	1.026567
H	4.237197	-0.828117	1.948863
H	4.761864	0.618492	-1.516422
H	5.208013	0.817751	0.191163
H	5.848736	-0.552534	-0.741682
O	2.657840	0.146014	-0.040251
H	1.858292	-0.348207	0.208938
