

Supporting information

A Theoretical Study of X Ligand Effect on Catalytic Activity of the Complexes RuHX(diamine)(PPh₃)₂ (X = NCMe, CO, Cl, OMe, OPh, CMe, H) in H₂-hydrogenation of Ketones

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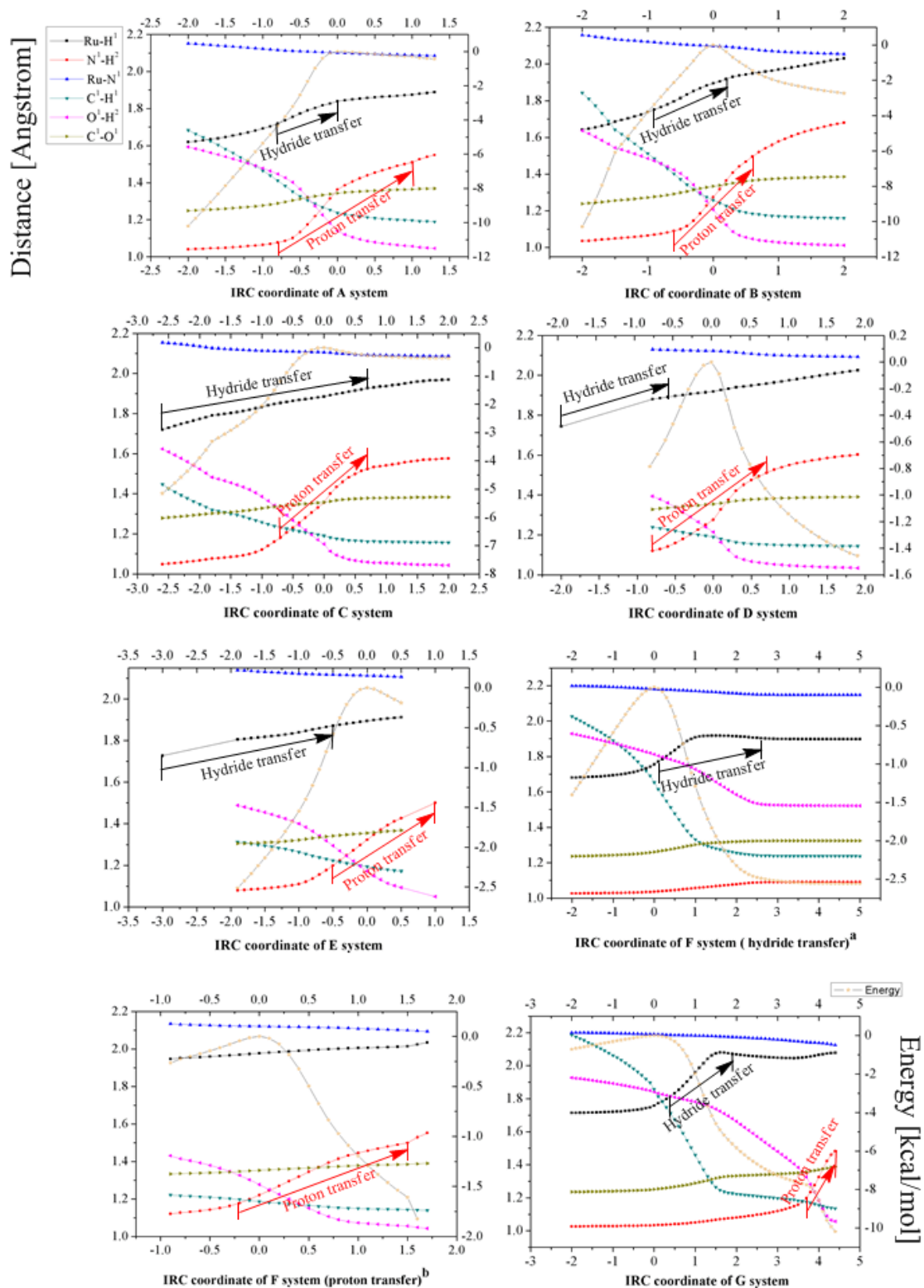
Abbreviations used in manuscript

TM :	Transition metal
HT :	Hydrogen transfer
DA :	Dihydrogen activation
HC :	Hydrogen coordination
HS :	Hydrogen splitting
TS:	Transition state
GI, GII:	Group I and II
DFT:	Density functional theory
TE:	Trans-effect
PMDs:	Proton-moved-distances
CD:	Charge difference between H ² and H ¹

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Figure S1. Structural changes along IRC pathway in HT for A-G systems.



Two hydrogen transfer modes in hydrogen transfer step are observed clearly through the structural changes along IRC pathways of all systems (Chen, Y.; Tang, Y.; Lei, M. *Dalton. Trans.* **2009**, 2359-2364.). Hydride and proton transfer synchronously

(mode 2 in the paper) could be predicted from frontier orbital interactions for GI (A, B), and for GII (C-G) hydride transfer precedes proton transfer (mode 1 in the paper). Because the IRC pathways for D and E systems could not go on successfully as other systems (The two transition states connect **2** and **3** via optimization of the break points were verified), we considered the hydride transfer begins when Ru-H¹ bond length are 1.744 and 1.727 Å for D and E, respectively. For F, the hydride and proton transfer via a stepwise mechanism: ^a hydride transfer (from **2_F** to **6_F** via **TS2-3_F**) and, ^b proton transfer (from **6_F** to **3_F** via **TS6-3_F**).

Figure S2. Potential energy profiles (without zero-point energy correction) of H₂-hydrogenation of ketone for A-G (in kcal/mol).

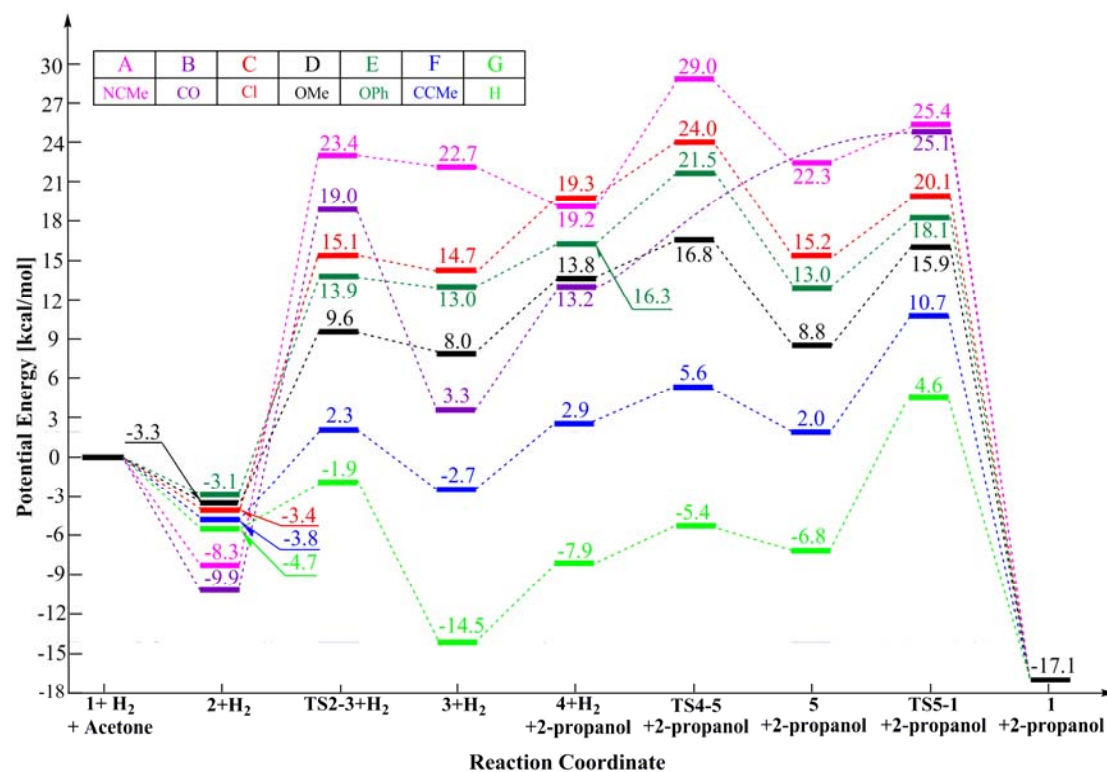
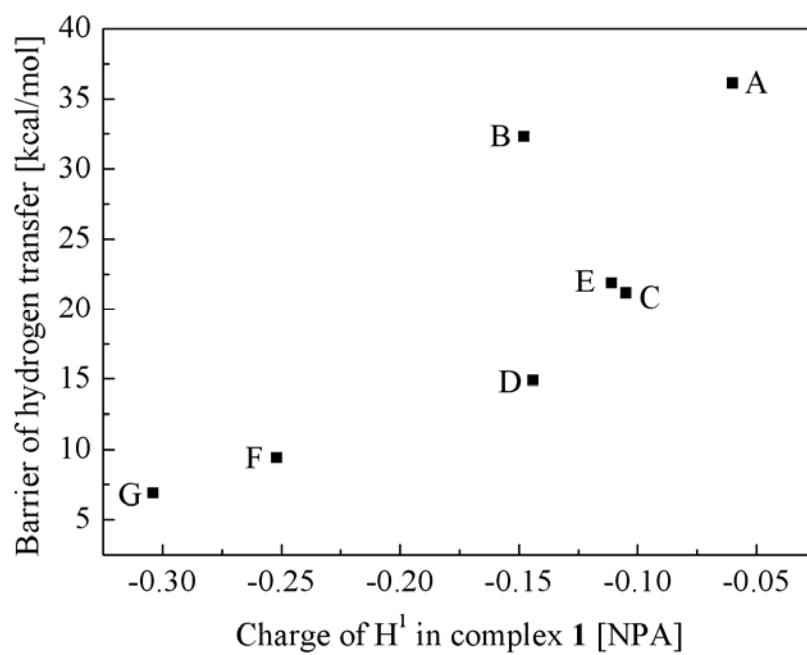
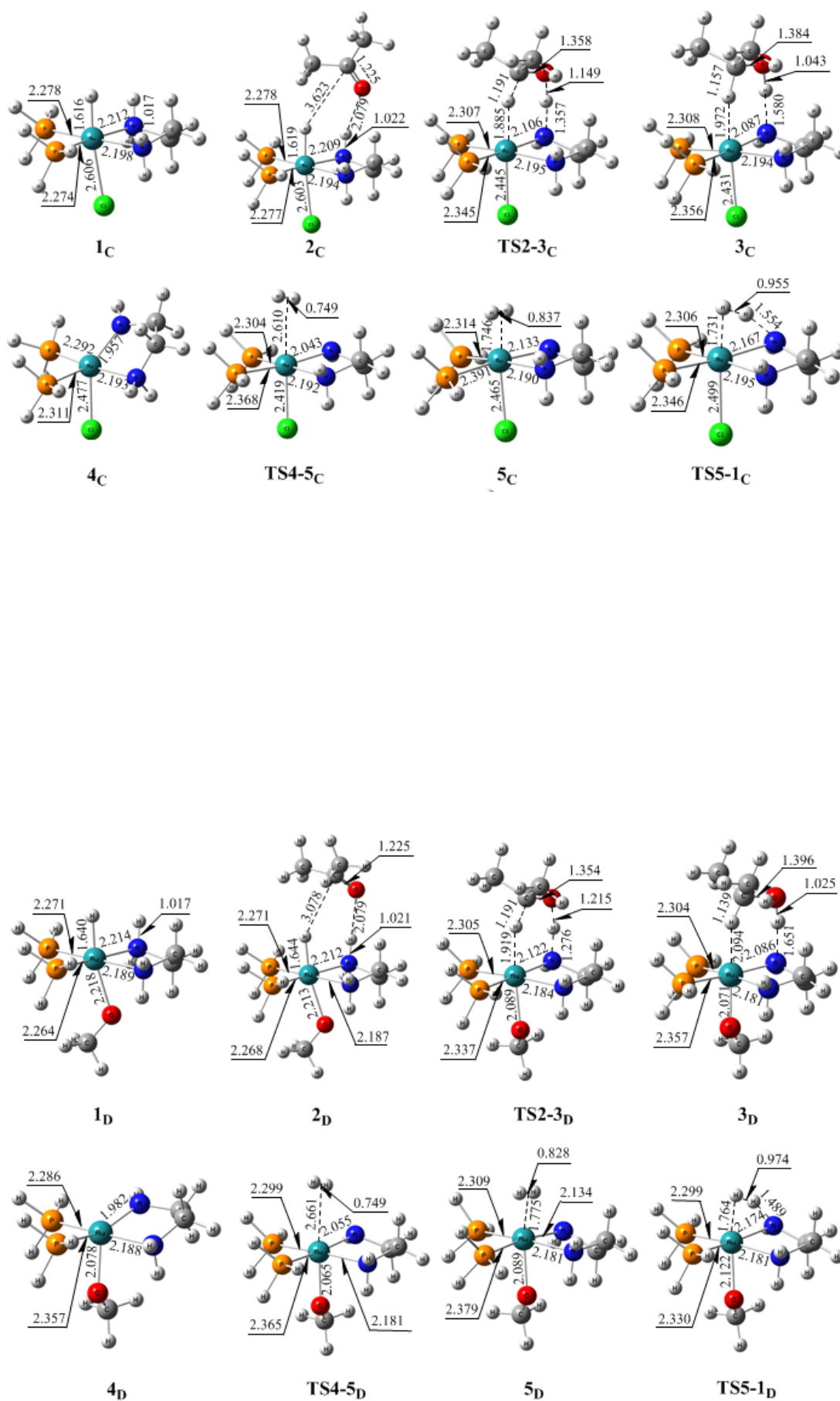
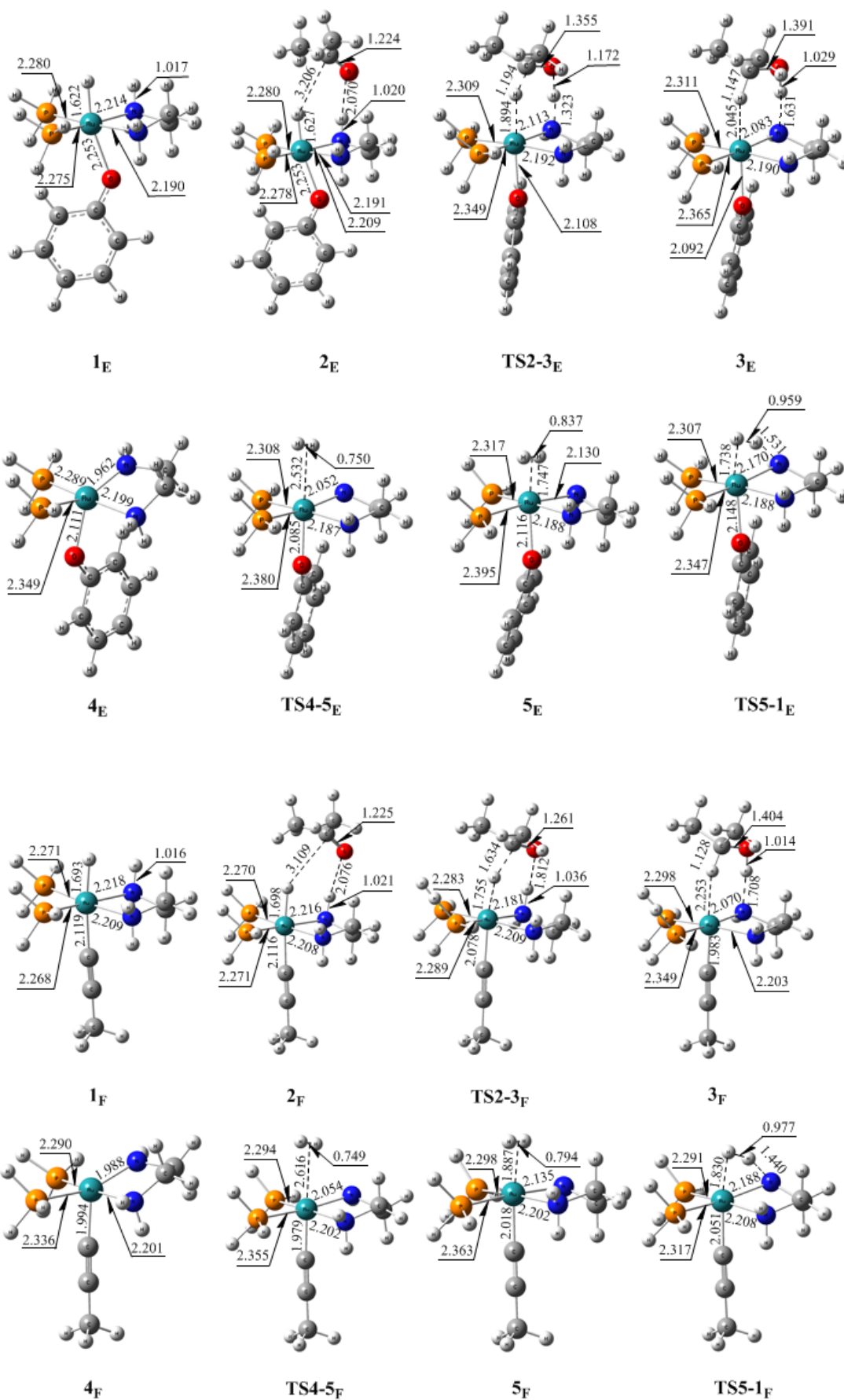


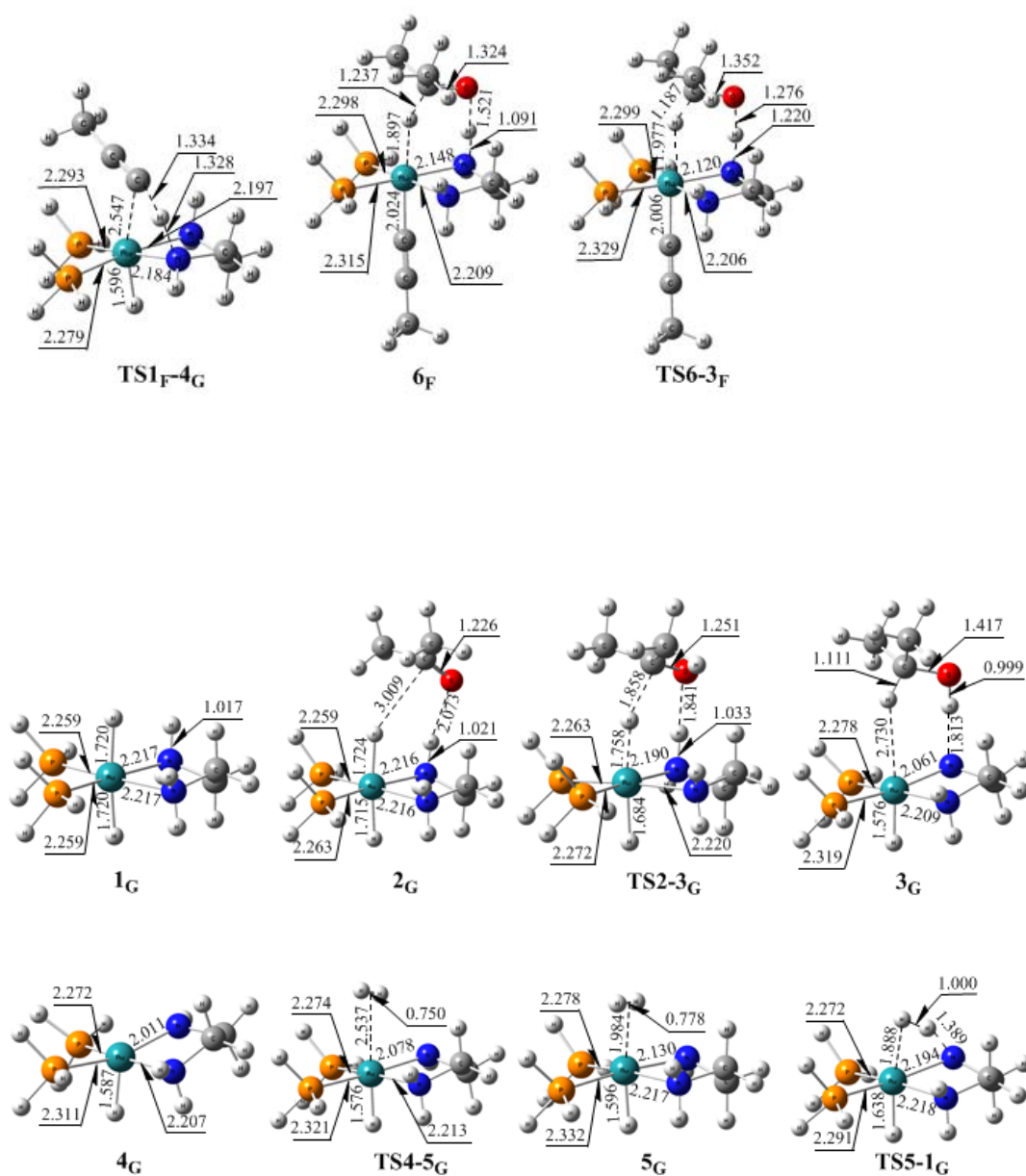
Figure S3. Correlation between the H¹ charge (NPA charge) in complex 1 and barrier of hydrogen transfer.











**Table S1. Calculated energies^a of stationary points at B3LYP/BSI level
(LANL2DZ basis set for Ru, 6-31+G** for other atoms).**

	1	2	TS2-3	3	4	TS4-5	5	TS5-1
A	-1103.99893	-1297.18664	-1297.13623	-1297.13719	-1102.76255	-1103.92542	-1103.93614	-1103.93112
B	-1084.56261	-1277.75297	-1277.70683	-1277.73180	-1083.33569	-	-	-1084.49537
C	-1431.64474	-1624.82464	-1624.79524	-1624.79583	-1430.40810	-1431.57915	-1431.59319	-1431.58534
D	-1086.52140	-1279.70113	-1279.68058	-1279.68317	-1085.29359	-1086.46746	-1086.48013	-1086.46889
E	-1278.29227	-1471.47172	-1471.44470	-1471.44599	-1277.06042	-1278.23071	-1278.24422	-1278.23616
F	-1087.45864	-1280.63923	-1280.62955	-1280.63744	-1086.24812	-1087.42249	-1087.42820	-1087.41424
G	-971.95733	-1165.13940	-1165.13486	-1165.15490	-970.76413	-971.93864	-971.94090	-971.92278

TS1 _F -4 _G	6 _F	TS6-3 _F
-1087.41638	-1280.63364	-1280.63293

^a Unit:a.u.

Table S2. Calculated imaginary frequencies of TS in the catalytic cycles at B3LYP/BSI level (LANL2DZ basis set for Ru, 6-31+G for other atoms).**

	TS2-3	TS4-5	TS5-1
A	721.1 <i>i</i>	298.6 <i>i</i>	752.6 <i>i</i>
B	1042.1 <i>i</i>	-	872.0 <i>i</i>
C	668.5 <i>i</i>	264.8 <i>i</i>	912.1 <i>i</i>
D	898.1 <i>i</i>	251.0 <i>i</i>	1053.7 <i>i</i>
E	784.3 <i>i</i>	300.3 <i>i</i>	923.0 <i>i</i>
F	305.6 <i>i</i>	213.9 <i>i</i>	1172.1 <i>i</i>
G	224.9 <i>i</i>	215.3 <i>i</i>	1301.9 <i>i</i>

TS1_F-4_G	TS6-3_F
-1258.8 <i>i</i>	724.2 <i>i</i>

The Cartesian coordinates of stationary points optimized for all systems.

Results of intermediate and TS calculated using B3LYP/BSI

1_A			

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.284266	-0.419107	0.013143
P	-0.600725	-1.736919	1.683117
N	1.419618	0.869156	1.421951
P	-0.541874	-1.796859	-1.634797
N	1.446815	0.826890	-1.401814
C	2.563661	1.477561	-0.662945
C	2.044400	1.992859	0.672322
H	1.823685	0.274111	-2.168894
H	2.142315	0.287300	1.841756
H	-0.603508	-3.143121	1.536932
H	0.023453	-1.685153	2.954673
H	-1.858758	-1.663200	-2.144690
H	-0.556245	-3.196429	-1.435148
H	3.333754	0.717746	-0.501274
H	3.009482	2.297735	-1.238109
H	2.856950	2.460542	1.240644
H	1.271917	2.751502	0.508981
H	1.528568	-1.435045	0.048520
H	-1.938055	-1.589744	2.132707
H	0.134612	-1.795844	-2.880785
H	0.859109	1.236032	2.188983
H	0.847181	1.536215	-1.823008
C	-2.314072	1.736873	-0.072640
N	-1.382436	1.043888	-0.040002
C	-3.497391	2.590625	-0.112691
H	-3.599797	3.139126	0.828258
H	-3.418570	3.308900	-0.933998
H	-4.392367	1.979652	-0.263848

2_A

Coordinates (Angstroms)

	X	Y	Z

Ru	0.811882	-0.348376	0.273240
P	0.698240	-2.019641	-1.300084
N	-0.631011	0.938936	-0.794822
P	2.092946	-1.631026	1.693244
N	0.540325	1.280574	1.746158
C	-0.671958	2.064549	1.375421
C	-0.685801	2.268270	-0.132187
H	0.436601	0.916605	2.690810
H	-1.563514	0.518454	-0.747494
H	0.580030	-3.368095	-0.888827
H	-0.405682	-2.003080	-2.189521
H	3.508333	-1.689522	1.602614
H	1.859181	-3.022938	1.790684
H	-1.547192	1.481762	1.673562
H	-0.702839	3.029799	1.894873
H	-1.582848	2.824751	-0.426314
H	0.192604	2.843142	-0.445528
H	-0.443300	-1.078951	0.955899
H	1.709136	-2.214921	-2.277538
H	2.021242	-1.342001	3.080237
H	-0.409132	1.060288	-1.781064
H	1.358836	1.888596	1.756634
C	-4.650175	0.029870	-0.321747
O	-3.521523	0.507458	-0.255019
C	-4.991419	-1.058833	-1.313695
H	-5.906399	-0.812428	-1.863530
H	-4.168347	-1.217749	-2.012124
H	-5.191436	-1.992649	-0.773431
C	-5.757495	0.508818	0.587801
H	-6.515891	1.033383	-0.006767
H	-6.263396	-0.338501	1.063805
H	-5.364775	1.186094	1.347492
C	3.419499	1.246229	-1.158258
N	2.498214	0.743216	-0.660555
C	4.583178	1.862348	-1.788390
H	4.319580	2.240779	-2.780459
H	4.948232	2.694174	-1.178849
H	5.384873	1.125314	-1.894113

TS2-3_A

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.235589	-0.183279	0.083289
P	0.263120	-1.797293	-1.604667
N	-0.239352	1.347609	-1.275038
P	0.387748	-1.786070	1.838392
N	0.183549	1.560615	1.435124
C	-0.322003	2.760655	0.688782
C	0.155897	2.670281	-0.752828
H	-0.374172	1.417538	2.275620
H	-1.599226	1.262168	-1.243025
H	-0.457819	-3.006017	-1.484152
H	-0.207001	-1.400341	-2.877913
H	1.620251	-2.411008	2.149537
H	-0.410181	-2.953259	1.811557
H	-1.413323	2.724406	0.710721
H	0.009350	3.686313	1.171001
H	-0.306350	3.477693	-1.336662
H	1.245657	2.814016	-0.804554
H	-1.596030	-0.326871	0.167180
H	1.510864	-2.335950	-1.994778
H	0.059420	-1.374931	3.153653
H	0.106392	1.250293	-2.229475
H	1.136175	1.732359	1.755246
C	-2.742594	0.010769	-0.152859
O	-2.686016	1.094174	-0.946802
C	-3.291195	-1.241848	-0.845247
H	-4.355157	-1.080173	-1.049905
H	-2.797075	-1.400380	-1.807508
H	-3.191692	-2.139162	-0.225304
C	-3.398176	0.275561	1.205949
H	-4.451570	0.523788	1.037036
H	-3.351238	-0.598877	1.863369
H	-2.937681	1.132192	1.706333
C	3.411252	0.188237	-0.165859
N	2.264578	0.044772	-0.053032
C	4.851751	0.364753	-0.315861
H	5.061418	1.249752	-0.924202
H	5.321423	0.488135	0.664559
H	5.285741	-0.511792	-0.806348

3A

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.253375	-0.168574	0.070965
P	0.281632	-1.764188	-1.640261
N	-0.180182	1.349017	-1.277961
P	0.367531	-1.794858	1.835097
N	0.213612	1.566984	1.427893
C	-0.286692	2.767623	0.677226
C	0.211255	2.669071	-0.756813
H	-0.341035	1.429433	2.271473
H	-1.816346	1.284616	-1.209002
H	-0.488697	-2.945805	-1.566014
H	-0.126760	-1.326628	-2.921261
H	1.583311	-2.463850	2.118755
H	-0.469362	-2.935294	1.824406
H	-1.378211	2.726731	0.688363
H	0.040064	3.692219	1.164749
H	-0.241740	3.475369	-1.350590
H	1.302970	2.825201	-0.786802
H	-1.673976	-0.320477	0.174156
H	1.521817	-2.343666	-1.993114
H	0.082062	-1.380619	3.159554
H	0.182445	1.249752	-2.225942
H	1.168498	1.734641	1.744134
C	-2.776588	-0.017239	-0.111626
O	-2.759854	1.160746	-0.826480
C	-3.320320	-1.194491	-0.925924
H	-4.376243	-1.008227	-1.147966
H	-2.797363	-1.280584	-1.882751
H	-3.243721	-2.141650	-0.380951
C	-3.488574	0.159829	1.228714
H	-4.532748	0.429965	1.039937
H	-3.473110	-0.760432	1.821680
H	-3.038436	0.971159	1.808403
N	2.258747	0.013098	-0.032883
C	3.408152	0.145732	-0.131650
C	4.851649	0.310587	-0.264253
H	5.285366	-0.571666	-0.744702
H	5.310053	0.435492	0.721336
H	5.075499	1.190938	-0.874400

4_A

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.208097	0.149127	-0.073469
P	-0.256663	0.405165	2.181470
N	1.095289	-1.867356	0.126494
P	-0.418506	2.317878	-0.649190
N	1.916917	0.400726	-0.939133
C	2.923285	-0.667764	-0.969057
C	2.578018	-1.687500	0.109919
H	2.273820	1.255798	-1.360349
H	0.799226	-2.407930	-0.687428
H	-1.553414	0.290726	2.747104
H	0.416203	-0.476011	3.062373
H	-0.601356	3.318883	0.333930
H	-1.617698	2.519967	-1.369839
H	2.934501	-1.143312	-1.962186
H	3.934713	-0.279425	-0.792298
H	3.097820	-2.639076	-0.049439
H	2.858817	-1.296498	1.091569
H	0.121342	1.626138	2.782822
H	0.462487	3.031276	-1.495486
H	0.814916	-2.410775	0.940784
C	-2.795309	-1.009273	-0.492214
N	-1.733751	-0.585735	-0.283450
C	-4.124980	-1.537441	-0.777092
H	-4.290958	-2.463234	-0.218179
H	-4.226581	-1.745900	-1.846599
H	-4.887842	-0.809439	-0.485043

TS4-5_A

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.199919	-0.400798	0.019793
P	-1.014796	-1.619124	-1.692530
N	1.523782	0.656141	-1.388541
P	-0.960853	-1.365453	1.810907
N	1.588474	0.323309	1.302287
C	2.433632	1.381912	0.751593

C	2.798399	0.985930	-0.670101
H	1.332262	0.555008	2.260830
H	1.056930	1.521129	-1.662982
H	-2.404667	-1.420775	-1.878049
H	-0.634475	-1.449939	-3.047282
H	-1.104252	-2.767375	1.914183
H	-2.305768	-0.998340	2.043325
H	1.940175	2.372613	0.740900
H	3.352901	1.496875	1.343249
H	3.349399	1.773239	-1.196199
H	3.406498	0.077444	-0.657544
H	-1.034123	-3.034976	-1.696305
H	-0.435538	-1.110944	3.098275
H	1.726195	0.159439	-2.254970
H	1.573743	-2.522947	-0.197088
H	1.899990	-2.107605	0.335798
C	-1.825715	2.003162	-0.078652
N	-1.099482	1.095869	-0.075986
C	-2.743628	3.137061	-0.075793
H	-3.122196	3.321423	-1.085777
H	-2.233239	4.036368	0.282334
H	-3.591072	2.927513	0.584144

5_A

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.222798	-0.509211	0.036129
P	-1.963267	-0.375782	-1.651378
N	1.413232	-0.927594	-1.379888
P	-1.653613	-0.115316	1.853258
N	1.395937	-0.728358	1.384202
C	2.653506	-0.519524	0.672244
C	2.615556	-1.362133	-0.591672
H	1.345102	-0.067434	2.158804
H	1.632263	-0.063902	-1.876094
H	-2.435324	0.906726	-2.018033
H	-1.705822	-0.853242	-2.959755
H	-2.807910	-0.906462	2.043034
H	-2.242304	1.159138	2.017157
H	2.853749	0.532285	0.382081
H	3.504137	-0.838667	1.292937

H	3.526573	-1.265264	-1.192012
H	2.472689	-2.414389	-0.330657
H	-3.222920	-0.996850	-1.484851
H	-1.073652	-0.263813	3.132674
H	1.193735	-1.615862	-2.098565
H	-0.662057	-2.244991	-0.012604
H	-0.115993	-2.180552	0.592867
C	0.417080	2.626776	-0.206158
N	0.167943	1.496127	-0.142188
C	0.732675	4.048710	-0.277272
H	0.543900	4.426475	-1.286446
H	1.785714	4.209624	-0.027596
H	0.111724	4.604725	0.431448

TS5-1_A

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.073441	-0.512583	0.017045
P	-1.359868	-1.078236	1.774147
N	1.691092	-0.109394	1.361958
P	-1.398082	-1.335297	-1.679664
N	1.654203	0.125417	-1.391421
C	2.949042	0.282349	-0.649375
C	2.633792	0.810183	0.743724
H	1.781773	-0.498514	-2.186549
H	1.309124	-1.534372	0.697381
H	-2.120681	-2.268349	1.742208
H	-0.771017	-1.241608	3.048636
H	-2.495389	-0.564116	-2.133850
H	-2.089728	-2.551884	-1.481833
H	3.404220	-0.709219	-0.573938
H	3.632116	0.940718	-1.195978
H	3.566660	0.867227	1.323202
H	2.245794	1.842584	0.654254
H	0.824824	-2.083246	0.145087
H	-2.390207	-0.176267	2.123458
H	-0.853440	-1.641416	-2.950278
H	1.431936	0.172395	2.302228
H	1.373272	1.025790	-1.778453
C	-1.153188	2.491331	-0.103033
N	-0.725897	1.412790	-0.089339

C	-1.689885	3.847501	-0.112769
H	-2.626613	3.881824	0.451472
H	-1.884365	4.168628	-1.140348
H	-0.974766	4.536606	0.346419

1_B

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.132374	0.013947	-0.134035
P	-1.709975	-1.629940	-0.635310
N	1.574254	-1.379831	-0.356733
P	-1.719361	1.713675	-0.324859
N	1.572301	1.433184	-0.095695
C	2.792536	0.733134	-0.592011
C	2.836962	-0.669778	-0.006196
H	1.387264	2.242516	-0.684929
H	1.602214	-1.670453	-1.332647
H	-2.691566	-1.341244	-1.606178
H	-1.206350	-2.827464	-1.192666
H	-2.531073	2.107063	0.762170
H	-2.720682	1.586743	-1.310388
H	2.720764	0.685682	-1.682529
H	3.703405	1.284390	-0.333339
H	3.716629	-1.209507	-0.374523
H	2.901313	-0.627158	1.085761
H	-0.063970	0.176458	-1.782316
H	-2.543023	-2.193749	0.356483
H	-1.226467	2.987494	-0.689910
H	1.494760	-2.230702	0.197217
H	1.737527	1.794875	0.842625
C	-0.265597	-0.178738	1.835512
O	-0.403191	-0.289478	2.973550

2_B

Coordinates (Angstroms)			
	X	Y	Z

Ru	-1.111162	-0.069478	-0.089841
P	-0.116978	-2.133505	0.335762

N	0.560495	1.002020	0.869319
P	-2.701248	-1.006370	-1.516934
N	-1.538436	2.008162	-0.732069
C	-0.297737	2.814072	-0.544875
C	0.318700	2.467476	0.802117
H	-1.817789	2.041325	-1.710283
H	1.434574	0.755588	0.394587
H	-0.097006	-3.095696	-0.696453
H	1.264257	-2.076753	0.619537
H	-3.948572	-1.479087	-1.049819
H	-2.331096	-2.124220	-2.295339
H	0.387232	2.544921	-1.353531
H	-0.504729	3.888564	-0.608286
H	1.246464	3.032240	0.950661
H	-0.368165	2.737287	1.611519
H	-0.156118	-0.139307	-1.443838
H	-0.537637	-2.969438	1.394979
H	-3.177372	-0.181166	-2.562743
H	0.696170	0.728868	1.840459
H	-2.304535	2.419407	-0.200722
C	4.372426	-0.229999	-0.093523
O	3.183137	-0.181445	0.212707
C	5.222948	-1.424637	0.266040
H	6.154081	-1.107128	0.748262
H	4.676286	-2.104209	0.921213
H	5.510658	-1.956180	-0.649715
C	5.043097	0.898158	-0.841921
H	5.776271	1.384711	-0.186559
H	5.600547	0.514604	-1.703520
H	4.309828	1.635498	-1.172196
C	-2.264777	-0.046886	1.518052
O	-2.954533	-0.097936	2.440577

TS2-3_B

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.567043	-0.043859	0.032406
P	0.718379	-1.737153	-1.609545
N	-0.317379	1.293869	-1.320955
P	1.069196	-1.537542	1.852337
N	0.196419	1.695580	1.350817

C	-0.584777	2.740582	0.601741
C	-0.181517	2.697787	-0.863021
H	-0.304703	1.441572	2.201292
H	-1.545717	0.971194	-1.218142
H	0.142316	-2.998590	-1.355770
H	0.110683	-1.445159	-2.849180
H	2.387268	-1.993501	2.068460
H	0.400583	-2.778515	1.926816
H	-1.642662	2.485235	0.689774
H	-0.420725	3.729315	1.040847
H	-0.844747	3.353852	-1.440687
H	0.845486	3.059021	-1.001516
H	-1.250122	-0.534768	0.252733
H	1.990853	-2.146107	-2.058064
H	0.793034	-1.075785	3.159294
H	-0.026010	1.230829	-2.296071
H	1.084285	2.088260	1.660636
C	-2.473893	-0.419433	-0.015428
O	-2.636796	0.604821	-0.853916
C	-2.820483	-1.789642	-0.612063
H	-3.905925	-1.833986	-0.752785
H	-2.364684	-1.910651	-1.598555
H	-2.525297	-2.619322	0.039268
C	-3.084895	-0.205334	1.375004
H	-4.173863	-0.160537	1.266458
H	-2.841758	-1.020595	2.064477
H	-2.763880	0.746654	1.807607
C	2.366024	0.439073	-0.248108
O	3.463800	0.739863	-0.435137

3_B

Coordinates (Angstroms)

X Y Z

Ru	1.211204	0.043398	0.032186
P	3.437538	-0.693962	-0.262153
N	1.840421	1.883041	0.028406
P	0.251728	-1.482712	-1.502579
N	-0.663329	1.129051	0.387791
C	-0.481085	2.521634	-0.116845
C	0.911385	2.990189	0.279431
H	-1.516504	0.714496	-0.008985

H	-3.412791	0.305344	-1.713353
H	3.810056	-1.467173	-1.383582
H	4.405179	0.328996	-0.369052
H	0.625797	-2.843410	-1.546686
H	0.447058	-1.158291	-2.863448
H	-0.562271	2.482340	-1.206960
H	-1.263085	3.185743	0.268110
H	1.190252	3.877349	-0.303230
H	0.937528	3.282516	1.341060
H	-4.563140	-1.523491	-0.704411
H	4.034024	-1.473499	0.750100
H	-1.153197	-1.615694	-1.487877
H	2.806931	2.202488	0.021847
H	-0.803495	1.154181	1.398334
C	-4.300729	-0.594120	-0.180821
O	-3.130859	-0.032725	-0.851825
C	-5.474669	0.377331	-0.248520
H	-5.234765	1.316568	0.261495
H	-5.746895	0.604111	-1.286252
H	-6.357242	-0.058255	0.230756
C	-3.875651	-0.924836	1.242502
H	-3.628141	-0.012241	1.797148
H	-4.690045	-1.427673	1.772001
H	-3.009184	-1.593808	1.250648
C	0.891358	-1.221844	1.395381
O	0.729440	-1.906620	2.313947

4_B

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.056116	0.056464	0.021954
P	1.223905	-1.527808	-1.308780
N	-1.720104	-1.212832	0.345106
P	1.625572	1.793329	-0.298054
N	-1.374863	1.356155	-0.158459
C	-2.774976	0.962670	0.035482
C	-2.889409	-0.520466	-0.282769
H	-1.280348	2.368331	-0.213455
H	-1.866997	-1.285455	1.352892
H	2.610094	-1.755218	-1.172288
H	0.782876	-2.870399	-1.282613

H	2.490255	1.783677	-1.413617
H	2.566350	2.058729	0.717287
H	-3.094606	1.167221	1.069157
H	-3.438045	1.536661	-0.623800
H	-3.834740	-0.946413	0.069943
H	-2.812603	-0.676229	-1.362225
H	1.170837	-1.302496	-2.701638
H	1.069417	3.081327	-0.454114
H	-1.653233	-2.171209	0.005828
C	0.984636	-0.607174	1.527118
O	1.477845	-0.933648	2.519958

TS5-1_B

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.110828	0.008896	-0.173586
P	-1.673261	-1.750122	-0.429695
N	1.531200	-1.312806	-0.514784
P	-1.779859	1.752709	-0.375706
N	1.603359	1.409395	-0.067269
C	2.868906	0.682502	-0.429451
C	2.749400	-0.753723	0.059112
H	1.489895	2.223805	-0.669413
H	0.765565	-0.601179	-1.689305
H	-2.593792	-1.690290	-1.496468
H	-1.126092	-3.028868	-0.666717
H	-2.862115	1.823328	0.527127
H	-2.500971	1.841767	-1.585455
H	2.953628	0.697733	-1.519517
H	3.737701	1.193271	-0.003554
H	3.629610	-1.321340	-0.273176
H	2.749781	-0.764928	1.163568
H	0.140628	-0.042057	-2.010890
H	-2.554434	-2.057005	0.626481
H	-1.351422	3.096613	-0.287946
H	1.387327	-2.281499	-0.246382
H	1.681926	1.775001	0.880685
C	-0.269651	-0.072200	1.721589
O	-0.363480	-0.138773	2.867079

1c

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.212251	0.020821	-0.307343
P	-1.785644	-1.625492	-0.361955
N	1.490101	-1.381300	-0.478613
P	-1.777076	1.661729	-0.138198
N	1.482052	1.418948	-0.237282
C	2.693027	0.747313	-0.762088
C	2.755996	-0.661721	-0.183481
H	1.333057	2.308962	-0.705662
H	1.512717	-1.807366	-1.401575
H	-2.927691	-1.548037	-1.201957
H	-1.389232	-2.931412	-0.767416
H	-2.422388	1.929231	1.098003
H	-2.939838	1.681592	-0.952806
H	2.605519	0.712578	-1.852780
H	3.611856	1.293458	-0.507409
H	3.631697	-1.195355	-0.574328
H	2.838601	-0.605266	0.905317
H	-0.300588	0.138359	-1.916162
H	-2.464309	-2.021900	0.820448
H	-1.379470	3.001524	-0.409371
H	1.350685	-2.114580	0.214167
H	1.569077	1.586811	0.768931
Cl	0.273584	-0.156786	2.246628

2c

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.787234	-0.189907	0.147456
P	0.759715	-1.973332	-1.268859
N	-0.479254	1.059106	-1.162139
P	2.101499	-1.258543	1.669234
N	0.731147	1.681058	1.291586
C	-0.384220	2.527602	0.804798
C	-0.402767	2.473875	-0.717943
H	0.691837	1.578674	2.302367
H	-1.451945	0.746597	-1.163624

H	0.471613	-3.294760	-0.831517
H	-0.170775	-1.968959	-2.346590
H	3.493182	-1.420946	1.439977
H	1.840405	-2.585358	2.104875
H	-1.314757	2.119566	1.210816
H	-0.285737	3.568682	1.142013
H	-1.242770	3.063348	-1.105600
H	0.531041	2.887316	-1.109165
H	-0.523349	-0.754736	0.912132
H	1.904084	-2.296050	-2.044271
H	2.215348	-0.695585	2.972621
H	-0.112873	0.991271	-2.109477
H	1.632491	2.095505	1.038798
Cl	2.776046	0.996234	-1.040648
C	-3.984071	-0.288991	-0.051871
O	-3.470511	0.628015	-0.680868
C	-5.100106	-0.033094	0.936628
H	-4.839391	-0.453344	1.915667
H	-5.294007	1.036896	1.026895
H	-6.011481	-0.546866	0.606153
C	-3.500459	-1.714112	-0.215007
H	-2.549538	-1.803830	0.327752
H	-4.207135	-2.449460	0.178260
H	-3.294940	-1.916851	-1.269585

TS2-3_C

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.432153	-0.121897	0.038621
P	0.677413	-1.728568	-1.598865
N	-0.357018	1.280138	-1.320779
P	1.111304	-1.539240	1.778581
N	0.358545	1.669195	1.305349
C	-0.379311	2.756887	0.599681
C	-0.065293	2.657758	-0.887929
H	0.007061	1.551629	2.253276
H	-1.678700	1.012897	-1.172566
H	0.020678	-2.985399	-1.573239
H	0.312190	-1.370296	-2.922220
H	2.429381	-2.060596	1.783735
H	0.442230	-2.747642	2.107695

H	-1.448017	2.590717	0.759454
H	-0.111404	3.742078	1.001003
H	-0.681876	3.387756	-1.433315
H	0.989805	2.908798	-1.063988
H	-1.395589	-0.503465	0.294648
H	1.984973	-2.191252	-1.871786
H	1.136510	-1.020642	3.102254
H	-0.051550	1.171230	-2.287263
H	1.352805	1.900690	1.367449
C	-2.550461	-0.345043	0.049506
O	-2.721257	0.690336	-0.812766
C	-2.994393	-1.694277	-0.534887
H	-4.080318	-1.674151	-0.682542
H	-2.530470	-1.855826	-1.511975
H	-2.746288	-2.533658	0.125263
C	-3.169717	-0.081294	1.429463
H	-4.255200	0.019798	1.317136
H	-2.965526	-0.896763	2.133037
H	-2.791030	0.855452	1.849094
Cl	2.760545	0.538060	-0.311475

3c

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.446220	-0.118260	0.033495
P	0.661504	-1.710816	-1.623092
N	-0.269461	1.299392	-1.319952
P	1.043293	-1.580201	1.781703
N	0.411037	1.664763	1.311161
C	-0.295998	2.770154	0.600811
C	0.043928	2.666919	-0.880464
H	0.052110	1.553447	2.257129
H	-1.817123	1.029540	-1.150944
H	-0.042909	-2.942188	-1.632461
H	0.335173	-1.315397	-2.946035
H	2.336460	-2.161296	1.794127
H	0.321745	-2.760607	2.105016
H	-1.369948	2.619946	0.742493
H	-0.017428	3.747702	1.013681
H	-0.547404	3.412044	-1.434870
H	1.107333	2.909626	-1.030858

H	-1.475541	-0.474186	0.292944
H	1.955038	-2.220161	-1.879149
H	1.085545	-1.071700	3.109143
H	0.056246	1.189830	-2.280032
H	1.409982	1.872878	1.380705
C	-2.597045	-0.315930	0.057077
O	-2.760639	0.762438	-0.794781
C	-3.075663	-1.626929	-0.578116
H	-4.155711	-1.566771	-0.753510
H	-2.590347	-1.782857	-1.545850
H	-2.873815	-2.490850	0.065897
C	-3.255405	-0.055461	1.415323
H	-4.332943	0.082943	1.272407
H	-3.100488	-0.890991	2.107504
H	-2.859219	0.858956	1.867165
Cl	2.793693	0.440452	-0.263262

4c

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.028280	0.133000	-0.051166
P	1.261882	-1.227306	-1.453620
N	-1.642932	-1.260396	0.221734
P	1.557913	1.840008	-0.029378
N	-1.490924	1.366973	-0.059186
C	-2.853201	0.861062	0.103244
C	-2.875305	-0.612892	-0.296576
H	-1.467256	2.384142	-0.047063
H	-1.666566	-1.382666	1.235529
H	2.459022	-1.890082	-1.069257
H	0.601714	-2.367990	-1.986950
H	2.479819	2.079807	-1.083294
H	2.483562	1.882279	1.040454
H	-3.185805	0.970748	1.150382
H	-3.578447	1.409189	-0.517181
H	-3.785762	-1.111957	0.061467
H	-2.837619	-0.693906	-1.386898
H	1.719065	-0.708380	-2.692365
H	1.081230	3.175457	0.068121
H	-1.515919	-2.188445	-0.175432
Cl	1.175279	-1.107987	1.760054

TS4-5_C

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.107287	0.022849	-0.275873
P	1.750649	-1.674012	-0.434816
N	-1.572391	-1.369206	-0.061266
P	1.610168	1.768380	-0.249413
N	-1.463020	1.320007	-0.433199
C	-2.724142	0.766925	0.054826
C	-2.829321	-0.666864	-0.446867
H	-1.346363	2.255151	-0.043677
H	-1.554570	-1.539578	0.947668
H	2.701780	-1.842879	0.605027
H	1.326931	-3.032278	-0.471238
H	2.542403	2.020450	-1.290598
H	2.506321	1.872067	0.840032
H	-2.793053	0.763384	1.158560
H	-3.588131	1.340270	-0.318431
H	-3.712325	-1.179950	-0.044513
H	-2.884097	-0.673022	-1.540264
H	2.669892	-1.794468	-1.514561
H	1.066589	3.077718	-0.187231
H	-1.499596	-2.271797	-0.525945
H	0.148278	-0.076758	-2.972219
H	-0.346306	0.427503	-2.723024
Cl	0.246941	-0.118981	2.135044

5_C

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.119729	0.011168	-0.374122
P	1.823094	-1.662371	-0.259554
N	-1.543572	-1.404276	-0.219066
P	1.583955	1.799265	-0.264538
N	-1.521621	1.373302	-0.338759
C	-2.702338	0.685436	0.183186
C	-2.812538	-0.669865	-0.498313

H	-1.298513	2.119128	0.320792
H	-1.503157	-1.659564	0.770582
H	2.808279	-1.526737	0.746420
H	1.426330	-2.983841	0.074986
H	2.363862	2.221410	-1.370841
H	2.610091	1.795890	0.708339
H	-2.675768	0.516525	1.275228
H	-3.617734	1.262493	-0.031243
H	-3.683474	-1.239672	-0.149230
H	-2.885660	-0.539811	-1.583090
H	2.698173	-2.032924	-1.316116
H	1.009885	3.055279	0.047575
H	-1.486356	-2.262100	-0.763696
H	0.188775	-0.242861	-2.110627
H	-0.249013	0.462963	-2.008046
Cl	0.145063	-0.080447	2.088662

TS5-1_c

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.127691	0.034247	-0.329663
P	1.645914	1.762468	-0.174447
N	-1.562404	1.382769	-0.476327
P	1.766599	-1.637591	-0.480893
N	-1.549543	-1.372533	-0.165524
C	-2.833818	-0.668382	-0.440544
C	-2.727668	0.745512	0.120450
H	-1.485858	-2.234935	-0.701733
H	-0.733762	0.771549	-1.639636
H	2.638179	2.027781	-1.153482
H	1.125048	3.079781	-0.101358
H	2.685645	-1.820090	0.580970
H	2.698525	-1.703349	-1.548614
H	-2.961889	-0.627698	-1.527355
H	-3.683818	-1.209937	-0.007464
H	-3.653667	1.290479	-0.125615
H	-2.660517	0.682909	1.219702
H	-0.064487	0.219296	-2.039478
H	2.474524	1.811562	0.969472
H	1.339858	-2.990292	-0.566234
H	-1.376988	2.291526	-0.062603

H	-1.480201	-1.610379	0.827630
Cl	0.205050	-0.228980	2.154388

1_D

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.161743	0.022415	-0.342683
P	-1.744112	-1.598357	-0.504321
N	1.537807	-1.390555	-0.464225
P	-1.700089	1.682762	-0.277166
N	1.532483	1.390393	-0.122698
C	2.781578	0.730804	-0.555784
C	2.774681	-0.697293	-0.022013
H	1.456487	2.327756	-0.507473
H	1.631999	-1.763504	-1.405391
H	-2.885828	-1.435525	-1.333424
H	-1.365577	-2.871397	-1.019862
H	-2.337794	2.095390	0.928986
H	-2.878742	1.636316	-1.068356
H	2.807587	0.737240	-1.650865
H	3.676296	1.253609	-0.188334
H	3.680262	-1.230420	-0.339151
H	2.734944	-0.670591	1.069651
H	-0.231664	0.129104	-1.977331
H	-2.448283	-2.105765	0.626401
H	-1.294832	2.985926	-0.682710
H	1.338326	-2.157482	0.173434
H	1.463420	1.408910	0.907119
O	0.437424	-0.052422	1.791344
C	-0.454869	-0.244074	2.836503
H	-1.325315	0.445217	2.809771
H	-0.877594	-1.270922	2.867663
H	0.036270	-0.082306	3.815694

2_D

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.639697	-0.166561	0.134475

P	0.528747	-1.947893	-1.269359
N	-0.410750	1.194698	-1.256484
P	1.661790	-1.348652	1.778494
N	0.750841	1.720287	1.235474
C	-0.195476	2.704712	0.668169
C	-0.139416	2.596453	-0.851219
H	0.705672	1.704888	2.250489
H	-1.414461	1.010609	-1.268142
H	0.135238	-3.238373	-0.820090
H	-0.374572	-1.893256	-2.369550
H	3.064704	-1.599284	1.791422
H	1.267151	-2.673703	2.106581
H	-1.199489	2.464723	1.032908
H	0.046417	3.732440	0.974636
H	-0.851355	3.295174	-1.308440
H	0.872392	2.831968	-1.190741
H	-0.789965	-0.653386	0.783072
H	1.651397	-2.391996	-2.025731
H	1.593088	-0.839862	3.107132
H	-0.045057	1.047463	-2.194105
H	1.714632	1.908965	0.915206
C	-3.711985	-0.175248	-0.058944
O	-3.424406	0.753066	-0.804020
C	-3.793040	-1.600263	-0.561042
H	-4.802183	-1.999548	-0.402477
H	-3.543949	-1.643811	-1.622535
H	-3.099102	-2.227819	0.009604
C	-3.976545	0.049863	1.413867
H	-4.819383	-0.550560	1.772002
H	-3.081454	-0.269539	1.962839
H	-4.155139	1.108987	1.608894
O	2.392393	0.934997	-0.646539
C	3.536443	0.315078	-1.125636
H	3.374678	-0.222433	-2.084810
H	4.337864	1.054288	-1.318560
H	3.963717	-0.432045	-0.423144

TS2-3_D

Coordinates (Angstroms)

X Y Z

Ru	0.419562	-0.156017	0.100471
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P	0.681663	-1.742995	-1.550390
N	-0.254666	1.333186	-1.253219
P	1.001478	-1.629280	1.818573
N	0.349557	1.589664	1.410798
C	-0.315805	2.730249	0.727827
C	0.056681	2.681820	-0.749177
H	0.008684	1.483272	2.363468
H	-1.512520	1.127324	-1.192639
H	-0.116111	-2.915046	-1.606140
H	0.485025	-1.344902	-2.899676
H	2.354026	-2.045518	1.900994
H	0.402285	-2.899973	2.023235
H	-1.396478	2.601977	0.834309
H	-0.027785	3.689541	1.176824
H	-0.509792	3.454417	-1.289457
H	1.126544	2.906708	-0.868560
H	-1.465123	-0.504051	0.196022
H	1.933353	-2.382271	-1.737479
H	0.877867	-1.192629	3.166436
H	0.066318	1.253282	-2.217111
H	1.369341	1.714625	1.426585
C	-2.591995	-0.256645	-0.098360
O	-2.655389	0.817401	-0.921144
C	-3.090488	-1.554160	-0.757489
H	-4.162973	-1.456603	-0.962517
H	-2.584057	-1.712190	-1.714283
H	-2.934490	-2.432048	-0.118487
C	-3.266803	-0.016884	1.262748
H	-4.338146	0.151383	1.102962
H	-3.143197	-0.870279	1.940570
H	-2.857425	0.878296	1.740553
O	2.420980	0.429721	0.217406
C	3.162982	0.643998	-0.944588
H	4.148726	1.053617	-0.667624
H	3.355543	-0.282811	-1.517624
H	2.696141	1.365582	-1.642749

3D

Coordinates (Angstroms)

X Y Z

Ru	0.451345	-0.149611	0.086159
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P	0.686520	-1.710606	-1.592065
N	-0.131517	1.353135	-1.238060
P	0.878700	-1.703428	1.806597
N	0.445189	1.579228	1.416179
C	-0.172766	2.750329	0.738189
C	0.205948	2.689636	-0.736790
H	0.094928	1.475254	2.365816
H	-1.767057	1.143329	-1.154273
H	-0.172951	-2.833173	-1.724257
H	0.586481	-1.269967	-2.939025
H	2.156638	-2.316803	1.846420
H	0.112341	-2.874514	2.051263
H	-1.258025	2.659819	0.841838
H	0.147777	3.694382	1.197620
H	-0.341111	3.477499	-1.278162
H	1.282090	2.917378	-0.841409
H	-1.615184	-0.466846	0.193607
H	1.907191	-2.419491	-1.724661
H	0.876982	-1.252810	3.155975
H	0.186960	1.274270	-2.203308
H	1.468182	1.662323	1.449643
C	-2.692772	-0.218369	-0.079612
O	-2.731632	0.913177	-0.896699
C	-3.250176	-1.449098	-0.804657
H	-4.304001	-1.278586	-1.052293
H	-2.711021	-1.618992	-1.741533
H	-3.178977	-2.352024	-0.186249
C	-3.416325	0.045135	1.244650
H	-4.467492	0.281854	1.044941
H	-3.376031	-0.826961	1.907913
H	-2.972987	0.902062	1.761392
O	2.477987	0.225897	0.288942
C	3.230833	0.553566	-0.842595
H	4.254757	0.802632	-0.518786
H	3.318755	-0.279586	-1.564889
H	2.839272	1.426031	-1.396424

4D

Coordinates (Angstroms)

X Y Z

Ru	-0.083462	0.008732	-0.225555
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P	-1.601415	1.799658	-0.438064
N	1.632091	1.265651	0.289705
P	-1.671501	-1.581750	-0.643665
N	1.409326	-1.179936	-0.761608
C	2.756183	-0.809492	-0.338907
C	2.856780	0.712843	-0.343858
H	1.339135	-2.184227	-0.911258
H	1.610124	1.146613	1.305573
H	-2.462892	2.156743	0.634995
H	-1.087841	3.105652	-0.676074
H	-2.651453	-1.427044	-1.662052
H	-2.567199	-1.982925	0.382168
H	2.981637	-1.187491	0.676820
H	3.530098	-1.219496	-1.006542
H	3.770793	1.059993	0.156632
H	2.864670	1.070149	-1.378219
H	-2.571593	1.844088	-1.474211
H	-1.251457	-2.884813	-1.030279
H	1.542073	2.261505	0.103919
O	-0.547056	0.320673	1.775832
C	-0.337929	-0.784074	2.604749
H	0.684674	-1.204277	2.527818
H	-0.487068	-0.472057	3.652719
H	-1.041318	-1.616273	2.413101

TS4-5_D

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.142444	0.095758	-0.278917
P	-1.796848	1.734082	0.135610
N	1.522353	1.405168	0.240092
P	-1.652097	-1.596283	-0.658756
N	1.447222	-1.069934	-0.859077
C	2.711837	-0.652369	-0.267295
C	2.784611	0.868542	-0.334661
H	1.364258	-2.083326	-0.787552
H	1.461867	1.236006	1.250765
H	-2.566332	1.636636	1.324983
H	-1.397735	3.088537	0.323511
H	-2.620474	-1.541636	-1.698342
H	-2.542041	-2.007797	0.366770

H	2.822620	-0.958878	0.793820
H	3.577126	-1.074434	-0.804498
H	3.664987	1.259480	0.192808
H	2.829530	1.188592	-1.380638
H	-2.877323	2.042377	-0.737331
H	-1.145125	-2.883961	-0.983373
H	1.433874	2.405264	0.075015
H	-0.316017	0.823661	-2.938535
H	0.227032	0.326626	-2.801543
O	-0.159319	-0.066834	1.779479
C	0.148906	-1.309468	2.341873
H	1.137574	-1.698410	2.037458
H	0.160231	-1.199910	3.438999
H	-0.596939	-2.091364	2.104782

5D

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.146387	0.107526	-0.395763
P	-1.791118	1.732730	0.165236
N	1.527515	1.449306	-0.005193
P	-1.625191	-1.653781	-0.605959
N	1.492163	-1.235256	-0.653627
C	2.666986	-0.686460	0.015552
C	2.799378	0.776020	-0.386429
H	1.287933	-2.142056	-0.233535
H	1.419469	1.438639	1.015894
H	-2.694359	1.392064	1.200224
H	-1.320280	2.937164	0.751668
H	-2.428565	-1.820521	-1.763618
H	-2.654102	-1.881273	0.343324
H	2.625715	-0.729046	1.121669
H	3.582792	-1.221265	-0.288976
H	3.662106	1.258095	0.092604
H	2.907478	0.854494	-1.473335
H	-2.740170	2.349069	-0.696253
H	-1.073616	-2.961127	-0.590833
H	1.495775	2.409825	-0.338851
H	-0.391756	0.596321	-2.097267
H	0.207498	0.025659	-2.119787
O	0.014650	0.072911	1.686309

C	-0.024577	-1.113026	2.416622
H	0.738969	-1.848832	2.100059
H	0.162563	-0.890804	3.480413
H	-1.007443	-1.622621	2.367814

TS5-1_D

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.165396	0.099820	-0.321483
P	-1.778063	1.735910	0.064639
N	1.507706	1.406252	0.178353
P	-1.711551	-1.577480	-0.610242
N	1.529528	-1.137538	-0.891042
C	2.736070	-0.662691	-0.231366
C	2.784619	0.858915	-0.345042
H	1.399673	-2.139598	-0.792719
H	1.402894	1.236531	1.189586
H	-2.450951	1.730433	1.311958
H	-1.371953	3.098521	0.094103
H	-2.798015	-1.468164	-1.517909
H	-2.461671	-2.046191	0.497883
H	2.768908	-0.932393	0.839370
H	3.645564	-1.076968	-0.696527
H	3.648682	1.266444	0.195710
H	2.864779	1.150271	-1.397724
H	-2.911431	1.940697	-0.765081
H	-1.254284	-2.843873	-1.062895
H	1.426370	2.402394	-0.010441
H	-0.010778	0.302813	-2.066575
H	0.703203	-0.308445	-1.810982
O	-0.075943	0.000757	1.796751
C	0.119265	-1.228869	2.420994
H	1.009048	-1.778236	2.052725
H	0.261781	-1.077529	3.505294
H	-0.742999	-1.916386	2.310824

1_E

Coordinates (Angstroms)		
X	Y	Z

Ru	-1.197598	-0.301932	-0.003209
P	-0.913647	-1.866376	-1.637997
N	-1.625696	1.329781	-1.436926
P	-0.928092	-1.816789	1.671929
N	-1.552920	1.370904	1.365430
C	-2.283312	2.447046	0.659746
C	-1.655331	2.630410	-0.717259
H	-1.984827	1.165216	2.262202
H	-2.498712	1.157844	-1.928788
H	-1.402231	-3.187673	-1.463504
H	-1.544997	-1.633250	-2.891934
H	0.337080	-2.152227	2.226437
H	-1.407608	-3.145362	1.531646
H	-3.330941	2.141028	0.572650
H	-2.247754	3.398803	1.208181
H	-2.195677	3.398511	-1.284545
H	-0.615744	2.944286	-0.600070
H	-2.756601	-0.749762	-0.011227
H	0.353892	-2.228394	-2.171193
H	-1.574629	-1.546939	2.910257
H	-0.867788	1.340894	-2.115995
H	-0.569572	1.632010	1.503042
O	0.728845	0.865112	0.044204
C	2.010434	0.547589	0.026488
C	2.995310	1.574199	0.057431
C	2.490257	-0.788009	-0.022279
C	4.357283	1.280265	0.041531
H	2.653372	2.606134	0.095067
C	3.857927	-1.070919	-0.037900
H	1.767795	-1.598240	-0.045489
C	4.809547	-0.045845	-0.006380
H	5.077114	2.096154	0.066903
H	4.183287	-2.109052	-0.074308
H	5.871802	-0.271599	-0.018561

2_E

Coordinates (Angstroms)			
	X	Y	Z
Ru	-0.277764	-0.264601	0.356794
P	-0.275834	-1.935247	-1.194871

N	-0.981910	1.248995	-1.089495
P	0.337124	-1.639232	2.066694
N	-0.375263	1.514864	1.630758
C	-1.200269	2.558216	0.978180
C	-0.832249	2.604004	-0.499733
H	-0.641278	1.394606	2.604384
H	-1.953901	1.086321	-1.354288
H	-0.724023	-3.241583	-0.861521
H	-1.112024	-1.774418	-2.335129
H	1.691900	-1.932305	2.381029
H	-0.142090	-2.974056	2.142931
H	-2.252764	2.285655	1.100600
H	-1.043103	3.546896	1.431474
H	-1.455166	3.340329	-1.021899
H	0.218664	2.884270	-0.603023
H	-1.808241	-0.713773	0.677382
H	0.881078	-2.342619	-1.913861
H	-0.049855	-1.264259	3.384120
H	-0.401978	1.186577	-1.923105
H	0.620472	1.758034	1.569620
C	-4.588863	0.076440	-0.708410
O	-4.019046	1.032014	-1.219202
C	-4.679595	-1.261789	-1.408275
H	-5.728852	-1.490865	-1.632385
H	-4.105961	-1.247218	-2.336280
H	-4.308812	-2.056156	-0.750824
C	-5.218206	0.178621	0.664422
H	-6.168245	-0.362803	0.718156
H	-4.531643	-0.286745	1.383424
H	-5.361747	1.225366	0.938900
O	1.637471	0.865167	-0.007029
C	2.888707	0.514849	-0.236161
C	3.327498	-0.833510	-0.312111
C	3.882673	1.516256	-0.422803
C	4.664524	-1.153019	-0.558709
H	2.594535	-1.621679	-0.171045
C	5.213836	1.185959	-0.667775
H	3.572253	2.557293	-0.369061
C	5.625520	-0.152501	-0.740115
H	4.958425	-2.200010	-0.608767
H	5.941989	1.983146	-0.805030
H	6.663990	-0.405959	-0.932123

TS2-3_E

	Coordinates (Angstroms)		
	X	Y	Z

Ru	0.493264	-0.292646	-0.191860
P	0.021723	-1.407400	1.774147
N	0.585711	1.614835	0.711671
P	0.667192	-2.284055	-1.424993
N	0.667587	0.995463	-1.957123
C	0.932083	2.403832	-1.551520
C	0.198778	2.668693	-0.242604
H	1.294400	0.711410	-2.706727
H	1.882901	1.678220	0.962744
H	0.865890	-2.434528	2.268612
H	-0.066149	-0.661887	2.977861
H	-0.523408	-2.979784	-1.752429
H	1.428728	-3.404543	-1.002945
H	2.009141	2.506749	-1.393641
H	0.620719	3.108471	-2.332700
H	0.475474	3.666620	0.128027
H	-0.887348	2.665021	-0.412644
H	2.342743	-0.257625	0.216042
H	-1.206870	-2.099321	1.887830
H	1.201239	-2.231846	-2.741325
H	0.069424	1.750558	1.579622
H	-0.297747	0.886211	-2.282315
C	3.324437	0.281618	0.628797
O	3.045936	1.546189	1.029469
C	3.782232	-0.630272	1.777877
H	4.748747	-0.271224	2.149835
H	3.070242	-0.582416	2.606878
H	3.895770	-1.673328	1.459308
C	4.285213	0.228022	-0.568483
H	5.253061	0.643071	-0.264746
H	4.440814	-0.796888	-0.925542
H	3.904849	0.839222	-1.392423
O	-1.479292	-0.269185	-0.935426
C	-2.634957	-0.032678	-0.316909
C	-3.832404	-0.372988	-0.998223
C	-2.763915	0.556880	0.961879
C	-5.079858	-0.133397	-0.428107
H	-3.746734	-0.825458	-1.982393
C	-4.022859	0.785993	1.527087

H	-1.870197	0.849560	1.502146
C	-5.192408	0.446030	0.843855
H	-5.976451	-0.406309	-0.980097
H	-4.083934	1.242321	2.512676
H	-6.166959	0.627464	1.286803

3_E

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.448025	-0.253733	-0.197529
P	-0.077783	-1.299943	1.794854
N	0.610883	1.633406	0.668393
P	0.611206	-2.287198	-1.394567
N	0.663958	0.997461	-1.982259
C	0.994242	2.396815	-1.592355
C	0.273943	2.699549	-0.284377
H	1.270553	0.676492	-2.733680
H	2.217796	1.653661	0.946170
H	0.737373	-2.321628	2.347953
H	-0.184579	-0.510248	2.968612
H	-0.576733	-3.006276	-1.681339
H	1.393242	-3.393377	-0.969691
H	2.075514	2.448568	-1.436344
H	0.715008	3.105903	-2.381805
H	0.598070	3.685885	0.081810
H	-0.811503	2.761231	-0.469678
H	2.450667	-0.303989	0.213765
H	-1.318419	-1.970547	1.900539
H	1.112345	-2.263467	-2.725189
H	0.118528	1.807658	1.543933
H	-0.306504	0.927417	-2.302172
C	3.424740	0.144826	0.621758
O	3.232694	1.484492	0.943447
C	3.794989	-0.687119	1.855301
H	4.753503	-0.336161	2.253797
H	3.042825	-0.562669	2.640072
H	3.885758	-1.753257	1.615734
C	4.449470	-0.000890	-0.506275
H	5.411818	0.406590	-0.176755
H	4.594423	-1.050519	-0.786878
H	4.132689	0.562049	-1.389591

O	-1.500379	-0.255155	-0.959095
C	-2.652973	-0.024569	-0.327567
C	-3.844133	-0.499031	-0.932693
C	-2.777292	0.684755	0.888086
C	-5.087991	-0.267563	-0.350118
H	-3.758876	-1.045936	-1.867614
C	-4.031297	0.904435	1.466719
H	-1.882669	1.075223	1.360358
C	-5.197705	0.433302	0.858938
H	-5.982400	-0.643976	-0.841297
H	-4.092528	1.457380	2.401461
H	-6.168717	0.607517	1.312552

4_E

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.053598	-0.095776	0.101883
P	1.906541	-1.873686	-1.175300
N	0.942812	1.346998	-1.553593
P	0.916990	-1.320363	2.031346
N	1.405835	1.582073	1.055609
C	1.337672	2.851196	0.331792
C	1.654160	2.584941	-1.137294
H	1.397008	1.730471	2.062764
H	-0.060628	1.505971	-1.657696
H	1.081045	-2.921689	-1.665599
H	2.532057	-1.555700	-2.411918
H	1.842216	-2.342833	2.372514
H	-0.268676	-2.063423	2.251110
H	0.334487	3.304837	0.419271
H	2.053650	3.589081	0.723921
H	1.387442	3.443295	-1.768019
H	2.724204	2.386154	-1.248291
H	2.962596	-2.677281	-0.675353
H	0.958219	-0.643601	3.280005
H	1.280025	1.016917	-2.454627
O	-0.724344	-0.921472	-0.682078
C	-1.924087	-0.442290	-0.362996
C	-2.152651	0.622074	0.543386
C	-3.060984	-1.030220	-0.978713
C	-3.451749	1.066088	0.814554

H	-1.300851	1.085254	1.033032
C	-4.346621	-0.576257	-0.698646
H	-2.896131	-1.849713	-1.672839
C	-4.560781	0.478639	0.201388
H	-3.592868	1.883532	1.518912
H	-5.194794	-1.051881	-1.186404
H	-5.565815	0.828751	0.417365

TS4-5_E

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.160893	-0.120222	0.160950
P	1.786731	-2.075169	-1.042610
N	1.545436	1.241252	-1.507411
P	0.414602	-1.272607	2.016390
N	1.040349	1.693710	1.112326
C	0.814223	2.810946	0.200827
C	1.739710	2.626397	-0.995542
H	0.446566	1.803459	1.933547
H	0.638439	1.142312	-1.972557
H	0.798603	-3.021851	-1.417147
H	2.351546	-1.924020	-2.340152
H	1.224869	-2.205461	2.717445
H	-0.738405	-2.084301	1.899200
H	-0.229824	2.871525	-0.163967
H	1.038655	3.778222	0.678632
H	1.551397	3.371426	-1.779486
H	2.781746	2.710420	-0.671266
H	2.753103	-3.011138	-0.583434
H	0.007696	-0.518796	3.147737
H	2.268531	0.993222	-2.179129
H	3.601000	-0.255372	1.069313
H	3.285962	0.391842	1.280975
O	-0.589774	-0.370491	-0.942547
C	-1.848644	-0.167516	-0.548556
C	-2.226686	0.559610	0.602093
C	-2.883957	-0.700569	-1.357607
C	-3.575668	0.739305	0.924747
H	-1.449481	0.994830	1.220612
C	-4.223473	-0.508592	-1.028285
H	-2.601477	-1.262127	-2.243811

C	-4.587187	0.210533	0.119057
H	-3.834262	1.306890	1.816065
H	-4.993474	-0.930235	-1.670483
H	-5.632682	0.354081	0.374961

5_E

Coordinates (Angstroms)			
	X	Y	Z

Ru	1.244863	-0.236310	0.193228
P	1.197527	-2.201842	-1.174247
N	1.906274	1.067067	-1.435480
P	0.298211	-1.272681	2.036468
N	1.228827	1.654852	1.172834
C	1.090363	2.699184	0.163183
C	2.140293	2.442559	-0.908712
H	0.448219	1.736339	1.823055
H	1.040378	1.047724	-1.982350
H	-0.052271	-2.851052	-1.306113
H	1.443395	-2.031243	-2.561867
H	1.014841	-2.260603	2.759474
H	-0.922572	-1.976004	1.914626
H	0.098588	2.733903	-0.325739
H	1.268418	3.695305	0.601751
H	2.098834	3.184670	-1.716299
H	3.138522	2.459949	-0.459604
H	1.991187	-3.369960	-1.022063
H	-0.049973	-0.459824	3.143327
H	2.673572	0.763803	-2.030953
H	2.874290	-0.732233	0.632555
H	2.709969	-0.061823	1.106328
O	-0.534936	0.112981	-0.896205
C	-1.814228	0.169581	-0.535420
C	-2.264364	0.646721	0.718187
C	-2.803109	-0.236656	-1.467118
C	-3.627456	0.705148	1.021325
H	-1.533868	1.000580	1.438224
C	-4.159912	-0.168727	-1.156666
H	-2.471864	-0.597028	-2.437638
C	-4.589826	0.297555	0.093062
H	-3.937729	1.083729	1.992918
H	-4.890979	-0.486974	-1.896624

H	-5.647804	0.346765	0.332761
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TS5-1_E

Coordinates (Angstroms)

	X	Y	Z
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Ru	1.218683	-0.143773	0.169418
P	0.484468	-1.404002	1.957278
N	1.084361	1.750067	1.219967
P	1.780199	-2.018680	-1.125196
N	1.560992	1.281136	-1.455335
C	1.679622	2.668582	-0.930199
C	0.753849	2.805496	0.275068
H	2.299735	1.080847	-2.125517
H	2.299783	0.822946	1.132449
H	1.266405	-2.440919	2.528956
H	0.175617	-0.736588	3.169890
H	0.748199	-2.867372	-1.595082
H	2.672403	-3.026670	-0.679693
H	2.718425	2.814629	-0.616361
H	1.439948	3.408590	-1.703857
H	0.900530	3.804321	0.716848
H	-0.292612	2.753590	-0.075232
H	2.792338	0.037972	0.884120
H	-0.723713	-2.126366	1.820548
H	2.408121	-1.801561	-2.381447
H	0.496419	1.769528	2.047283
H	0.654322	1.133849	-1.912135
O	-0.607680	-0.250143	-0.956422
C	-1.869588	-0.115720	-0.565452
C	-2.260750	0.484348	0.656335
C	-2.904705	-0.575891	-1.420743
C	-3.609991	0.607703	1.001461
H	-1.489445	0.869527	1.315861
C	-4.245723	-0.442815	-1.068277
H	-2.618650	-1.036038	-2.362983
C	-4.616970	0.146962	0.148633
H	-3.874222	1.077147	1.946915
H	-5.012534	-0.807070	-1.748663
H	-5.663614	0.246613	0.420472

1_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.481328	-0.296133	0.011426
P	-1.764670	0.615413	1.648099
N	0.873508	-1.326136	1.433452
P	-1.779677	0.561054	-1.638257
N	0.869320	-1.339202	-1.390574
C	1.608538	-2.388882	-0.654763
C	2.054461	-1.825547	0.690372
H	0.387116	-1.736849	-2.192066
H	0.369663	-2.085576	1.883552
H	-3.182652	0.542400	1.614085
H	-1.621037	0.103261	2.969537
H	-1.675880	1.914436	-2.061247
H	-3.197848	0.514709	-1.575012
H	0.921944	-3.228482	-0.505980
H	2.482026	-2.751425	-1.214488
H	2.607955	-2.587580	1.255293
H	2.711895	-0.965973	0.528961
H	-1.479630	-1.662940	0.034231
H	-1.678369	1.989151	2.004306
H	-1.669065	-0.016847	-2.935730
H	1.170541	-0.663773	2.146028
H	1.502869	-0.609670	-1.718931
C	0.937384	1.277884	-0.021155
C	1.805248	2.154284	-0.058782
C	2.803247	3.230295	-0.098319
H	2.683615	3.926650	0.742725
H	2.726111	3.824740	-1.018791
H	3.831323	2.845776	-0.051107

2_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.462254	-0.343297	0.198228
P	0.355584	-1.883441	-1.466241
N	-0.343054	1.288145	-1.066202
P	1.236922	-1.845479	1.715356

N	0.487973	1.339698	1.627516
C	-0.351277	2.439162	1.096485
C	-0.081383	2.583886	-0.396241
H	0.193005	1.085005	2.566241
H	-1.344948	1.171877	-1.223307
H	-0.313096	-3.130212	-1.319904
H	-0.295304	-1.510447	-2.676855
H	2.587478	-2.289404	1.717078
H	0.643678	-3.125793	1.882985
H	-1.397605	2.165584	1.259927
H	-0.155338	3.391065	1.609424
H	-0.700161	3.389258	-0.812516
H	0.972799	2.828239	-0.558971
H	-1.116503	-0.720381	0.697330
H	1.530191	-2.402125	-2.074182
H	1.191971	-1.483626	3.092804
H	0.131362	1.273151	-1.965767
H	1.469350	1.617432	1.659058
C	-3.886294	0.223513	-0.354454
O	-3.394591	1.207315	-0.894077
C	-3.884633	-1.132046	-1.024380
H	-4.829651	-1.663055	-0.869315
H	-3.679104	-1.028034	-2.091497
H	-3.083388	-1.722437	-0.561982
C	-4.490486	0.304580	1.030522
H	-5.533150	-0.033837	1.015844
H	-3.939028	-0.365584	1.700822
H	-4.439323	1.327307	1.407863
C	2.390970	0.313942	-0.373806
C	3.509246	0.743144	-0.668285
C	4.851077	1.218044	-1.027489
H	5.224549	0.730042	-1.937896
H	5.582324	1.015449	-0.233181
H	4.872099	2.300622	-1.213470

TS2-3_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.232883	-0.254280	0.084441
P	0.315315	-1.853843	-1.542364
N	-0.193149	1.357527	-1.322169

P	0.568509	-1.760603	1.775074
N	0.261449	1.495751	1.431903
C	-0.284599	2.681742	0.721671
C	0.199639	2.654386	-0.722327
H	-0.218403	1.360414	2.318449
H	-1.220752	1.339600	-1.454208
H	-0.595532	-2.941581	-1.613160
H	0.155871	-1.428838	-2.889941
H	1.802345	-2.449112	1.910464
H	-0.276114	-2.883952	1.982142
H	-1.375484	2.608488	0.735679
H	0.014615	3.618945	1.208772
H	-0.232354	3.500819	-1.272098
H	1.290786	2.726400	-0.761355
H	-1.511375	-0.367173	0.242033
H	1.502096	-2.602847	-1.739234
H	0.506131	-1.280414	3.113706
H	0.268704	1.239618	-2.220874
H	1.256145	1.618955	1.624129
C	-3.027528	0.147995	-0.171562
O	-2.920101	1.212599	-0.838604
C	-3.426377	-1.135622	-0.901044
H	-4.508936	-1.091962	-1.087481
H	-2.923361	-1.191433	-1.868935
H	-3.208744	-2.034270	-0.317567
C	-3.519465	0.240871	1.275034
H	-4.604414	0.415493	1.250137
H	-3.326237	-0.674218	1.841408
H	-3.057996	1.092172	1.781228
C	2.275601	0.069703	-0.120188
C	3.479594	0.309196	-0.215903
C	4.917774	0.570365	-0.347613
H	5.343254	0.055256	-1.218963
H	5.477964	0.228813	0.532858
H	5.132482	1.640280	-0.470967

3_F

Coordinates (Angstroms)

X Y Z

Ru	0.288631	-0.175563	0.060920
P	0.401152	-1.760494	-1.599255

N	-0.305136	1.280450	-1.284741
P	0.690997	-1.686531	1.814393
N	0.357721	1.612847	1.345475
C	-0.274093	2.758031	0.627542
C	0.074812	2.631049	-0.849673
H	-0.018587	1.521460	2.286779
H	-2.001567	1.151609	-1.136082
H	-0.506662	-2.845912	-1.717422
H	0.284590	-1.296851	-2.935616
H	1.840706	-2.517447	1.786412
H	-0.226551	-2.691066	2.229565
H	-1.356765	2.670830	0.756066
H	0.056599	3.718271	1.043247
H	-0.471501	3.405343	-1.410886
H	1.151789	2.823581	-0.987401
H	-1.940327	-0.400152	0.300104
H	1.598607	-2.497518	-1.754010
H	0.918292	-1.158800	3.115771
H	-0.007600	1.155137	-2.251601
H	1.365429	1.759835	1.430737
C	-2.989250	-0.118164	-0.004198
O	-2.957071	1.022493	-0.822770
C	-3.579391	-1.319486	-0.753353
H	-4.614552	-1.100791	-1.038760
H	-3.015124	-1.514532	-1.670697
H	-3.571683	-2.226505	-0.136471
C	-3.758006	0.186867	1.284353
H	-4.785945	0.476559	1.038997
H	-3.792247	-0.684728	1.948532
H	-3.295146	1.021053	1.821533
C	2.255451	0.024278	-0.093670
C	3.467293	0.207759	-0.167130
C	4.912450	0.425613	-0.291559
H	5.387002	-0.362746	-0.889905
H	5.411734	0.432398	0.686026
H	5.140400	1.382401	-0.779319

4F

Coordinates (Angstroms)

X Y Z

Ru	-0.268349	-0.353172	0.064187
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P	0.936285	-1.003410	1.956752
N	-1.227557	1.378025	1.026737
P	0.586773	-1.969272	-1.314126
N	-1.870099	-0.120427	-1.090895
C	-2.670295	1.086931	-0.913171
C	-2.640072	1.453134	0.566377
H	-1.963423	-0.480198	-2.038207
H	-0.673983	2.156810	0.664705
H	2.353920	-0.934063	2.040537
H	0.681047	-0.290782	3.162745
H	0.766505	-3.325115	-0.926655
H	1.868854	-1.771814	-1.881558
H	-2.282650	1.936245	-1.506502
H	-3.716750	0.936955	-1.221936
H	-3.075504	2.444336	0.751102
H	-3.201116	0.706240	1.136682
H	0.797722	-2.300574	2.523487
H	-0.116646	-2.243009	-2.518374
H	-1.169104	1.418217	2.041810
C	1.312979	0.813617	-0.276326
C	2.237814	1.592470	-0.496138
C	3.334833	2.514881	-0.807179
H	3.659089	3.081075	0.076029
H	3.050177	3.247142	-1.574666
H	4.215407	1.978958	-1.185086

TS4-5_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.220281	-0.478767	0.018751
P	1.148767	-1.358522	1.721303
N	-1.413855	0.783275	1.372208
P	0.921014	-1.452779	-1.716845
N	-1.679083	0.179024	-1.268603
C	-2.400313	1.348828	-0.773850
C	-2.701342	1.119245	0.701055
H	-1.404885	0.350616	-2.235025
H	-0.822831	1.614774	1.440059
H	2.557009	-1.188254	1.664639
H	0.993433	-0.841427	3.038621
H	0.977668	-2.855891	-1.937441

H	2.302314	-1.187806	-1.874631
H	-1.828417	2.291397	-0.872681
H	-3.352348	1.496234	-1.310252
H	-3.178061	1.992248	1.166035
H	-3.362853	0.253986	0.812185
H	1.176377	-2.726613	2.121278
H	0.506326	-1.096440	-3.026780
H	-1.569410	0.441193	2.318089
C	1.048346	1.037342	-0.074438
C	1.783437	2.020867	-0.107859
C	2.664356	3.191147	-0.181659
H	3.082528	3.453195	0.799173
H	2.136062	4.077998	-0.556115
H	3.512693	3.013770	-0.855502
H	-1.748689	-2.664899	0.421286
H	-2.047616	-2.229485	-0.109575

5_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.083232	-0.606722	-0.013286
P	-1.556576	-0.991617	-1.670517
N	1.605750	0.144574	-1.416120
P	-1.295687	-1.043250	1.772634
N	1.644094	-0.103346	1.354250
C	2.596104	0.791216	0.699177
C	2.902455	0.238998	-0.685220
H	1.251611	0.410511	2.142733
H	1.262369	1.083195	-1.626441
H	-2.834272	-0.408668	-1.484753
H	-1.325238	-0.446836	-2.963018
H	-1.598304	-2.356949	2.218116
H	-2.617249	-0.536254	1.790412
H	2.226805	1.827769	0.575409
H	3.539551	0.854435	1.268520
H	3.621511	0.863719	-1.231787
H	3.307774	-0.774689	-0.599998
H	-2.022303	-2.254202	-2.136411
H	-0.872690	-0.525161	3.021630
H	1.712132	-0.350347	-2.299077
H	0.658174	-2.389815	-0.322331

H	1.066830	-2.168364	0.321003
C	-0.623658	1.283136	0.032300
C	-1.030435	2.441932	0.026459
C	-1.518108	3.824693	0.040033
H	-1.912379	4.128259	-0.938532
H	-0.722863	4.534082	0.303967
H	-2.326777	3.959611	0.769982

TS5-1_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.143630	-0.550462	0.033075
P	1.318351	-1.193620	1.711493
N	-1.495267	0.559120	1.381544
P	1.171901	-1.348864	-1.664712
N	-1.832960	-0.127105	-1.290856
C	-2.574038	1.009202	-0.768302
C	-2.811713	0.777471	0.721363
H	-1.589956	-0.014450	-2.269826
H	-0.990969	1.442289	1.474498
H	2.683000	-0.809758	1.669557
H	1.063687	-0.722245	3.029184
H	1.380679	-2.730310	-1.919941
H	2.525226	-0.941442	-1.736636
H	-2.025180	1.958921	-0.892881
H	-3.552961	1.124446	-1.262588
H	-3.350310	1.619106	1.174958
H	-3.404450	-0.132107	0.862712
H	1.530823	-2.550214	2.075346
H	0.800919	-0.990678	-2.986604
H	-1.618645	0.168072	2.312640
H	-1.261486	-1.999408	0.040676
H	-1.679644	-1.368249	-0.577401
C	0.889201	1.217194	-0.091806
C	1.461522	2.304614	-0.140330
C	2.153574	3.595123	-0.226017
H	2.593020	3.889602	0.736143
H	1.476716	4.403134	-0.533733
H	2.971793	3.565153	-0.957367

TS1_F-4_G

Coordinates (Angstroms)			
	X	Y	Z

Ru	-0.028765	-0.372635	0.177699
P	1.102589	-1.838974	-1.150434
N	-1.772755	-0.413747	-1.135529
P	1.649055	-0.212638	1.731896
N	-1.447201	0.885633	1.288351
C	-2.817756	0.400460	0.965013
C	-2.921723	0.289754	-0.557074
H	-1.301631	0.896513	2.295218
H	-2.032929	-1.319412	-1.512606
H	1.835728	-2.927929	-0.609613
H	0.341612	-2.599086	-2.079032
H	2.817771	0.595139	1.596512
H	2.336752	-1.370835	2.184377
H	-2.925616	-0.582723	1.430285
H	-3.587664	1.075108	1.368739
H	-3.874603	-0.184281	-0.824381
H	-2.953450	1.313754	-0.969093
H	-0.555102	-1.623584	1.017042
H	2.097601	-1.407150	-2.069332
H	1.311759	0.266151	3.031679
H	-1.018224	0.491035	-1.747901
H	-1.325432	1.841705	0.950496
C	-0.036876	1.390118	-1.660154
C	0.956792	1.958095	-1.195193
C	2.145076	2.726235	-0.809626
H	3.024661	2.080648	-0.695161
H	2.002129	3.258711	0.138771
H	2.384233	3.475177	-1.574232

6_F

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.213367	-0.227396	0.072471
P	0.367559	-1.823692	-1.572987
N	-0.286959	1.332015	-1.317204
P	0.624938	-1.734082	1.780953

N	0.216861	1.535253	1.398592
C	-0.340731	2.713413	0.675019
C	0.109964	2.651582	-0.778238
H	-0.257791	1.411896	2.290355
H	-1.376729	1.277464	-1.332153
H	-0.563492	-2.883412	-1.720742
H	0.327599	-1.372678	-2.917853
H	1.793920	-2.535082	1.752361
H	-0.285880	-2.760233	2.145321
H	-1.431042	2.639752	0.709469
H	-0.028320	3.654562	1.144277
H	-0.362470	3.469129	-1.339116
H	1.197494	2.758231	-0.852427
H	-1.677446	-0.339015	0.184181
H	1.551522	-2.592379	-1.671658
H	0.811656	-1.219035	3.092527
H	0.086869	1.216578	-2.256799
H	1.210680	1.670353	1.588815
C	-2.823687	0.021439	-0.108853
O	-2.819448	1.093110	-0.886484
C	-3.396807	-1.249359	-0.772007
H	-4.468700	-1.098069	-0.947748
H	-2.922068	-1.409936	-1.744747
H	-3.264589	-2.145495	-0.152593
C	-3.436457	0.246883	1.290888
H	-4.503192	0.472675	1.174394
H	-3.331862	-0.631691	1.939849
H	-2.969464	1.109141	1.778385
C	2.206933	0.073387	-0.102101
C	3.411575	0.303369	-0.180669
C	4.850337	0.565038	-0.298936
H	5.288068	0.026341	-1.149206
H	5.398179	0.250964	0.598916
H	5.060964	1.631704	-0.450481

TS6-3_F

Coordinates (Angstroms)			
	X	Y	Z
Ru	0.225719	-0.217218	0.083233
P	0.368581	-1.805868	-1.572483
N	-0.345634	1.298719	-1.284162

P	0.686859	-1.723118	1.799403
N	0.261899	1.558547	1.391302
C	-0.329892	2.724847	0.673989
C	0.054390	2.632963	-0.797078
H	-0.165768	1.449812	2.308458
H	-1.561318	1.204240	-1.237445
H	-0.545705	-2.882329	-1.706281
H	0.291361	-1.346885	-2.912699
H	1.853496	-2.526418	1.740209
H	-0.210221	-2.748131	2.201718
H	-1.416770	2.653982	0.765619
H	0.002563	3.673055	1.114485
H	-0.460435	3.430587	-1.351765
H	1.135910	2.775664	-0.916712
H	-1.738984	-0.370077	0.237026
H	1.564176	-2.551703	-1.696614
H	0.917097	-1.204232	3.102774
H	-0.010760	1.176536	-2.238330
H	1.263991	1.698040	1.530151
C	-2.829686	-0.032204	-0.086240
O	-2.787848	1.017309	-0.938139
C	-3.435877	-1.301017	-0.715184
H	-4.492050	-1.113871	-0.941590
H	-2.931801	-1.531926	-1.658506
H	-3.368297	-2.171155	-0.049909
C	-3.507928	0.302582	1.256186
H	-4.555846	0.564203	1.069201
H	-3.476999	-0.540632	1.957708
H	-3.029997	1.169817	1.723715
C	2.199396	0.075247	-0.120266
C	3.402652	0.303382	-0.214517
C	4.838908	0.566137	-0.356539
H	5.394325	0.308989	0.554659
H	5.041318	1.623209	-0.572581
H	5.274632	-0.019338	-1.176312

1_G

Coordinates (Angstroms)

X Y Z

Ru	0.179019	0.000026	0.000050
P	1.733303	1.639611	-0.034419

N	-1.530310	1.410691	-0.067642
P	1.733284	-1.639596	0.034371
N	-1.530282	-1.410657	0.067604
C	-2.759189	-0.688969	-0.327005
C	-2.759215	0.688985	0.326929
H	-1.373575	-2.205135	-0.546337
H	-1.598262	1.752546	-1.022745
H	2.651223	1.826894	-1.106763
H	1.269954	2.989534	-0.013687
H	2.650542	-1.827714	1.107114
H	2.697089	-1.808060	-0.999376
H	-2.735088	-0.582175	-1.416472
H	-3.672552	-1.235367	-0.052633
H	-3.672584	1.235360	0.052530
H	-2.735138	0.582191	1.416397
H	0.091277	0.065543	1.716171
H	0.091437	-0.067374	-1.716030
H	2.696570	1.808884	0.999727
H	1.269922	-2.989492	0.012337
H	-1.373651	2.205185	0.546290
H	-1.598248	-1.752517	1.022704

2_G

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.969221	0.062114	-0.075985
P	1.272535	-1.851199	-1.238221
N	-0.492681	0.874870	-1.529347
P	2.478705	-0.505009	1.512161
N	0.600296	2.072993	0.779577
C	-0.586646	2.669235	0.123085
C	-0.547872	2.344267	-1.365186
H	0.464432	2.030027	1.785447
H	-1.418975	0.477670	-1.363884
H	0.750139	-3.125254	-0.862815
H	0.769819	-1.892757	-2.572660
H	3.809702	-0.898432	1.195678
H	2.263490	-1.529747	2.478021
H	-1.474537	2.212515	0.569767
H	-0.640781	3.756312	0.274207
H	-1.423514	2.781506	-1.863820

H	0.358242	2.763077	-1.815498
H	2.189999	0.790162	-1.035472
H	-0.334210	-0.531089	0.883010
H	2.571576	-2.333982	-1.559260
H	2.852562	0.494037	2.460817
H	-0.214322	0.645266	-2.479583
H	1.432024	2.627770	0.595381
C	-3.290500	-0.703509	0.349179
O	-3.285241	0.164464	-0.516906
C	-2.976704	-2.146353	0.026276
H	-3.639072	-2.835411	0.560736
H	-3.040945	-2.317426	-1.050188
H	-1.947450	-2.331591	0.359446
C	-3.571095	-0.368988	1.797314
H	-4.369003	-1.004180	2.198748
H	-2.662332	-0.569693	2.377680
H	-3.845669	0.682674	1.898095

TS2-3_G

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.772137	0.209778	-0.077585
P	1.503766	-1.386549	-1.504860
N	-0.644523	1.043454	-1.524366
P	2.164610	-0.446146	1.593889
N	0.023017	1.980341	1.033012
C	-1.164356	2.531565	0.330898
C	-0.936610	2.451074	-1.173431
H	-0.208982	1.765884	1.999288
H	-1.509869	0.487765	-1.425739
H	1.123956	-2.758605	-1.438835
H	1.194695	-1.221738	-2.885880
H	3.556813	-0.646374	1.382919
H	1.974316	-1.625166	2.370428
H	-2.022895	1.906148	0.590117
H	-1.376018	3.565905	0.633217
H	-1.825667	2.826187	-1.698478
H	-0.076165	3.062724	-1.464576
H	1.980472	1.211056	-0.688778
H	-0.590182	-0.716407	0.536573
H	2.891414	-1.630392	-1.688752

H	2.315735	0.426619	2.712206
H	-0.322832	0.984881	-2.487234
H	0.784090	2.654457	1.039103
C	-2.378417	-1.165343	0.306071
O	-2.865333	-0.319934	-0.477694
C	-2.062272	-2.566293	-0.201265
H	-3.000859	-3.140850	-0.205360
H	-1.691110	-2.522825	-1.226978
H	-1.338512	-3.084459	0.431786
C	-2.670646	-1.052964	1.798629
H	-3.675276	-1.465391	1.976340
H	-1.953147	-1.609375	2.405819
H	-2.682618	-0.005164	2.106750

3_G

Coordinates (Angstroms)			
	X	Y	Z

Ru	0.941830	0.060584	-0.068537
P	1.174544	-1.635479	-1.571313
N	-0.217864	1.148451	-1.380177
P	1.865602	-1.096027	1.716638
N	0.756067	1.972782	1.022231
C	-0.305177	2.799482	0.374479
C	-0.201822	2.593307	-1.130540
H	0.589944	1.894011	2.023584
H	-1.901288	0.670660	-0.906829
H	0.515361	-2.892104	-1.461480
H	0.783711	-1.376914	-2.913955
H	3.134464	-1.738435	1.655513
H	1.207524	-2.181333	2.365646
H	-1.271162	2.422024	0.722487
H	-0.213213	3.857621	0.651911
H	-1.050937	3.102762	-1.613690
H	0.718137	3.080199	-1.503256
H	2.433535	0.439254	-0.406591
H	-1.558758	-0.786128	0.628259
H	2.458011	-2.162339	-1.867528
H	2.143609	-0.381656	2.919722
H	-0.126455	0.979676	-2.380767
H	1.664560	2.419087	0.907957
C	-2.625259	-0.684936	0.333325

O	-2.780350	0.467492	-0.477258
C	-3.025583	-1.950768	-0.435311
H	-4.076943	-1.886178	-0.738061
H	-2.421031	-2.056890	-1.342250
H	-2.893156	-2.851888	0.176619
C	-3.456742	-0.503250	1.604549
H	-4.513070	-0.370638	1.343682
H	-3.370277	-1.372909	2.266635
H	-3.132389	0.387430	2.152820

4_G

Coordinates (Angstroms)

X Y Z

Ru	-0.158979	-0.011354	0.087590
P	-1.659170	1.724623	-0.186930
N	1.603619	1.290111	0.350643
P	-1.697951	-1.680646	-0.006772
N	1.336731	-1.293624	-0.313549
C	2.693920	-0.854683	-0.021801
C	2.768416	0.639443	-0.313361
H	1.259403	-2.305633	-0.244305
H	1.748018	1.324836	1.358859
H	-2.727988	2.048889	0.700521
H	-1.136369	3.052694	-0.231584
H	-2.728633	-1.760126	-0.986746
H	-2.531439	-1.970089	1.105216
H	2.990214	-1.028196	1.032439
H	3.441165	-1.372968	-0.644569
H	3.719963	1.076521	0.019233
H	2.655984	0.804942	-1.389267
H	-0.531535	0.180327	1.618011
H	-2.444501	1.858994	-1.369632
H	-1.212644	-3.005083	-0.198384
H	1.493780	2.250851	0.033065

TS4-5_G

Coordinates (Angstroms)

X Y Z

Ru	-0.158454	0.000136	-0.002086
P	-1.768649	-1.671569	-0.027769
N	1.557641	-1.384264	-0.190541
P	-1.634887	1.728762	-0.047266
N	1.435615	1.320631	0.181450
C	2.692281	0.762515	-0.299334
C	2.795430	-0.662634	0.226060
H	1.317463	2.253309	-0.210659
H	1.604028	-1.598869	-1.185207
H	-2.866086	-1.644177	-0.934213
H	-1.371201	-3.002893	-0.356241
H	-2.468527	2.087713	1.050540
H	-2.653936	1.795562	-1.033419
H	2.782590	0.728240	-1.405990
H	3.563881	1.333083	0.065307
H	3.697766	-1.175032	-0.133930
H	2.808017	-0.646949	1.320526
H	-0.254636	0.013012	-1.575299
H	-2.560025	-2.069207	1.095050
H	-1.104540	3.030197	-0.264645
H	1.472769	-2.272848	0.298808
H	-0.144696	-0.190255	2.618345
H	0.323080	0.341372	2.371618

5G

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_G

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
