

Mechanism and Optimization of Ruthenium-Catalyzed Oxalamide Synthesis Using DFT

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Table S1. BP86-D3/Def2-SVP-SDD Cartesian coordinates of the optimized geometries of the species calculated in this study.

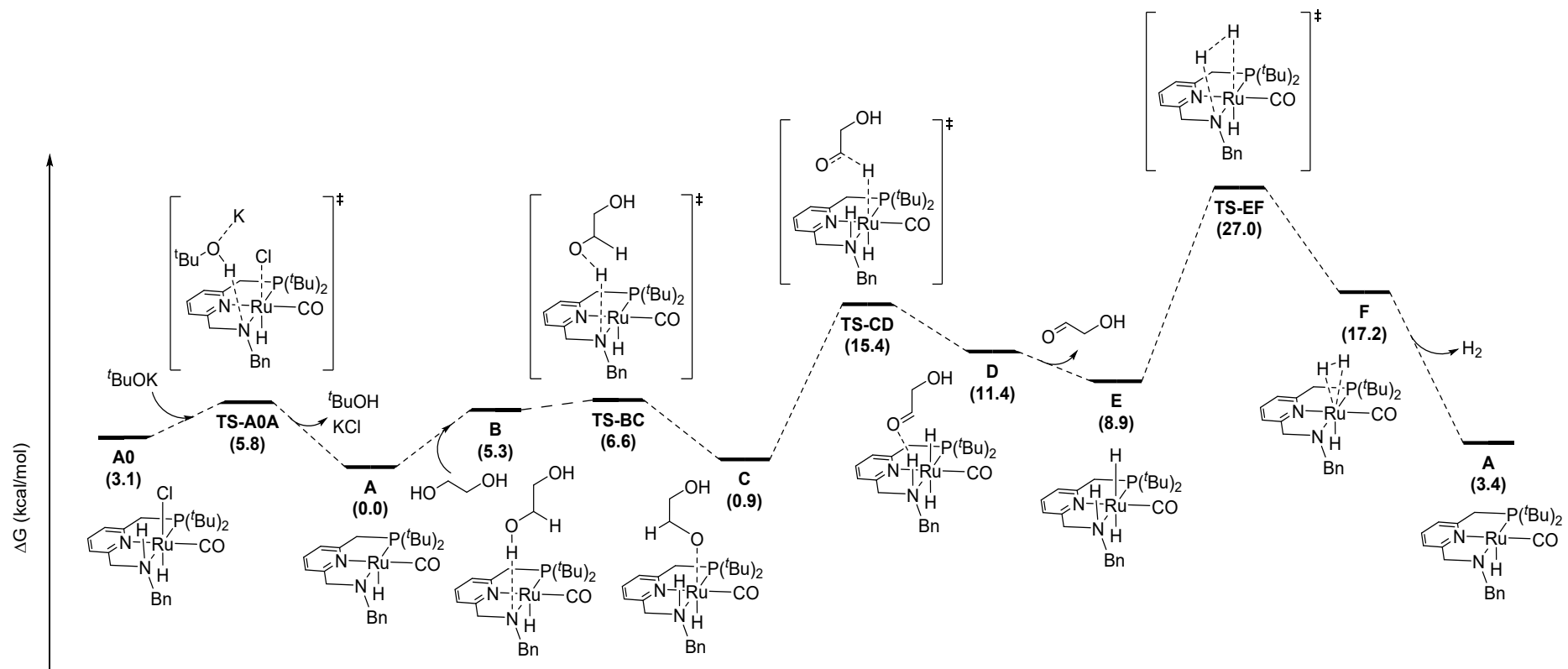


Figure S1. Reaction path for the formation of hydroxyacetaldehyde from ethyleneglycol (relative Gibbs energies in kcal/mol).

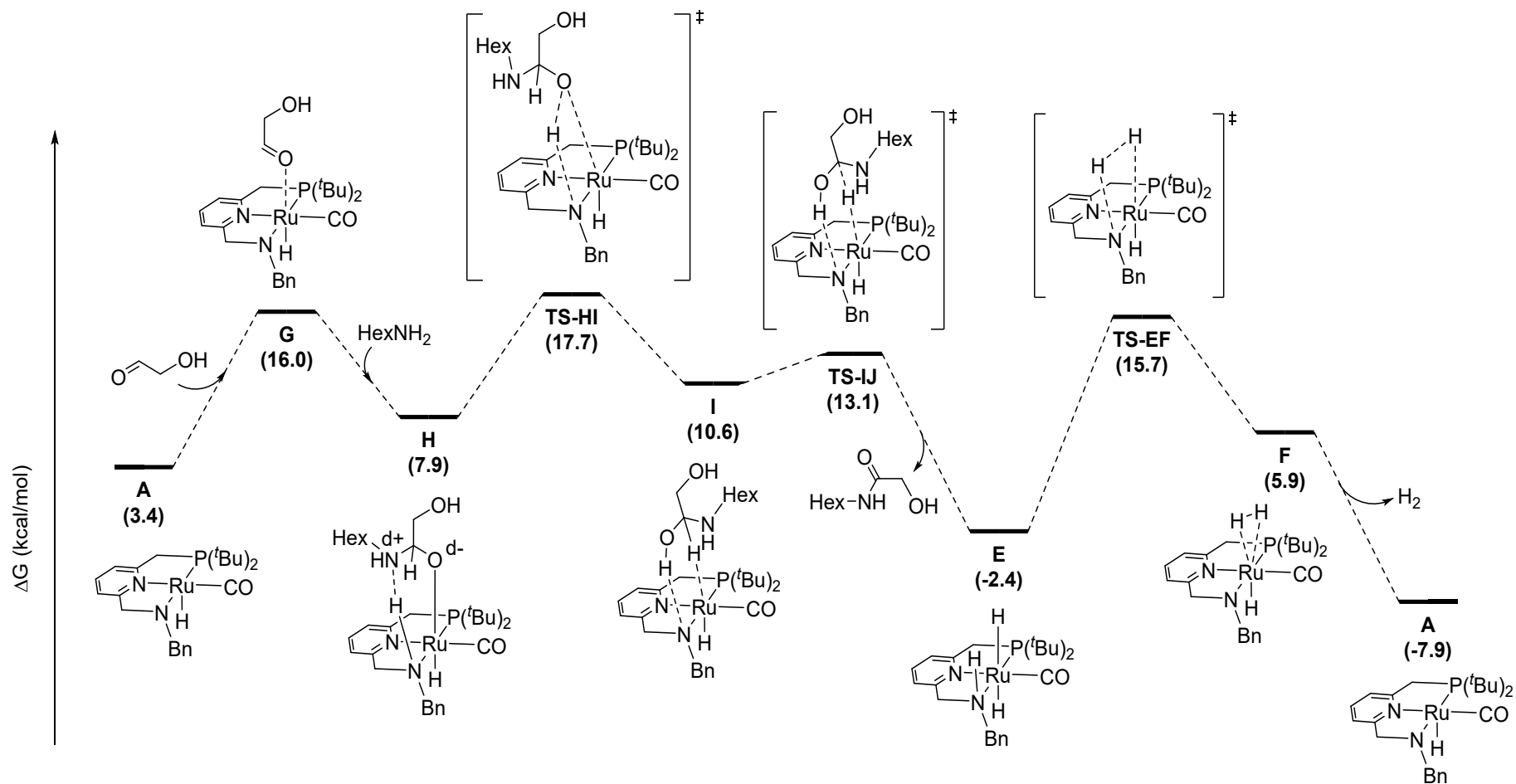


Figure S2. Reaction path for the formation of hydroxyacetamide from hydroxyacetaldehyde (relative Gibbs energies in kcal/mol).

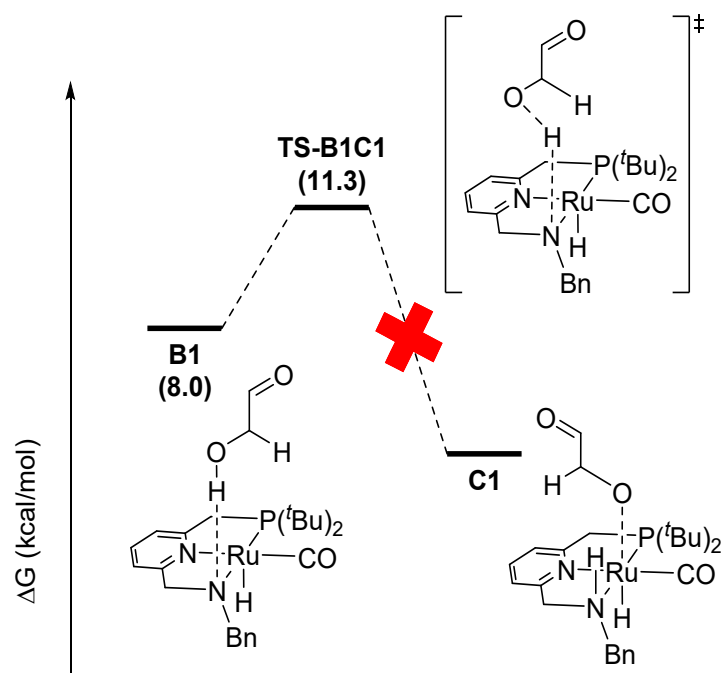


Figure S3. Reaction path leading to the oxalaldehyde **C1** from hydroxyacetaldehyde **B1** through **TS-B1C1** (relative Gibbs energies in kcal/mol).

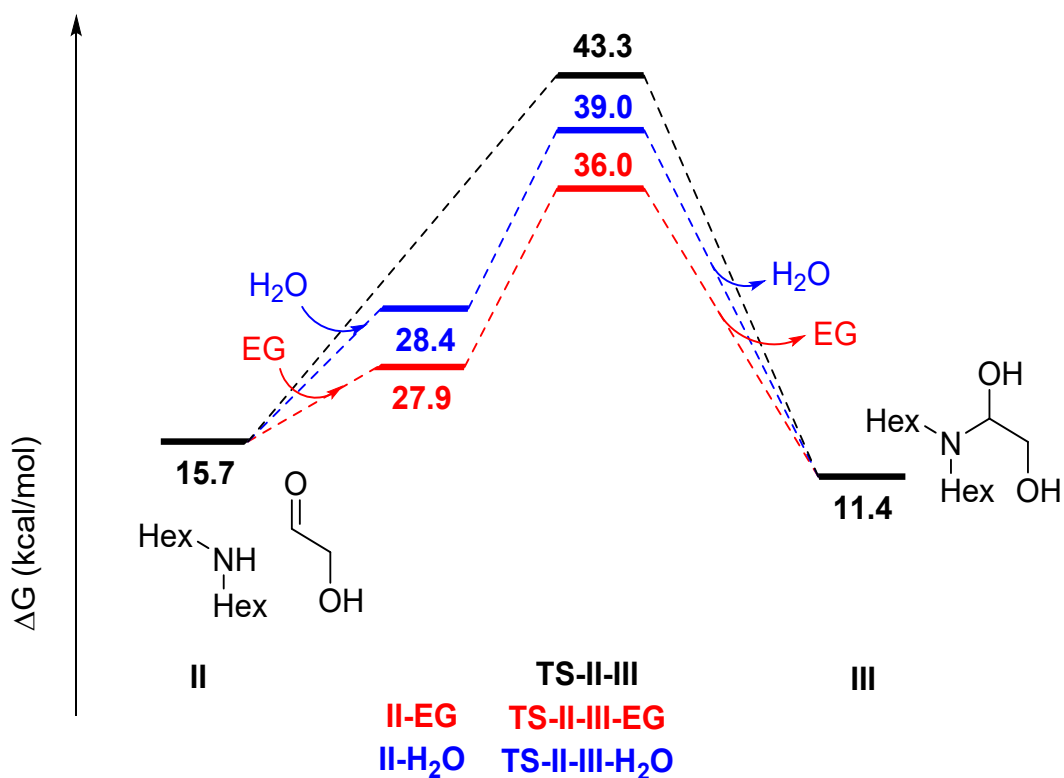


Figure S4. Reaction path for the non-assisted (in black), water-assisted (in blue) and ethyleneglycol(EG)-assisted (in red) non-metal catalyzed coupling of hydroxyacetaldehyde (**II**) with amines to form aminoalcohol species **III**.

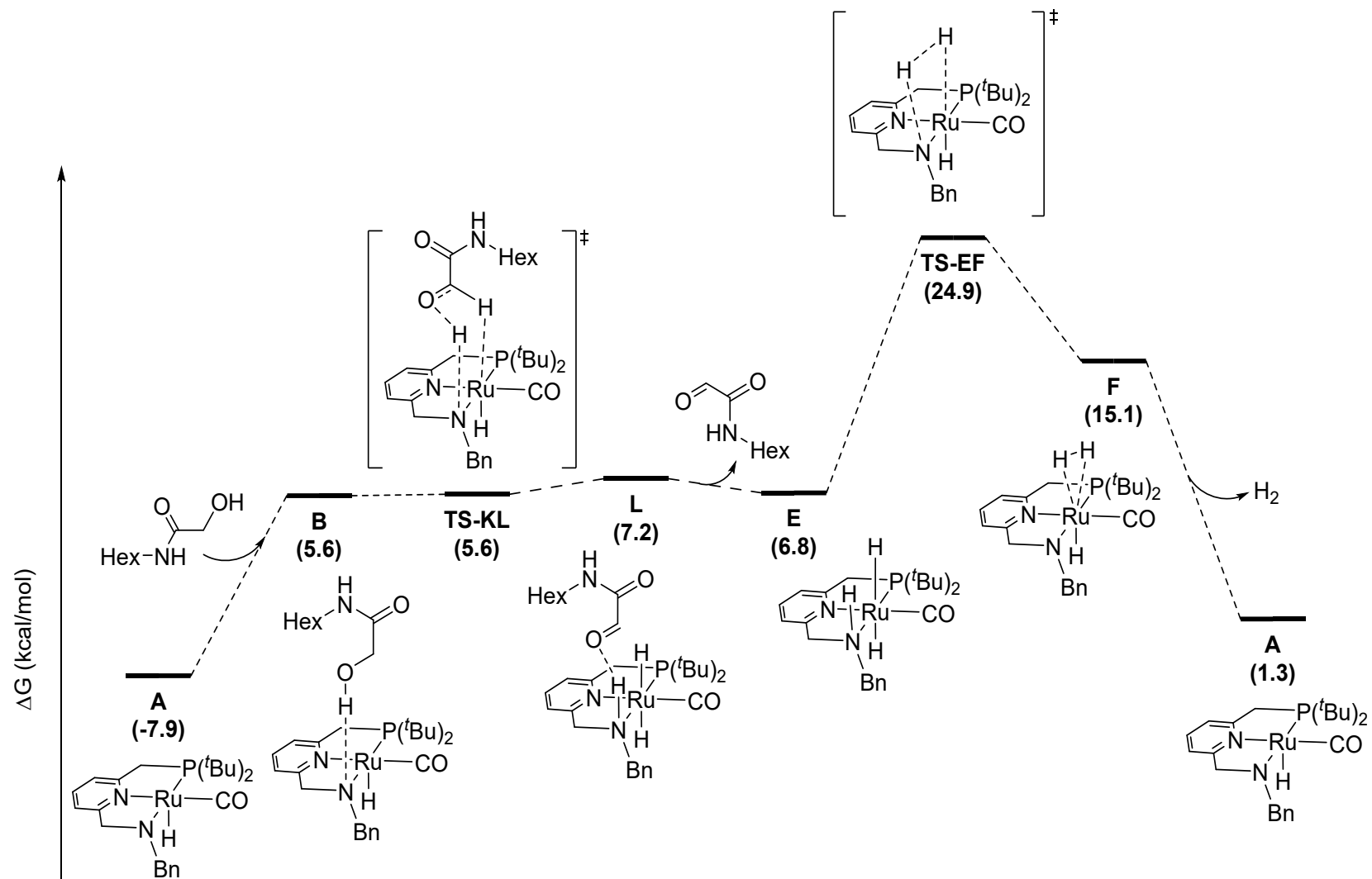


Figure S5. Reaction path for the formation of oxoacetamide from hydroxyacetamide (relative Gibbs energies in kcal/mol).

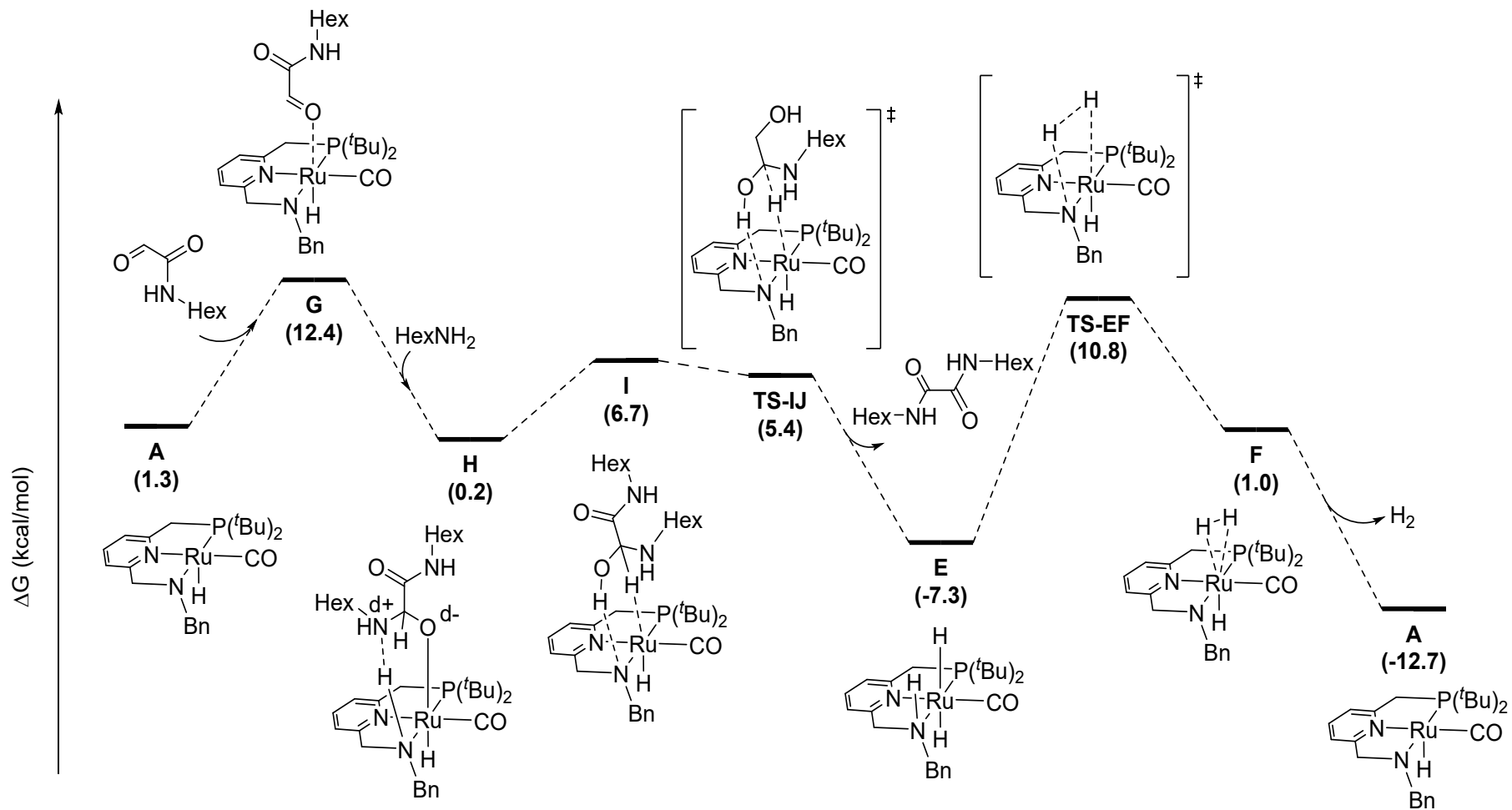


Figure S6. Reaction path for the formation of oxalamide from oxoacetamide (relative Gibbs energies in kcal/mol).

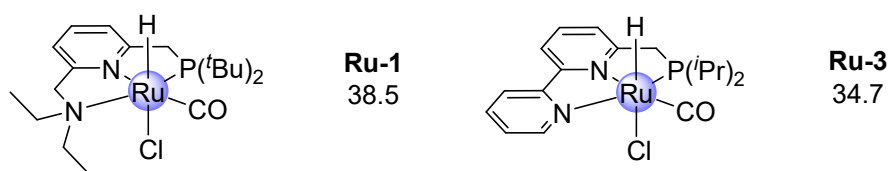


Figure S7. Ru-PNN catalyst derivatives tested experimentally that contain a labile C-H bond in the side arm of the pincer ligand, and the activation energy of the rds (relative Gibbs energies in kcal/mol).

Table S1. BP86-D3/Def2-SVP-SDD Cartesian coordinates and absolute energies (in a.u.) of the optimized geometries of the species calculated in this study.

63

A0 SCF Done: -1978.84134638 A.U.

Number of imaginary frequencies = 0

C	-0.916023	-0.049544	-0.763384
H	-1.186397	1.075984	-2.613989
N	-1.602724	0.478637	3.157843
C	-0.470239	-0.439255	2.891132
C	-0.416794	-0.803935	1.424861
N	-0.901349	0.142034	0.583055
C	-1.589706	1.022052	-1.582113
P	-1.599171	2.666470	-0.657064
H	-2.504011	-0.010798	2.953703
H	-0.511122	-1.352815	3.525384
H	0.464822	0.105719	3.155760
H	-2.668651	0.753612	-1.644144
C	0.121823	-2.001671	0.932607
H	0.503193	-2.761193	1.631167
C	0.162124	-2.202046	-0.457501
H	0.587870	-3.128586	-0.872824
C	-0.363956	-1.220182	-1.312475
H	-0.368316	-1.362501	-2.403273
Ru	-1.749984	1.860431	1.465692
C	-1.626873	1.015294	4.542000
H	-0.733801	1.661206	4.670200
H	-2.518649	1.670791	4.604069
C	-1.681484	-0.073051	5.597660
C	-2.846364	-0.861604	5.728638
C	-0.568530	-0.363052	6.412787
C	-2.895567	-1.915474	6.655143
C	-0.616058	-1.415213	7.344995
C	-1.779472	-2.194568	7.466363
H	-3.723175	-0.642959	5.095383
H	0.345937	0.245711	6.315255
H	-3.811602	-2.520049	6.749531
H	0.259970	-1.627484	7.978506
H	-1.818842	-3.019388	8.195490
C	0.094694	3.471491	-1.124450
C	-3.044123	3.632580	-1.481348
C	-4.354343	3.105800	-0.856726
H	-5.209828	3.638894	-1.326849
H	-4.499339	2.018076	-1.008488
H	-4.391285	3.273336	0.236234
C	-3.117371	3.434814	-3.011208
H	-2.215278	3.783043	-3.546383
H	-3.298093	2.375231	-3.284388
H	-3.979043	4.017448	-3.405067
C	-2.909025	5.130285	-1.132473
H	-3.831122	5.660681	-1.455597

H	-2.802703	5.287706	-0.039280
H	-2.055505	5.616205	-1.645817
C	0.192562	3.932537	-2.591067
H	1.227043	4.288382	-2.792570
H	-0.013534	3.110076	-3.307848
H	-0.489588	4.774573	-2.819300
C	0.352680	4.658860	-0.170547
H	-0.358087	5.492931	-0.323763
H	0.281865	4.336019	0.887468
H	1.376229	5.055807	-0.347895
C	1.184040	2.401962	-0.874198
H	2.184245	2.869068	-1.006511
H	1.127373	1.998831	0.156696
H	1.121452	1.555924	-1.589248
Cl	-3.895356	0.486376	1.224223
H	-0.279599	2.411530	1.808530
C	-2.407132	3.405361	2.229870
O	-2.791712	4.414331	2.699415

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tBuOK SCF Done: -833.157686603 A.U.

Number of imaginary frequencies = 0

C	0.696406	-0.255236	0.116679
C	1.008036	-1.775193	0.222641
H	0.792206	-2.263725	-0.752014
H	2.089177	-1.914695	0.439145
H	0.420991	-2.293887	1.013709
C	1.008038	0.413285	1.485842
H	2.089209	0.295698	1.714839
H	0.792017	1.501575	1.421412
H	0.421114	-0.012394	2.330694
C	-0.817757	-0.077857	-0.190608
H	-1.052054	1.005496	-0.272075
H	-1.052122	-0.549476	-1.169297
H	-1.482282	-0.524261	0.583101
O	1.456592	0.319831	-0.879619
K	2.692546	1.253529	-2.497275

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A0-ad SCF Done: -2812.03091528 A.U.

Number of imaginary frequencies = 0

C	-2.616287	0.568057	-0.441697
H	-2.226366	1.400614	-2.419014
N	-2.703196	1.787995	3.375844
C	-2.052292	0.461259	3.209099
C	-2.399358	-0.069669	1.843455
N	-2.423095	0.881677	0.873532
C	-2.554638	1.726120	-1.410236
P	-1.536750	3.139729	-0.664943
H	-3.729168	1.508349	3.446130
H	-2.362647	-0.251811	3.994965

H	-0.947539	0.604734	3.255562
H	-3.569181	2.176081	-1.499174
C	-2.627746	-1.418705	1.524125
H	-2.640818	-2.168789	2.326660
C	-2.851455	-1.768267	0.184020
H	-3.034585	-2.818636	-0.091471
C	-2.838297	-0.767984	-0.812544
H	-2.989338	-1.022269	-1.872560
Ru	-2.175140	2.873683	1.508887
C	-2.283374	2.515714	4.605664
H	-1.196117	2.719981	4.514974
H	-2.801571	3.494260	4.576522
C	-2.588224	1.805464	5.909648
C	-3.825893	2.005416	6.555905
C	-1.659874	0.913549	6.488037
C	-4.134179	1.325723	7.745679
C	-1.965460	0.226677	7.675283
C	-3.205600	0.430712	8.306157
H	-4.557579	2.698509	6.109887
H	-0.684084	0.757989	5.998799
H	-5.108408	1.488092	8.233041
H	-1.232162	-0.470307	8.111344
H	-3.448284	-0.107985	9.235772
C	0.299680	2.644889	-1.037355
C	-2.020760	4.660848	-1.744952
C	-3.368382	5.192871	-1.214297
H	-3.661384	6.079880	-1.818123
H	-4.181813	4.444728	-1.279513
H	-3.306947	5.494315	-0.151632
C	-2.188886	4.319639	-3.241699
H	-1.271407	3.923307	-3.713246
H	-3.009237	3.592221	-3.409747
H	-2.466777	5.246691	-3.790092
C	-0.963106	5.768793	-1.552530
H	-1.329883	6.703788	-2.029241
H	-0.795224	5.988986	-0.477876
H	0.010201	5.523111	-2.021014
C	0.681979	2.717805	-2.528496
H	1.714551	2.325055	-2.658331
H	0.016439	2.097885	-3.165268
H	0.679041	3.752752	-2.922310
C	1.231848	3.549013	-0.199808
H	1.207922	4.607054	-0.521182
H	0.958355	3.508640	0.873711
H	2.279632	3.192100	-0.306723
C	0.496348	1.185364	-0.562758
H	1.570891	0.919123	-0.664780
H	0.212813	1.059546	0.500519
H	-0.079393	0.457684	-1.170590
Cl	-4.689365	3.216447	1.080839
H	-0.661386	2.544390	1.911095

C	-1.836563	4.602161	2.064218
O	-1.573252	5.699848	2.396991
C	-5.445526	-0.822692	4.192260
C	-6.137145	-1.997906	3.431693
H	-5.401784	-2.486568	2.755916
H	-6.558197	-2.774361	4.107799
H	-6.985345	-1.622573	2.811435
C	-4.377071	-1.447850	5.132098
H	-4.814607	-2.146534	5.877830
H	-3.631134	-2.016912	4.535697
H	-3.843980	-0.650702	5.684698
C	-6.514665	-0.111758	5.068029
H	-6.991958	-0.784620	5.815069
H	-6.040627	0.731436	5.607366
H	-7.315313	0.310564	4.421231
O	-4.886247	0.074517	3.292261
K	-5.958798	0.620487	1.160507

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TS-A0A SCF Done: -2812.02211727 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -513.69 cm⁻¹

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N	-2.040522	0.719387	3.365993
C	-1.112100	-0.370697	2.998105
C	-1.239101	-0.767903	1.550825
N	-1.590631	0.242253	0.710552
C	-2.063291	1.264935	-1.455094
P	-1.680920	2.852005	-0.498011
H	-3.085171	0.041742	3.586701
H	-1.273598	-1.268272	3.636527
H	-0.051774	-0.037104	3.135895
H	-3.175505	1.281802	-1.514672
C	-0.974436	-2.055969	1.048194
H	-0.704229	-2.865334	1.743066
C	-1.051847	-2.273688	-0.339951
H	-0.839707	-3.269985	-0.759130
C	-1.395066	-1.206503	-1.191348
H	-1.455441	-1.348155	-2.280751
Ru	-2.093148	2.060787	1.611952
C	-1.576369	1.447523	4.577308
H	-0.538998	1.817835	4.394157
H	-2.207169	2.352169	4.664664
C	-1.614216	0.727564	5.922120
C	-2.397324	1.266891	6.967545
C	-0.846999	-0.425050	6.208548
C	-2.448659	0.664061	8.235354
C	-0.906334	-1.043381	7.468732
C	-1.713557	-0.506214	8.487038
H	-2.984747	2.180258	6.779744

H	-0.176087	-0.844971	5.445397
H	-3.075697	1.106018	9.025981
H	-0.307949	-1.948740	7.660277
H	-1.760481	-0.992614	9.474275
C	0.193251	3.173871	-0.879514
C	-2.749144	4.187655	-1.391144
C	-4.182225	4.084084	-0.828301
H	-4.810266	4.862988	-1.314393
H	-4.645873	3.096539	-1.014526
H	-4.211071	4.242291	0.266466
C	-2.813776	3.998369	-2.922140
H	-1.827923	4.052778	-3.418724
H	-3.290902	3.035871	-3.198412
H	-3.445897	4.804366	-3.356226
C	-2.200689	5.586336	-1.035622
H	-2.915692	6.356365	-1.398770
H	-2.102840	5.717591	0.061994
H	-1.221727	5.801331	-1.507442
C	0.480407	3.582983	-2.337047
H	1.580666	3.652257	-2.486060
H	0.100192	2.837510	-3.066808
H	0.056937	4.572721	-2.595769
C	0.716389	4.253533	0.094480
H	0.272161	5.249641	-0.089009
H	0.505469	3.970497	1.145397
H	1.817498	4.352920	-0.025907
C	0.958367	1.860284	-0.591091
H	2.048746	2.051527	-0.694038
H	0.771512	1.496457	0.438530
H	0.701349	1.051715	-1.306065
Cl	-4.539323	1.354305	1.004335
H	-0.568617	2.325764	2.006911
C	-2.488438	3.692306	2.385782
O	-2.713044	4.747495	2.855668
C	-4.999456	-0.703612	4.574063
C	-6.289842	-1.346153	3.995556
H	-6.124069	-2.427581	3.783245
H	-7.142275	-1.280289	4.704540
H	-6.608482	-0.823045	3.065314
C	-4.676662	-1.382426	5.924784
H	-5.481754	-1.239801	6.678463
H	-4.529105	-2.472233	5.767498
H	-3.735450	-0.972670	6.336679
C	-5.259916	0.809939	4.756633
H	-6.136258	1.008316	5.410081
H	-4.379436	1.295850	5.217096
H	-5.423838	1.280687	3.765023
O	-3.927015	-0.911130	3.677491
K	-4.493312	-1.535665	1.332880

A-ad SCF Done: -2812.02643182 A.U.

Number of imaginary frequencies = 0

C	-1.287080	-0.019090	-0.533704
H	-1.263510	1.152214	-2.370422
N	-2.083207	0.563251	3.431933
C	-0.989810	-0.379519	3.135983
C	-0.940129	-0.794726	1.690177
N	-1.354122	0.162635	0.816241
C	-1.784316	1.117392	-1.390935
P	-1.770641	2.732865	-0.406669
H	-3.398017	-0.159924	3.713478
H	-1.000831	-1.282525	3.793629
H	0.007079	0.104888	3.329884
H	-2.870045	0.947495	-1.571497
C	-0.461052	-2.032505	1.218282
H	-0.131295	-2.798740	1.936826
C	-0.387793	-2.248725	-0.170648
H	-0.004985	-3.203276	-0.565241
C	-0.797310	-1.232637	-1.052806
H	-0.745736	-1.374409	-2.142562
Ru	-2.220551	1.864735	1.671717
C	-1.739240	1.310775	4.660051
H	-0.899303	2.021216	4.464339
H	-2.612448	1.951559	4.910157
C	-1.366397	0.480085	5.886387
C	-0.322813	0.919287	6.730051
C	-2.039968	-0.715606	6.225293
C	0.029888	0.203024	7.887295
C	-1.683224	-1.438474	7.376893
C	-0.650278	-0.982716	8.215950
H	0.222332	1.843365	6.472483
H	-2.851665	-1.073894	5.571975
H	0.845161	0.570022	8.531925
H	-2.223928	-2.367165	7.623757
H	-0.374397	-1.549807	9.119651
C	0.048959	3.371177	-0.620297
C	-2.965059	3.879429	-1.398170
C	-4.402885	3.525103	-0.963490
H	-5.110593	4.201426	-1.491928
H	-4.675973	2.479836	-1.203829
H	-4.548073	3.645844	0.127097
C	-2.862171	3.704102	-2.928467
H	-1.861484	3.938261	-3.335195
H	-3.134999	2.676508	-3.244651
H	-3.586107	4.392422	-3.418402
C	-2.695852	5.345547	-0.996564
H	-3.495208	5.989573	-1.423724
H	-2.719011	5.476191	0.105370
H	-1.728983	5.728299	-1.378533
C	0.390685	3.840655	-2.047505
H	1.472129	4.096760	-2.098518

H	0.207700	3.051073	-2.806412
H	-0.170536	4.747597	-2.345146
C	0.295500	4.511833	0.392626
H	-0.294231	5.420350	0.168700
H	0.045592	4.184545	1.421966
H	1.369994	4.797903	0.368388
C	0.994935	2.200836	-0.259879
H	2.042924	2.572098	-0.267295
H	0.782343	1.799341	0.750660
H	0.940211	1.367885	-0.990911
Cl	-4.428716	0.690304	0.752258
H	-0.811518	2.395741	2.182901
C	-2.957078	3.383170	2.425135
O	-3.401633	4.371498	2.885012
C	-5.437360	-0.214638	4.378110
C	-6.605631	-0.716250	3.500761
H	-6.668079	-1.827644	3.536101
H	-7.581337	-0.321666	3.853949
H	-6.459605	-0.377037	2.452982
C	-5.664683	-0.637072	5.843581
H	-6.624740	-0.241050	6.237346
H	-5.682644	-1.744652	5.924046
H	-4.844204	-0.260878	6.487743
C	-5.343714	1.317713	4.268190
H	-6.297235	1.793240	4.577936
H	-4.543860	1.708972	4.927956
H	-5.115932	1.614913	3.225590
O	-4.231028	-0.840656	3.903274
K	-3.989080	-2.015498	1.664050

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tBuOH-KCl SCF Done: -1294.07238215 A.U.

Number of imaginary frequencies = 0

C	-0.388128	0.288768	-0.098320
C	-1.844888	0.338451	-0.583090
H	-2.516303	-0.156941	0.148768
H	-2.188424	1.391262	-0.691000
H	-1.936718	-0.189235	-1.558073
C	-0.203795	0.998104	1.252746
H	-0.799040	0.500806	2.045770
H	0.863512	0.988912	1.555804
H	-0.542789	2.056259	1.197778
C	0.115260	-1.158514	-0.043779
H	-0.101482	-1.679360	-1.004188
H	1.202873	-1.184520	0.182236
H	-0.411991	-1.710303	0.760250
O	0.464543	0.975846	-1.082343
H	0.162067	1.905274	-1.093293
K	1.202526	-0.254885	-3.367080
Cl	-1.030076	-1.845336	-3.478620

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A SCF Done: -1517.92483419 A.U.

Number of imaginary frequencies = 0

C	-0.565358	-0.126532	-0.728805
H	-0.985202	1.115906	-2.476339
N	-0.340804	0.601145	3.173855
C	0.167216	-0.715014	2.848644
C	0.119868	-0.992018	1.370960
N	-0.350165	0.037406	0.612296
C	-1.316075	0.981988	-1.426491
H	-0.405916	-1.526828	3.369288
H	1.227149	-0.844725	3.200511
H	-2.381399	0.666410	-1.478479
C	0.494211	-2.211460	0.781375
H	0.884144	-3.022952	1.414304
C	0.359757	-2.368326	-0.604757
H	0.658178	-3.309253	-1.092266
C	-0.194507	-1.318600	-1.364567
H	-0.360595	-1.430060	-2.446523
Ru	-0.634815	1.856576	1.638886
C	-0.376713	0.845460	4.608705
H	0.597198	0.581344	5.096207
H	-0.528640	1.931625	4.773339
C	-1.499183	0.071909	5.298681
C	-2.824687	0.211413	4.832190
C	-1.249678	-0.798456	6.377422
C	-3.875724	-0.492870	5.439243
C	-2.300351	-1.509828	6.988055
C	-3.616417	-1.357953	6.520705
H	-3.013233	0.875778	3.972152
H	-0.216124	-0.920448	6.744158
H	-4.906309	-0.368193	5.068908
H	-2.087440	-2.188811	7.829669
H	-4.440725	-1.914075	6.995441
C	-0.043003	3.681483	-1.436282
C	-3.088147	3.242298	-0.651535
C	-3.946345	2.386397	0.309702
H	-5.007646	2.712885	0.244607
H	-3.914878	1.304889	0.057583
H	-3.607171	2.492920	1.359987
C	-3.665268	3.114925	-2.076843
H	-3.134983	3.741878	-2.816242
H	-3.660319	2.068556	-2.446558
H	-4.727548	3.445268	-2.068848
C	-3.140253	4.711863	-0.184883
H	-4.200319	5.040532	-0.114449
H	-2.681593	4.843873	0.816363
H	-2.633361	5.394898	-0.895961
C	-0.554403	4.146657	-2.811561
H	0.269116	4.657702	-3.357885
H	-0.892210	3.301724	-3.448071

H	-1.386465	4.873442	-2.726550
C	0.331794	4.901358	-0.566705
H	-0.530897	5.567847	-0.373964
H	0.739491	4.584058	0.413671
H	1.109544	5.501504	-1.087773
C	1.222306	2.814145	-1.637121
H	1.573089	2.377859	-0.678976
H	1.063059	1.986342	-2.358522
H	2.039623	3.449117	-2.042934
H	0.765253	2.446704	1.228543
C	-0.971176	3.445848	2.514244
O	-1.194988	4.484208	3.028424
P	-1.284587	2.590050	-0.436615

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ethyleneglycol SCF Done: -230.359711835 A.U.

Number of imaginary frequencies = 0

C	-1.699129	0.348093	0.000009
H	-1.280114	0.867328	0.898983
H	-1.280090	0.867324	-0.898957
C	-1.191591	-1.089528	0.000017
H	-1.610615	-1.608757	0.898990
H	-1.610619	-1.608767	-0.898950
O	0.227830	-1.041366	0.000012
H	0.554677	-1.958530	0.000109
O	-3.118549	0.299930	-0.000011
H	-3.445396	1.217094	-0.000009

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B SCF Done: -1748.31429827 A.U.

Number of imaginary frequencies = 0

C	-1.800961	-0.268933	-0.780816
H	-1.751210	1.265548	-2.330435
N	-2.344754	-0.404094	3.197924
C	-1.485082	-1.490944	2.701143
C	-1.503561	-1.552847	1.194783
N	-1.806465	-0.378702	0.579525
C	-2.214497	1.070453	-1.341558
H	-1.769776	-2.484883	3.122682
H	-0.415567	-1.326396	3.006822
H	-3.315914	1.054277	-1.500528
C	-1.181645	-2.693395	0.439956
H	-0.956344	-3.638601	0.955052
C	-1.154217	-2.598627	-0.957735
H	-0.898527	-3.477662	-1.569707
C	-1.462986	-1.372955	-1.576851
H	-1.455179	-1.272806	-2.672332
Ru	-2.113362	1.288477	1.881644
C	-2.170185	-0.232054	4.647866
H	-1.118302	0.061666	4.894827
H	-2.806049	0.624016	4.964079

C	-2.545192	-1.456138	5.477817
C	-3.758107	-2.143966	5.249170
C	-1.691162	-1.922865	6.498357
C	-4.105673	-3.261881	6.025169
C	-2.039461	-3.037034	7.282878
C	-3.250156	-3.711138	7.048211
H	-4.426829	-1.820634	4.435610
H	-0.735824	-1.401708	6.679514
H	-5.053421	-3.788281	5.827405
H	-1.358068	-3.383578	8.076751
H	-3.524645	-4.587720	7.656767
C	-0.145918	3.075972	-0.526455
C	-3.248012	3.750505	-0.567415
C	-4.579890	3.190035	-0.018290
H	-5.396340	3.914141	-0.231224
H	-4.858883	2.231022	-0.504570
H	-4.537412	3.009705	1.073804
C	-3.399507	3.992106	-2.083818
H	-2.504649	4.449309	-2.543386
H	-3.635124	3.060585	-2.638666
H	-4.248347	4.690530	-2.254578
C	-2.928929	5.072040	0.162132
H	-3.784480	5.772783	0.047240
H	-2.768985	4.913945	1.248523
H	-2.034240	5.576459	-0.255188
C	-0.058522	3.854865	-1.851457
H	1.008321	4.072020	-2.079478
H	-0.464963	3.279466	-2.709471
H	-0.584683	4.828699	-1.802899
C	0.359835	3.951201	0.641758
H	-0.246983	4.866348	0.783335
H	0.350644	3.387787	1.595713
H	1.404937	4.270166	0.436127
C	0.751198	1.819123	-0.623621
H	0.663693	1.184106	0.281277
H	0.517924	1.196087	-1.511416
H	1.812175	2.137907	-0.716212
H	-0.547113	1.320217	2.048190
C	-2.169874	2.751942	3.003275
O	-2.157937	3.705881	3.693899
P	-1.914712	2.451934	-0.083612
O	-4.650215	0.954975	2.426226
C	-5.649884	0.197516	1.735682
C	-5.051760	-1.019957	1.035447
H	-5.857556	-1.582260	0.512892
H	-4.341065	-0.656031	0.248527
O	-4.421429	-1.901735	1.943142
H	-3.743319	-1.367774	2.461323
H	-4.085821	0.313688	2.947642
H	-6.435144	-0.134905	2.456648
H	-6.129421	0.878659	1.000284

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TS-BC SCF Done: -1748.30960410 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -671.10 cm⁻¹

C	-1.664615	-0.249776	-0.662843
H	-1.737038	1.236092	-2.260971
N	-1.876050	-0.237162	3.350462
C	-1.157747	-1.400812	2.830075
C	-1.250971	-1.474701	1.327483
N	-1.539145	-0.306920	0.695020
C	-2.142478	1.060461	-1.243410
H	-1.542954	-2.356229	3.255266
H	-0.070506	-1.341655	3.101412
H	-3.247788	0.994313	-1.349358
C	-1.044521	-2.654021	0.591895
H	-0.837866	-3.593791	1.123746
C	-1.122866	-2.608203	-0.805580
H	-0.958322	-3.518978	-1.402285
C	-1.437723	-1.393553	-1.442544
H	-1.533480	-1.334820	-2.536936
Ru	-1.769740	1.430735	1.946286
C	-1.808702	-0.140232	4.815443
H	-0.754088	-0.173228	5.181733
H	-2.226995	0.844207	5.106404
C	-2.630073	-1.256652	5.448208
C	-4.041056	-1.218532	5.340911
C	-2.029227	-2.388161	6.032897
C	-4.824898	-2.289156	5.802138
C	-2.811787	-3.463208	6.497021
C	-4.210600	-3.418965	6.378893
H	-4.511988	-0.337092	4.874572
H	-0.930327	-2.429884	6.119183
H	-5.922822	-2.240974	5.718105
H	-2.324020	-4.342115	6.948602
H	-4.824246	-4.260148	6.738621
C	-0.187094	3.258341	-0.701007
C	-3.332647	3.660087	-0.437298
C	-4.552615	2.978075	0.226056
H	-5.441215	3.637363	0.116519
H	-4.803389	2.011478	-0.260229
H	-4.388740	2.769416	1.302625
C	-3.635288	3.865690	-1.936438
H	-2.843268	4.425135	-2.466511
H	-3.799121	2.907927	-2.472274
H	-4.574299	4.453660	-2.036444
C	-3.082801	5.018812	0.249657
H	-4.008250	5.633001	0.198931
H	-2.818476	4.898861	1.319973
H	-2.278614	5.597990	-0.247749
C	-0.295916	3.977974	-2.057442

H	0.722098	4.261449	-2.404852
H	-0.743112	3.336480	-2.845593
H	-0.887454	4.912411	-1.990652
C	0.347932	4.227754	0.375654
H	-0.321476	5.094888	0.537197
H	0.476016	3.712056	1.347834
H	1.337423	4.622091	0.056699
C	0.800994	2.075183	-0.834805
H	0.851981	1.481012	0.100334
H	0.538693	1.392372	-1.669229
H	1.817674	2.473306	-1.044151
H	-0.196133	1.598960	1.980008
C	-1.853868	2.928010	3.013412
O	-1.877370	3.901607	3.677601
P	-1.840305	2.505539	-0.061839
O	-4.070900	0.503278	2.543044
C	-5.101718	-0.236762	1.957349
C	-4.658861	-1.553317	1.307621
H	-5.566130	-2.071586	0.900685
H	-3.986800	-1.347005	0.445457
O	-3.926596	-2.399829	2.189817
H	-4.288727	-2.296530	3.094938
H	-3.150824	-0.113169	2.983457
H	-5.880799	-0.491188	2.731318
H	-5.640874	0.367994	1.185198

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C SCF Done: -1748.32306359 A.U.

Number of imaginary frequencies = 0

C	-2.402717	-0.154274	-0.875944
H	-2.511228	1.350202	-2.454859
N	-3.174386	-0.395497	3.036836
C	-2.090997	-1.323969	2.619553
C	-2.036320	-1.398074	1.111557
N	-2.392704	-0.251233	0.480981
C	-2.910891	1.147987	-1.440554
H	-2.216695	-2.337832	3.059874
H	-1.127766	-0.907401	2.991919
H	-4.019311	1.064674	-1.505714
C	-1.633288	-2.524267	0.379171
H	-1.359066	-3.451541	0.903304
C	-1.594369	-2.437500	-1.022901
H	-1.275247	-3.303944	-1.622697
C	-1.983506	-1.245517	-1.656966
H	-1.981198	-1.160770	-2.753727
Ru	-3.033330	1.343596	1.693756
C	-3.216008	-0.155160	4.496425
H	-2.292426	0.388644	4.785321
H	-4.059302	0.546506	4.670943
C	-3.398297	-1.408347	5.339964
C	-4.323596	-2.407543	4.958907

C	-2.661269	-1.582711	6.529040
C	-4.504900	-3.549457	5.757018
C	-2.849309	-2.721334	7.332448
C	-3.772490	-3.708927	6.947752
H	-4.892642	-2.303299	4.018615
H	-1.930624	-0.813579	6.830829
H	-5.226654	-4.321282	5.445104
H	-2.266589	-2.839733	8.260020
H	-3.918439	-4.604354	7.572699
C	-0.861535	3.150058	-0.493321
C	-3.926312	3.881673	-0.783752
C	-5.310786	3.466947	-0.235192
H	-6.075048	4.170864	-0.631570
H	-5.587662	2.430958	-0.512264
H	-5.337182	3.509453	0.870523
C	-4.016940	3.988049	-2.321746
H	-3.055553	4.244826	-2.803841
H	-4.397454	3.052231	-2.779296
H	-4.741586	4.790234	-2.583742
C	-3.551459	5.245685	-0.166266
H	-4.376123	5.966413	-0.357957
H	-3.423462	5.174062	0.933608
H	-2.630047	5.678928	-0.603732
C	-0.648867	3.873802	-1.836257
H	0.433122	4.099242	-1.962106
H	-0.954201	3.250994	-2.703277
H	-1.189523	4.838882	-1.891328
C	-0.452866	4.061049	0.685545
H	-1.013046	5.014998	0.704146
H	-0.614686	3.545415	1.653788
H	0.627241	4.310591	0.597740
C	0.036718	1.890981	-0.464156
H	-0.117311	1.305651	0.464512
H	-0.135387	1.225957	-1.335422
H	1.101668	2.208168	-0.499385
H	-1.523922	1.553608	2.237394
C	-3.476466	2.772531	2.767956
O	-3.718374	3.706009	3.447042
P	-2.670307	2.550063	-0.197279
O	-5.000598	0.672979	0.904012
C	-6.103069	0.712453	1.770138
C	-6.577352	-0.770570	1.979874
H	-6.975598	-0.943588	3.004399
H	-7.380190	-1.042575	1.251374
O	-5.418272	-1.577715	1.759457
H	-4.953750	-0.902990	1.121524
H	-4.078397	-0.847474	2.741128
H	-5.842042	1.152671	2.767290
H	-6.944793	1.331852	1.365858

B1 SCF Done: -1747.10389755 A.U.

Number of imaginary frequencies = 0

C	0.530521	0.074398	-0.614147
H	0.994645	1.390401	-2.287640
N	0.178760	0.352382	3.418811
C	0.624110	-0.973261	2.954856
C	0.521874	-1.098617	1.449160
N	0.604839	0.064447	0.747705
C	0.506640	1.422098	-1.291701
H	0.060435	-1.799624	3.446550
H	1.695125	-1.100694	3.240968
H	-0.568026	1.665461	-1.454613
C	0.377436	-2.328161	0.789312
H	0.298046	-3.256620	1.374035
C	0.334750	-2.344539	-0.614223
H	0.225646	-3.297185	-1.155408
C	0.410055	-1.134861	-1.321078
H	0.349247	-1.114715	-2.418940
Ru	0.698172	1.879908	1.875896
C	0.343770	0.567925	4.868724
H	1.419014	0.476072	5.135013
H	0.048159	1.618192	5.068406
C	-0.509676	-0.382605	5.693286
C	-1.910562	-0.392582	5.502047
C	0.058280	-1.282516	6.616140
C	-2.721608	-1.282072	6.223990
C	-0.753513	-2.172389	7.343858
C	-2.145036	-2.174366	7.148375
H	-2.359879	0.304515	4.773234
H	1.150852	-1.285538	6.767406
H	-3.812378	-1.277695	6.068584
H	-0.295438	-2.869148	8.064083
H	-2.782386	-2.871104	7.715833
C	3.063269	2.813324	-0.605334
C	0.311581	4.374047	-0.772923
C	-1.131973	4.324549	-0.222357
H	-1.609552	5.315568	-0.383728
H	-1.742036	3.573490	-0.757933
H	-1.168061	4.088646	0.860204
C	0.234431	4.505645	-2.309146
H	1.220304	4.644037	-2.788485
H	-0.265568	3.633705	-2.778091
H	-0.379612	5.398936	-2.558240
C	1.042324	5.587640	-0.160491
H	0.458228	6.508480	-0.376523
H	1.133946	5.502909	0.941589
H	2.053798	5.735294	-0.588930
C	3.362849	3.390841	-2.001706
H	4.444111	3.258242	-2.226549
H	2.796724	2.876568	-2.806261
H	3.149869	4.475949	-2.064321

C	3.816790	3.621317	0.474039
H	3.522573	4.687907	0.492349
H	3.636789	3.200898	1.483310
H	4.908604	3.578503	0.267730
C	3.565453	1.350423	-0.558862
H	3.325879	0.867085	0.409488
H	3.145077	0.728629	-1.375846
H	4.670608	1.344878	-0.679502
H	2.261105	1.705832	2.113122
C	0.831177	3.448397	2.832633
O	0.954595	4.456165	3.430810
P	1.180351	2.771699	-0.163110
C	-2.521985	0.620833	1.324438
H	-1.988001	-0.260657	0.873360
H	-3.421537	0.211502	1.864993
O	-1.750591	1.435051	2.152685
H	-0.840037	0.568022	3.107835
O	-2.641831	1.423655	-0.978130
C	-2.990286	1.515136	0.194292
H	-3.596515	2.402445	0.551960

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TS-B1C1 SCF Done: -1747.08792120 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -712.39 cm⁻¹

C	-1.582320	-0.268527	-0.749692
H	-1.550900	1.278212	-2.285483
N	-2.243676	-0.475159	3.189406
C	-1.289253	-1.495762	2.727919
C	-1.261507	-1.545854	1.224183
N	-1.610241	-0.385306	0.608219
C	-2.047349	1.049523	-1.319925
H	-1.526944	-2.503044	3.141998
H	-0.253456	-1.250990	3.077375
H	-3.137542	0.972147	-1.529059
C	-0.862356	-2.663732	0.472924
H	-0.597452	-3.598202	0.988912
C	-0.807099	-2.559635	-0.924045
H	-0.491101	-3.420244	-1.533891
C	-1.167697	-1.349405	-1.542935
H	-1.142628	-1.242711	-2.637482
Ru	-2.151256	1.203726	1.890477
C	-2.195134	-0.285872	4.658253
H	-1.198605	0.113415	4.958444
H	-2.954704	0.481800	4.904316
C	-2.502199	-1.563914	5.420673
C	-3.802439	-2.115612	5.358928
C	-1.504722	-2.242817	6.149888
C	-4.089887	-3.321664	6.017941
C	-1.793898	-3.449145	6.813642
C	-3.088958	-3.991631	6.747385

H	-4.576636	-1.585889	4.780250
H	-0.487625	-1.817638	6.198770
H	-5.107094	-3.742273	5.964863
H	-1.005222	-3.966580	7.383711
H	-3.319519	-4.936552	7.265534
C	-0.112277	3.118764	-0.342973
C	-3.214140	3.694499	-0.621257
C	-4.574062	3.141207	-0.141232
H	-5.385031	3.827099	-0.469471
H	-4.801016	2.137812	-0.559321
H	-4.611574	3.063664	0.962263
C	-3.276232	3.892920	-2.150856
H	-2.342017	4.302046	-2.575541
H	-3.517382	2.952645	-2.687693
H	-4.088393	4.614784	-2.388129
C	-2.959428	5.039776	0.091069
H	-3.821922	5.718578	-0.085717
H	-2.855378	4.910374	1.188267
H	-2.055050	5.554151	-0.290290
C	0.053008	3.895252	-1.662566
H	1.124582	4.160369	-1.798147
H	-0.248030	3.296535	-2.547647
H	-0.518650	4.844098	-1.670291
C	0.269002	4.015985	0.855429
H	-0.357610	4.925758	0.924060
H	0.176068	3.464913	1.812357
H	1.325111	4.345438	0.745518
C	0.838303	1.897667	-0.364472
H	0.716657	1.267002	0.539117
H	0.691828	1.258935	-1.259684
H	1.889057	2.259400	-0.389058
H	-0.618943	1.421808	2.230510
C	-2.493366	2.636878	3.010852
O	-2.665698	3.580562	3.690939
P	-1.887994	2.427958	-0.039509
O	-4.440627	-1.192560	2.244493
C	-4.830501	0.028526	1.861410
C	-5.337731	0.970260	2.955844
H	-5.694033	1.981226	2.577103
O	-5.352045	0.699388	4.142567
H	-3.416563	-0.944198	2.814223
H	-3.972715	0.704779	1.348624
H	-5.551451	0.054512	0.998077

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II SCF Done: -521.709353387 A.U.

Number of imaginary frequencies = 0

C	-2.322716	1.361662	0.082655
H	-2.612585	1.810179	-0.899283
H	-3.262560	1.277590	0.687673
C	-1.878977	-0.081296	-0.170729

H	-1.161304	-0.468301	0.614680
O	-1.315087	2.091225	0.769633
H	-1.736084	2.864097	1.185714
O	-2.421743	-0.798385	-0.994675
N	0.255041	0.770787	-1.153067
H	0.412413	0.313702	-2.060222
H	0.091159	1.772162	-1.315512
C	1.364423	0.568616	-0.224247
H	1.066841	1.037338	0.739067
H	1.452029	-0.523133	-0.021936
C	2.728232	1.118777	-0.676981
H	2.628580	2.211178	-0.877799
H	3.004982	0.654899	-1.652652
C	3.851662	0.883795	0.342370
H	3.563692	1.340854	1.317474
H	3.944888	-0.209002	0.542133
C	5.214933	1.437153	-0.095844
H	5.122330	2.530280	-0.295398
H	5.501952	0.980156	-1.071545
C	6.338311	1.201158	0.924954
H	6.047511	1.657693	1.898737
H	6.427185	0.108383	1.122750
C	7.695486	1.757875	0.477230
H	7.644206	2.854856	0.306416
H	8.487172	1.573430	1.232938
H	8.026999	1.292275	-0.475886

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TS-II-III SCF Done: -521.668339812 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -1345.99 cm⁻¹

C	-2.715130	1.324465	-0.285807
H	-2.756214	1.624494	-1.363440
H	-3.674237	0.804670	-0.048236
C	-1.586711	0.286513	-0.157772
H	-1.556236	-0.090011	0.909025
O	-2.440650	2.421774	0.586916
H	-3.173524	3.059769	0.513360
O	-1.477466	-0.603267	-1.153236
N	-0.224773	1.060143	-0.408528
H	-0.392372	0.312877	-1.338374
H	-0.340983	2.086035	-0.502291
C	0.905043	0.716026	0.474972
H	0.730674	1.146621	1.485437
H	0.894655	-0.390906	0.576115
C	2.246844	1.186837	-0.092323
H	2.224123	2.292922	-0.229548
H	2.380445	0.753469	-1.108891
C	3.438001	0.806223	0.798420
H	3.292082	1.236518	1.816122
H	3.452960	-0.298976	0.939251

C	4.791824	1.267157	0.240313
H	4.774910	2.372795	0.097532
H	4.935948	0.837059	-0.777925
C	5.987644	0.887555	1.126549
H	5.838634	1.317138	2.143607
H	6.000038	-0.217340	1.267782
C	7.335210	1.352186	0.560670
H	7.363109	2.456803	0.442115
H	8.179997	1.064852	1.220442
H	7.525938	0.908956	-0.440348

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III SCF Done: -521.719790545 A.U.

Number of imaginary frequencies = 0

C	-2.492176	1.339751	-0.028360
H	-2.547524	2.106668	-0.843631
H	-3.528070	0.946403	0.121321
C	-1.604274	0.196159	-0.537794
H	-1.527969	-0.566798	0.281317
O	-1.919765	1.846540	1.169050
H	-2.473105	2.586467	1.475527
O	-2.266342	-0.311687	-1.686434
N	-0.244279	0.566316	-0.881588
H	-1.568709	-0.811050	-2.156934
H	-0.243790	1.449798	-1.410745
C	0.755694	0.602252	0.189054
H	0.537955	1.381645	0.958696
H	0.712412	-0.373950	0.723814
C	2.164653	0.806590	-0.378234
H	2.203010	1.778647	-0.924542
H	2.360660	0.021256	-1.142292
C	3.259295	0.790913	0.696921
H	3.033982	1.565756	1.465863
H	3.229956	-0.183136	1.238316
C	4.672602	1.020201	0.143302
H	4.703703	1.995907	-0.395638
H	4.895844	0.247315	-0.628613
C	5.771377	0.998446	1.216476
H	5.543473	1.770232	1.987004
H	5.737387	0.022619	1.752990
C	7.178852	1.229884	0.652733
H	7.251006	2.214166	0.141670
H	7.951723	1.208725	1.449109
H	7.446086	0.451806	-0.094484

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II-EG SCF Done: -752.082162450 A.U.

Number of imaginary frequencies = 0

C	-2.873424	1.273638	-0.162062
H	-3.124350	1.771878	-1.131380
H	-3.845204	0.994337	0.319925

C	-2.179537	-0.047401	-0.484882
H	-1.671074	-0.502985	0.413660
O	-2.060363	2.067108	0.691026
H	-2.619662	2.765009	1.075738
O	-2.565424	-0.739120	-1.448778
N	-0.294933	0.771274	-1.033339
H	-0.112113	0.108585	-1.812971
H	-0.422724	1.726363	-1.391102
C	0.735663	0.694088	0.003756
H	0.401670	1.317929	0.858915
H	0.754545	-0.354771	0.371503
C	2.152152	1.087426	-0.451813
H	2.228025	2.194570	-0.553042
H	2.326742	0.677100	-1.472974
C	3.240439	0.555577	0.492047
H	3.048879	0.921827	1.527185
H	3.144111	-0.553868	0.541407
C	4.666432	0.933287	0.070753
H	4.762348	2.043361	0.030156
H	4.846714	0.581914	-0.972397
C	5.754507	0.362480	0.992687
H	5.570953	0.713580	2.033801
H	5.652747	-0.746567	1.032123
C	7.178077	0.737190	0.562620
H	7.317432	1.839652	0.550734
H	7.941883	0.310654	1.245628
H	7.400110	0.367528	-0.461729
O	-0.355973	-1.804554	-2.426431
H	-1.304290	-1.591067	-2.171950
C	0.187743	-2.555006	-1.355486
H	-0.142010	-3.623480	-1.373818
H	-0.116370	-2.153915	-0.356642
C	1.712852	-2.486761	-1.431074
H	1.995917	-1.432225	-1.670210
H	2.078958	-3.118927	-2.276261
O	2.235336	-2.906215	-0.171710
H	3.201389	-2.991995	-0.262816

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TS-II-III-EG SCF Done: -752.069863036 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = 805.46 cm^{-1}

C	-1.371624	1.703509	-0.472552
H	-1.106224	2.239200	-1.409447
H	-2.416019	2.003759	-0.218835
C	-1.414690	0.196609	-0.765238
H	-1.457675	-0.364430	0.222824
O	-0.428139	2.095800	0.519085
H	-0.709385	1.699407	1.365252
O	-2.341109	-0.117739	-1.670062
N	0.005692	-0.309143	-1.313745

H	-0.358512	-1.296698	-1.773826
H	0.252698	0.296870	-2.113207
C	1.155971	-0.480984	-0.384692
H	0.742184	-0.534446	0.644780
H	1.621192	-1.469570	-0.591436
C	2.199496	0.633208	-0.483643
H	1.691893	1.600655	-0.286025
H	2.600950	0.668742	-1.523213
C	3.359650	0.444298	0.503402
H	2.955276	0.415765	1.541666
H	3.838314	-0.549067	0.339454
C	4.425085	1.545376	0.405941
H	3.942286	2.537664	0.561796
H	4.833578	1.571749	-0.631065
C	5.581302	1.377789	1.403060
H	5.169251	1.351898	2.437809
H	6.057421	0.382882	1.246097
C	6.640739	2.481473	1.295642
H	6.198434	3.483582	1.482712
H	7.462622	2.336199	2.027035
H	7.094824	2.506446	0.281690
O	-1.338833	-2.249937	-2.219904
H	-2.008972	-1.278395	-2.036063
C	-1.606570	-3.173890	-1.182138
H	-1.113039	-4.150747	-1.397434
H	-1.208430	-2.835802	-0.185971
C	-3.110849	-3.401996	-1.018026
H	-3.587505	-2.408236	-0.821296
H	-3.516619	-3.771563	-1.993553
O	-3.301883	-4.326146	0.046661
H	-4.260288	-4.467692	0.144531

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II-H2O SCF Done: -598.185363585 A.U.

Number of imaginary frequencies = 0

C	-2.569885	1.250258	0.134470
H	-2.626344	2.092979	-0.598421
H	-3.625412	1.001897	0.418554
C	-2.048586	0.020937	-0.601573
H	-1.599931	-0.745784	0.096521
O	-1.761544	1.526996	1.266604
H	-2.213196	2.204827	1.799866
O	-2.516983	-0.284438	-1.715996
N	-0.060638	0.672370	-0.998870
H	0.101892	-0.101730	-1.682688
H	-0.135684	1.555592	-1.521730
C	0.953585	0.725990	0.054632
H	0.657741	1.513940	0.777763
H	0.897999	-0.232637	0.618201
C	2.388878	0.948099	-0.448530
H	2.431675	1.906469	-1.016716

H	2.648413	0.149532	-1.180699
C	3.427454	0.975007	0.681780
H	3.152599	1.767500	1.416030
H	3.380520	0.015718	1.247741
C	4.865021	1.207548	0.195881
H	4.912606	2.167955	-0.368459
H	5.137444	0.416257	-0.540662
C	5.905840	1.230327	1.325405
H	5.629060	2.020675	2.060303
H	5.854858	0.269618	1.887242
C	7.338092	1.463900	0.829018
H	7.425672	2.434168	0.294238
H	8.068058	1.475253	1.664991
H	7.652975	0.668451	0.119711
O	-0.422674	-1.641262	-2.657867
H	-0.378666	-2.401723	-2.047442
H	-1.340734	-1.274998	-2.471069

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TS-II-III-H2O SCF Done: -598.172451561 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -892.26 cm⁻¹

C	-1.234424	1.979267	-0.306284
H	-0.868681	2.466692	-1.235499
H	-2.244913	2.404855	-0.098225
C	-1.446165	0.483633	-0.587160
H	-1.559564	-0.054945	0.413038
O	-0.291108	2.272342	0.720634
H	-0.653811	1.925401	1.557288
O	-2.389906	0.268671	-1.498335
N	-0.097836	-0.196909	-1.112641
H	-0.596895	-1.194384	-1.476508
H	0.162685	0.303699	-1.978369
C	1.068759	-0.374791	-0.210467
H	0.692124	-0.323528	0.833189
H	1.470355	-1.402262	-0.357480
C	2.175137	0.661333	-0.420658
H	1.740286	1.670467	-0.263654
H	2.533304	0.607268	-1.475135
C	3.362104	0.460657	0.531436
H	3.000258	0.524207	1.583708
H	3.771194	-0.569908	0.414522
C	4.488797	1.482214	0.321967
H	4.075809	2.511330	0.433003
H	4.852933	1.418472	-0.729860
C	5.674619	1.301940	1.281408
H	5.306957	1.366036	2.331129
H	6.081167	0.270672	1.169627
C	6.794677	2.326408	1.062230
H	6.423609	3.364449	1.202291
H	7.637073	2.173587	1.768366

H	7.204936	2.260130	0.031583
O	-1.650643	-1.991365	-1.943084
H	-1.983827	-2.550956	-1.215210
H	-2.218001	-0.950988	-1.804019

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TS-CD SCF Done: -1748.29392612 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -56.62 cm⁻¹

Ru	-0.121526	-0.750161	-0.731325
H	-0.607269	-2.260054	-1.266879
P	-2.175528	-0.086834	-0.023082
O	-0.615915	0.421126	-3.472511
N	1.926361	-1.625814	-0.711650
N	0.026255	-1.457795	1.255979
C	-1.891674	-0.064285	1.833744
C	-0.828887	-1.050091	2.235744
C	-0.644943	-1.484479	3.560072
H	-1.347512	-1.150568	4.337532
C	0.449178	-2.303291	3.878264
H	0.612793	-2.636081	4.914790
C	1.344041	-2.676766	2.861506
H	2.223172	-3.303102	3.074434
C	1.095046	-2.241148	1.552447
C	1.915388	-2.656889	0.359018
H	2.945666	-2.953574	0.663479
H	1.424965	-3.555400	-0.081193
C	-0.363990	-0.062127	-2.427036
C	-2.811971	1.694318	-0.375650
C	-1.581383	2.630148	-0.422740
H	-1.940838	3.671992	-0.573071
H	-0.991146	2.609743	0.516260
H	-0.904469	2.375174	-1.259571
C	-3.509428	1.724556	-1.752669
H	-3.738038	2.779832	-2.018073
H	-2.861133	1.314175	-2.552860
H	-4.470159	1.171972	-1.755147
C	-3.769048	2.213706	0.721433
H	-4.674782	1.592643	0.845952
H	-3.265833	2.300251	1.705489
H	-4.107434	3.236000	0.443742
C	-3.593249	-1.375495	-0.260657
C	-3.687167	-1.723716	-1.762118
H	-4.034205	-0.871251	-2.376981
H	-2.700219	-2.050837	-2.147543
H	-4.412529	-2.554922	-1.901928
C	-4.964149	-0.923352	0.275731
H	-5.686039	-1.764947	0.185598
H	-4.927066	-0.641636	1.349162
H	-5.385584	-0.072433	-0.294904
C	-3.152616	-2.644341	0.506946

H	-2.141898	-2.972755	0.189174
H	-3.151986	-2.496779	1.606937
H	-3.867880	-3.466514	0.286768
C	2.490130	-2.218130	-1.961004
H	1.807840	-3.042642	-2.250993
H	3.487200	-2.666620	-1.728055
H	-2.816665	-0.174967	2.435487
C	1.376540	1.427104	1.444692
H	0.461496	0.701235	-0.027556
O	0.547440	1.960440	2.188809
C	2.229471	2.189342	0.426375
H	3.122599	2.567560	0.976479
H	1.656398	3.078894	0.070896
O	2.704932	1.367543	-0.625197
H	1.788517	0.395022	1.667884
H	-1.461286	0.940300	2.050109
H	1.871158	1.004014	-1.032800
H	2.525248	-0.829258	-0.419062
C	2.629750	-1.240896	-3.103735
C	3.564609	-0.185859	-3.041751
C	1.832682	-1.380248	-4.257468
C	3.679013	0.726617	-4.102274
H	4.190208	-0.054384	-2.145331
C	1.956098	-0.477954	-5.325749
H	1.085512	-2.188486	-4.302082
C	2.876327	0.580871	-5.248110
H	4.398227	1.557560	-4.030756
H	1.313718	-0.590380	-6.212774
H	2.965520	1.297882	-6.079681

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D SCF Done: -1748.29662462 A.U.

Number of imaginary frequencies = 0

Ru	-0.113020	-0.762569	-0.794152
H	-0.600702	-2.307488	-1.244973
P	-2.151604	-0.073941	-0.077769
O	-0.598995	0.251343	-3.601193
N	1.937499	-1.636654	-0.760195
N	0.065056	-1.409676	1.204815
C	-1.850737	-0.012523	1.779196
C	-0.781645	-0.988227	2.188493
C	-0.585446	-1.400795	3.517562
H	-1.277318	-1.048454	4.296570
C	0.504214	-2.225695	3.838194
H	0.677886	-2.541069	4.878432
C	1.376193	-2.634160	2.814301
H	2.244706	-3.276038	3.024858
C	1.117909	-2.218119	1.501005
C	1.905844	-2.674354	0.300736
H	2.928658	-3.008463	0.592604
H	1.371125	-3.551398	-0.131978

C	-0.361120	-0.168075	-2.527363
C	-2.788137	1.704700	-0.451453
C	-1.561440	2.645223	-0.498432
H	-1.923142	3.684148	-0.663505
H	-0.979415	2.637416	0.446066
H	-0.871697	2.378792	-1.320800
C	-3.468438	1.713249	-1.837402
H	-3.695414	2.763204	-2.124640
H	-2.810407	1.288053	-2.622149
H	-4.428141	1.158825	-1.841692
C	-3.758790	2.238492	0.626695
H	-4.672129	1.627125	0.739282
H	-3.272633	2.325928	1.619449
H	-4.083278	3.262411	0.338337
C	-3.582038	-1.358804	-0.268739
C	-3.684760	-1.746907	-1.760030
H	-4.019616	-0.906000	-2.397584
H	-2.704091	-2.100207	-2.138144
H	-4.423930	-2.569772	-1.875242
C	-4.949277	-0.887747	0.259947
H	-5.673038	-1.730384	0.198510
H	-4.907416	-0.573537	1.324163
H	-5.372020	-0.054236	-0.335044
C	-3.143743	-2.608987	0.530190
H	-2.133061	-2.945198	0.219889
H	-3.144790	-2.435059	1.626328
H	-3.859167	-3.435871	0.328868
C	2.511565	-2.198749	-2.012945
H	1.880924	-3.068731	-2.287426
H	3.540641	-2.583006	-1.801144
H	-2.771268	-0.124865	2.387901
C	1.467823	1.488219	1.937255
H	0.455866	0.758063	-0.283964
O	0.567834	2.125696	2.463515
C	2.488390	2.052850	0.954106
H	3.431753	2.220272	1.526619
H	2.128054	3.049214	0.601792
O	2.766118	1.148690	-0.096424
H	1.643826	0.396898	2.181074
H	-1.441643	1.002729	1.982280
H	1.832892	0.928440	-0.459342
H	2.536790	-0.856258	-0.427363
C	2.554128	-1.223593	-3.167938
C	3.193012	0.029251	-3.048231
C	1.952871	-1.567821	-4.395046
C	3.207032	0.923798	-4.130381
H	3.657002	0.332702	-2.096757
C	1.980419	-0.680013	-5.482433
H	1.429959	-2.533368	-4.488742
C	2.603501	0.571723	-5.350922
H	3.691824	1.906417	-4.016156

H	1.491257	-0.958916	-6.428820
H	2.611991	1.277615	-6.196560

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E SCF Done: -1519.12514861 A.U.

Number of imaginary frequencies = 0

Ru	-0.269919	-0.853997	-0.919707
H	-0.749214	-2.465999	-1.219436
P	-2.243551	-0.117477	-0.109439
O	-1.017655	-0.062473	-3.740103
N	1.793748	-1.702775	-0.944441
N	0.062938	-1.346664	1.100027
C	-1.786982	0.113385	1.708265
C	-0.715048	-0.862999	2.112910
C	-0.472192	-1.247709	3.441517
H	-1.118148	-0.856825	4.241903
C	0.599208	-2.109293	3.734822
H	0.805939	-2.409669	4.773394
C	1.404384	-2.577309	2.682156
H	2.253153	-3.252550	2.868681
C	1.098098	-2.187101	1.371367
C	1.797947	-2.710595	0.144132
H	2.826902	-3.068237	0.384918
H	1.207390	-3.576261	-0.238720
C	-0.673861	-0.387833	-2.657812
C	-2.945050	1.614487	-0.587618
C	-1.742596	2.550388	-0.844605
H	-2.128934	3.566709	-1.080819
H	-1.074991	2.635285	0.036953
H	-1.118550	2.199727	-1.687259
C	-3.750191	1.486155	-1.899128
H	-4.017888	2.502734	-2.262112
H	-3.160251	0.992215	-2.697409
H	-4.697888	0.928489	-1.762115
C	-3.821431	2.245826	0.517799
H	-4.711221	1.642349	0.772374
H	-3.250587	2.431722	1.450599
H	-4.186461	3.235343	0.164235
C	-3.679997	-1.417358	-0.051223
C	-3.903867	-1.944583	-1.485005
H	-4.306064	-1.170669	-2.166834
H	-2.951263	-2.322201	-1.909516
H	-4.635697	-2.781765	-1.458989
C	-5.001035	-0.901620	0.547534
H	-5.719338	-1.747564	0.627853
H	-4.870548	-0.489542	1.570511
H	-5.482345	-0.128121	-0.083009
C	-3.163867	-2.587371	0.818826
H	-2.178319	-2.945856	0.455817
H	-3.078358	-2.314693	1.891193
H	-3.883424	-3.432501	0.752186

C	2.349431	-2.264974	-2.205575
H	1.588209	-2.961291	-2.611812
H	3.269259	-2.855784	-1.970775
H	-2.652091	0.093587	2.402516
H	0.448112	0.639065	-0.604383
H	-1.347645	1.135377	1.748677
H	2.369550	-0.893358	-0.666022
C	2.691590	-1.182062	-3.202727
C	3.783088	-0.320480	-2.956337
C	1.927274	-0.995658	-4.369722
C	4.090507	0.719886	-3.847276
H	4.405975	-0.468749	-2.056761
C	2.234205	0.041559	-5.266125
H	1.067554	-1.653781	-4.565106
C	3.312449	0.903879	-5.005237
H	4.942279	1.387270	-3.640747
H	1.614621	0.183924	-6.165042
H	3.549319	1.721189	-5.704844

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hydroxyacetaldehyde SCF Done: -229.145086713 A.U.

Number of imaginary frequencies = 0

C	-0.330883	-0.621166	-0.010586
H	0.012597	-0.133583	0.939035
H	-1.450580	-0.651054	0.043419
C	0.154323	-2.066876	0.031807
H	0.797630	-2.347927	-0.860849
O	0.171920	-0.014705	-1.182556
H	-0.139366	0.907410	-1.208085
O	-0.114534	-2.844523	0.923828

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TS-EF SCF Done: -1519.08660283 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -935.90 cm⁻¹

C	-0.603774	0.052826	-0.714578
H	-0.849460	1.224051	-2.539747
N	-1.301497	0.523850	3.209203
C	-0.201582	-0.387035	2.940243
C	-0.126592	-0.733602	1.472763
N	-0.620236	0.216509	0.636859
C	-1.288726	1.125496	-1.525879
H	-2.464402	0.713864	2.351693
H	-0.263836	-1.323575	3.546949
H	0.785864	0.092310	3.205660
H	-2.350519	0.821613	-1.661682
C	0.445101	-1.909128	0.958449
H	0.834977	-2.671561	1.648992
C	0.516098	-2.079761	-0.432947
H	0.974056	-2.985818	-0.859559
C	-0.015496	-1.091245	-1.279030

H	0.008438	-1.207275	-2.372740
Ru	-1.362086	1.967006	1.575643
C	-1.351757	0.987697	4.584398
H	-0.422181	1.551978	4.861445
H	-2.184705	1.721631	4.661041
C	-1.583969	-0.128072	5.600579
C	-2.518357	-1.151238	5.329778
C	-0.887858	-0.158597	6.825610
C	-2.756556	-2.172992	6.263321
C	-1.127294	-1.176379	7.766661
C	-2.062950	-2.187892	7.488145
H	-3.047900	-1.137499	4.362906
H	-0.145797	0.628234	7.043356
H	-3.489699	-2.964051	6.035886
H	-0.574364	-1.182982	8.720002
H	-2.248870	-2.988863	8.221590
C	0.230941	3.674218	-1.154698
C	-2.937118	3.594601	-1.296651
C	-4.145975	2.913826	-0.615685
H	-5.083319	3.356347	-1.018367
H	-4.183076	1.820876	-0.807536
H	-4.130523	3.053660	0.482244
C	-3.087024	3.447957	-2.826280
H	-2.269185	3.928544	-3.392736
H	-3.149518	2.386605	-3.143114
H	-4.036021	3.933337	-3.144166
C	-2.925389	5.084882	-0.895087
H	-3.909295	5.540241	-1.141748
H	-2.760418	5.215019	0.194382
H	-2.151761	5.662445	-1.439308
C	0.191144	4.164703	-2.613881
H	1.186940	4.578824	-2.886210
H	-0.027254	3.346246	-3.331732
H	-0.549323	4.974091	-2.769664
C	0.480901	4.860867	-0.198145
H	-0.308662	5.634331	-0.261874
H	0.540423	4.514819	0.852956
H	1.446272	5.346221	-0.460741
C	1.394751	2.666271	-0.999532
H	1.417208	2.229686	0.019815
H	1.345340	1.840846	-1.739464
H	2.356939	3.197597	-1.166217
H	0.180054	2.451736	1.750994
C	-1.843860	3.553266	2.392945
O	-2.114271	4.588977	2.881764
P	-1.363030	2.754936	-0.573253
H	-3.015310	1.139619	1.626316

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F SCF Done: -1519.10134640 A.U.

Number of imaginary frequencies = 0

C	-0.742012	0.019513	-0.766199
H	-0.903993	1.232994	-2.568372
N	-1.417984	0.465714	3.176276
C	-0.299165	-0.403280	2.875473
C	-0.243138	-0.766226	1.418807
N	-0.807862	0.150328	0.588355
C	-1.392564	1.115233	-1.578941
H	-3.270784	0.972773	1.777389
H	-0.296953	-1.331988	3.499156
H	0.703927	0.088479	3.086181
H	-2.452157	0.835575	-1.773370
C	0.395155	-1.903749	0.892435
H	0.836983	-2.641846	1.578131
C	0.467521	-2.064539	-0.498290
H	0.967599	-2.944795	-0.931740
C	-0.099449	-1.088799	-1.339230
H	-0.048776	-1.183535	-2.434073
Ru	-1.666442	1.828494	1.562800
C	-1.325684	0.977669	4.532198
H	-0.379613	1.563223	4.717290
H	-2.158854	1.698521	4.686479
C	-1.436865	-0.105053	5.606494
C	-2.345568	-1.173865	5.445289
C	-0.658846	-0.056435	6.780933
C	-2.478687	-2.161000	6.435356
C	-0.792920	-1.038972	7.778733
C	-1.704186	-2.096105	7.609217
H	-2.932428	-1.216932	4.512951
H	0.065412	0.765724	6.912037
H	-3.192523	-2.989043	6.292498
H	-0.176164	-0.982742	8.690645
H	-1.807260	-2.870237	8.386749
C	0.203441	3.575415	-0.960691
C	-2.928772	3.665515	-1.425293
C	-4.238981	3.049646	-0.884788
H	-5.103191	3.553659	-1.369736
H	-4.325699	1.965168	-1.109543
H	-4.333486	3.182970	0.210671
C	-2.939350	3.561198	-2.965634
H	-2.036783	3.989502	-3.437098
H	-3.046429	2.513382	-3.313883
H	-3.814419	4.122365	-3.361363
C	-2.872020	5.142296	-0.979543
H	-3.802485	5.659786	-1.299788
H	-2.799830	5.234669	0.124127
H	-2.021569	5.687940	-1.433985
C	0.334679	4.109333	-2.399467
H	1.368582	4.489235	-2.553134
H	0.162123	3.321107	-3.162064
H	-0.353275	4.952980	-2.604795
C	0.403869	4.722046	0.055235

H	-0.336503	5.535857	-0.065408
H	0.336160	4.347231	1.095812
H	1.413230	5.165446	-0.088996
C	1.307584	2.516528	-0.725715
H	1.223156	2.053104	0.277729
H	1.295426	1.711660	-1.488928
H	2.299682	3.013794	-0.789565
H	-0.170012	2.304225	1.890503
C	-2.203327	3.382832	2.412602
O	-2.500062	4.404658	2.913475
P	-1.480890	2.715400	-0.579890
H	-3.339662	1.246454	0.988251

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H2 SCF Done: -1.17937423914 A.U.

Number of imaginary frequencies = 0

H	-0.848630	-0.249205	0.000000
H	-1.616058	-0.249205	0.000000

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G SCF Done: -1747.08030260 A.U.

Number of imaginary frequencies = 0

C	-0.944162	-0.061065	-0.732280
H	-1.493871	1.081029	-2.503708
N	-0.764080	0.590757	3.194663
C	0.139996	-0.454113	2.790049
C	-0.031628	-0.798691	1.332021
N	-0.721847	0.121454	0.603497
C	-1.754189	1.006990	-1.427391
H	0.017266	-1.400121	3.384293
H	1.226166	-0.173091	2.927306
H	-2.828982	0.723595	-1.371762
C	0.480372	-1.957775	0.724737
H	1.034509	-2.688602	1.332851
C	0.270390	-2.161281	-0.646121
H	0.659743	-3.063657	-1.142437
C	-0.452301	-1.201728	-1.382742
H	-0.640476	-1.337243	-2.458130
Ru	-1.333092	1.858866	1.642666
C	-0.716361	0.917030	4.612887
H	0.239690	0.588088	5.092142
H	-0.784072	2.016182	4.757574
C	-1.897492	0.232188	5.287194
C	-3.178395	0.827466	5.220691
C	-1.788731	-1.072662	5.815631
C	-4.319747	0.133253	5.651679
C	-2.931437	-1.777409	6.242972
C	-4.203285	-1.178488	6.159271
H	-3.273846	1.837825	4.790678
H	-0.794808	-1.544288	5.890784
H	-5.309540	0.613649	5.593227

H	-2.828008	-2.796190	6.650094
H	-5.098060	-1.724637	6.497242
C	-0.086443	3.489823	-1.278456
C	-3.238703	3.564239	-1.060962
C	-4.387672	2.971901	-0.216872
H	-5.341061	3.467939	-0.503655
H	-4.516004	1.881913	-0.377903
H	-4.221448	3.119632	0.866691
C	-3.582830	3.389263	-2.555183
H	-2.814961	3.803496	-3.233163
H	-3.745540	2.325727	-2.825945
H	-4.534684	3.923302	-2.771331
C	-3.101508	5.060358	-0.707591
H	-4.084247	5.561344	-0.848667
H	-2.802244	5.205445	0.351168
H	-2.371442	5.584939	-1.355586
C	-0.275453	3.960074	-2.732648
H	0.696518	4.331482	-3.126400
H	-0.605068	3.139322	-3.403803
H	-0.999038	4.794241	-2.818959
C	0.321720	4.679676	-0.381866
H	-0.435660	5.486655	-0.371508
H	0.484073	4.350363	0.663792
H	1.271191	5.117183	-0.761105
C	1.052584	2.442838	-1.246349
H	1.194033	2.023424	-0.230114
H	0.879749	1.603744	-1.951261
H	2.003053	2.933936	-1.549127
H	0.148482	2.389204	1.639392
C	-1.783247	3.430633	2.493365
O	-2.056319	4.460153	3.000930
P	-1.641833	2.645361	-0.495429
O	-3.583839	0.935149	1.895122
C	-4.003963	-0.122799	2.360253
H	-5.070855	-0.203085	2.721422
C	-3.181372	-1.375317	2.530977
H	-2.854911	-1.715518	1.520744
H	-2.249037	-1.017094	3.044127
O	-3.870634	-2.418200	3.180278
H	-3.845007	-2.218363	4.140221

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hexanamine SCF Done: -292.558489620 A.U.

Number of imaginary frequencies = 0

N	-3.216866	0.554861	0.021678
H	-2.874900	-0.416311	0.067810
H	-2.872158	0.998205	0.885889
C	-2.620628	1.223966	-1.137265
H	-3.010057	0.735192	-2.060023
H	-3.007008	2.268700	-1.173087
C	-1.080519	1.254388	-1.195254

H	-0.694369	1.746478	-0.271385
H	-0.697529	0.207023	-1.161440
C	-0.517494	1.968219	-2.431950
H	-0.910809	1.476023	-3.351880
H	-0.907586	3.012274	-2.463669
C	1.016385	1.998702	-2.490279
H	1.410503	2.491218	-1.570721
H	1.407250	0.954799	-2.458922
C	1.577622	2.713437	-3.728729
H	1.180933	2.219691	-4.645406
H	1.184219	3.755477	-3.757568
C	3.110492	2.737751	-3.776431
H	3.487592	3.259742	-4.680573
H	3.532687	3.257036	-2.889044
H	3.529422	1.708283	-3.784553

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H SCF Done: -2039.68927508 A.U.

Number of imaginary frequencies = 0

C	-0.820796	1.033906	-1.012607
H	-1.417201	2.756859	-2.218457
N	-1.801102	-0.542623	2.601418
C	-0.427790	-0.867106	2.142599
C	-0.184487	-0.462347	0.707179
N	-0.908439	0.596138	0.270906
C	-1.829537	2.069237	-1.451611
H	-0.178882	-1.940947	2.294666
H	0.275823	-0.285033	2.781432
H	-2.673289	1.520347	-1.924595
C	0.747877	-1.091389	-0.132013
H	1.325821	-1.952411	0.235507
C	0.919324	-0.602009	-1.437685
H	1.652851	-1.068291	-2.113678
C	0.122449	0.463287	-1.886082
H	0.201872	0.834888	-2.918432
Ru	-2.451940	1.251738	1.548032
C	-1.895948	-0.513081	4.079929
H	-1.281742	0.334729	4.447783
H	-2.948340	-0.263179	4.322581
C	-1.494502	-1.809789	4.762876
C	-2.021573	-3.045072	4.322551
C	-0.600460	-1.807153	5.852764
C	-1.665882	-4.244315	4.960876
C	-0.247150	-3.005825	6.498075
C	-0.778767	-4.228541	6.053140
H	-2.713447	-3.057624	3.465055
H	-0.176832	-0.850533	6.201697
H	-2.086146	-5.198865	4.605416
H	0.451230	-2.984287	7.349957
H	-0.500790	-5.168991	6.554900
C	-1.453075	4.451095	0.317409

C	-4.324488	3.510475	-0.631208
C	-5.285271	2.304932	-0.521307
H	-6.280267	2.612350	-0.911822
H	-4.962080	1.416261	-1.096838
H	-5.415224	1.986829	0.531098
C	-4.282733	3.980661	-2.101078
H	-3.594912	4.829786	-2.271003
H	-4.002448	3.159878	-2.791942
H	-5.300481	4.314681	-2.400303
C	-4.861331	4.633799	0.281655
H	-5.918207	4.845117	0.008996
H	-4.849133	4.332936	1.349582
H	-4.299201	5.582447	0.173112
C	-1.524143	5.517961	-0.791652
H	-0.758272	6.300464	-0.595269
H	-1.308603	5.098573	-1.796983
H	-2.506500	6.028321	-0.830242
C	-1.785697	5.075812	1.690310
H	-2.778980	5.562555	1.709536
H	-1.761875	4.305767	2.487675
H	-1.029002	5.854126	1.931805
C	-0.010769	3.893777	0.377000
H	0.078817	3.086119	1.131003
H	0.336839	3.503777	-0.602072
H	0.680959	4.714858	0.665652
H	-1.442087	2.107248	2.474888
C	-3.796797	1.847411	2.651027
O	-4.650270	2.257693	3.357641
P	-2.612406	2.934806	0.028299
O	-3.361406	-0.230781	0.199014
C	-4.453848	-0.986582	0.528894
C	-4.942960	-1.656099	-0.807007
H	-4.422572	-2.650945	-0.907942
H	-6.037270	-1.862055	-0.783181
O	-4.621570	-0.798296	-1.879855
H	-3.855752	-0.314686	-1.438788
H	-2.521909	-1.220527	2.220930
N	-4.142767	-2.021496	1.568473
H	-3.813128	-2.861593	1.069927
C	-5.285263	-2.381786	2.431019
H	-6.244869	-2.418916	1.855682
H	-5.126823	-3.413401	2.816732
C	-5.437391	-1.416019	3.611965
H	-4.559828	-1.540872	4.283440
H	-5.389300	-0.371093	3.236294
C	-6.726610	-1.608955	4.417796
H	-7.606259	-1.454584	3.750599
H	-6.797902	-2.664850	4.770010
C	-6.826530	-0.659524	5.620456
H	-6.723187	0.391313	5.264548
H	-5.955354	-0.830946	6.295088

C	-8.126912	-0.804669	6.424264
H	-8.994840	-0.628972	5.748076
H	-8.227427	-1.858885	6.771272
C	-8.207358	0.145683	7.625609
H	-8.141602	1.206929	7.302646
H	-9.156946	0.023545	8.187468
H	-7.371553	-0.032924	8.336136
H	-5.286642	-0.367325	0.960677

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TS-HI SCF Done: -2039.67297640 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -106.41 cm⁻¹

C	-0.835960	0.879147	-0.867376
H	-1.562067	2.444812	-2.202564
N	-1.851394	-0.583669	2.729288
C	-0.439528	-0.813070	2.407165
C	-0.117490	-0.422929	0.987705
N	-0.976469	0.469766	0.426651
C	-1.939287	1.745983	-1.427677
H	-0.136528	-1.874902	2.576630
H	0.227687	-0.203210	3.076365
H	-2.675657	1.074205	-1.924712
C	0.980229	-0.910064	0.258232
H	1.663852	-1.635696	0.723231
C	1.176178	-0.462223	-1.056056
H	2.032963	-0.825520	-1.644752
C	0.255353	0.433572	-1.629298
H	0.364853	0.770883	-2.670481
Ru	-2.595482	1.055280	1.649182
C	-2.109238	-0.784556	4.153316
H	-1.499095	-0.087219	4.783192
H	-3.168397	-0.515283	4.348074
C	-1.876876	-2.214739	4.632362
C	-2.254865	-3.317108	3.831305
C	-1.310324	-2.465669	5.899089
C	-2.074378	-4.631122	4.295428
C	-1.134281	-3.780091	6.367186
C	-1.516008	-4.869454	5.564711
H	-2.703864	-3.146468	2.838901
H	-1.001592	-1.613794	6.528715
H	-2.377677	-5.477684	3.658087
H	-0.690788	-3.953784	7.361091
H	-1.375645	-5.900974	5.925905
H	-1.772493	2.122477	2.442591
C	-4.019070	1.606081	2.679961
O	-4.931768	2.005132	3.313616
P	-2.901555	2.587132	-0.042492
O	-3.020027	-1.598074	0.653913
C	-4.415407	-1.834848	0.469071
C	-4.549380	-2.056331	-1.054874

H	-4.289721	-3.126586	-1.273192
H	-5.599305	-1.889087	-1.379459
O	-3.691811	-1.173493	-1.763670
H	-2.931067	-1.098800	-1.132386
H	-2.710604	-1.368055	1.631045
N	-4.932100	-2.933559	1.247500
H	-5.105839	-3.773925	0.687529
C	-6.006871	-2.631220	2.194099
H	-6.866809	-2.090545	1.713918
H	-6.418897	-3.595793	2.562988
C	-5.496516	-1.807840	3.381944
H	-4.709614	-2.394787	3.901003
H	-4.990991	-0.895585	2.993497
C	-6.577073	-1.383476	4.380680
H	-7.353861	-0.776645	3.859948
H	-7.105528	-2.285436	4.769614
C	-6.003861	-0.575782	5.554459
H	-5.490125	0.325935	5.152101
H	-5.214091	-1.178351	6.060972
C	-7.053447	-0.139785	6.586625
H	-7.841113	0.458150	6.073430
H	-7.573391	-1.040509	6.987189
C	-6.460209	0.674068	7.743576
H	-5.964296	1.595803	7.370335
H	-7.236295	0.981908	8.475364
H	-5.692822	0.088259	8.294416
H	-4.977146	-0.912147	0.750492
C	-1.965513	4.260907	0.182905
C	-4.633506	2.885600	-0.819558
C	-5.384487	1.541274	-0.690361
H	-4.846635	0.708174	-1.187518
H	-5.538711	1.267705	0.372841
H	-6.384929	1.637259	-1.166918
C	-5.384458	3.949360	0.007566
H	-4.971891	4.968414	-0.132119
H	-6.447235	3.978123	-0.317929
H	-5.375412	3.708025	1.090596
C	-4.588544	3.286302	-2.309284
H	-4.132277	2.495922	-2.939164
H	-5.628996	3.427366	-2.676460
H	-4.046179	4.232588	-2.490745
C	-2.122619	5.236385	-0.998482
H	-1.472870	6.123679	-0.830866
H	-1.812765	4.784802	-1.964205
H	-3.160128	5.609530	-1.105192
C	-2.448443	4.924809	1.491527
H	-3.504251	5.251486	1.440456
H	-2.347036	4.233394	2.352008
H	-1.830341	5.826147	1.696453
C	-0.466719	3.908554	0.339606
H	-0.300581	3.168543	1.148135

H	-0.022873	3.507537	-0.594634
H	0.096412	4.831056	0.599820

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I SCF Done: -2039.68403442 A.U.

Number of imaginary frequencies = 0

C	-0.821697	0.236893	-1.032279
H	-1.211542	1.413965	-2.827589
N	-2.298493	0.019334	2.702164
C	-0.911387	-0.460223	2.597714
C	-0.458492	-0.563509	1.168286
N	-1.136788	0.224692	0.292980
C	-1.736663	1.027315	-1.930329
H	-0.767236	-1.442141	3.107975
H	-0.209868	0.247886	3.114457
H	-2.516845	0.316266	-2.283370
C	0.600573	-1.375915	0.730445
H	1.125114	-2.020502	1.451172
C	0.971809	-1.337954	-0.621269
H	1.805774	-1.957388	-0.986254
C	0.256152	-0.520860	-1.511702
H	0.502567	-0.497205	-2.583113
Ru	-2.741586	1.358412	1.118082
C	-2.606299	0.372244	4.096032
H	-1.982692	1.236868	4.432739
H	-3.657298	0.731158	4.127912
C	-2.453269	-0.763234	5.103709
C	-2.832380	-2.087824	4.787303
C	-1.964729	-0.497335	6.399915
C	-2.716307	-3.112701	5.740902
C	-1.866093	-1.517838	7.362212
C	-2.238400	-2.833037	7.033850
H	-3.232208	-2.319180	3.788291
H	-1.658951	0.530320	6.659737
H	-3.013574	-4.139267	5.473374
H	-1.488759	-1.285295	8.371084
H	-2.157394	-3.636938	7.782513
H	-1.754540	2.456409	1.659870
C	-4.100074	2.389094	1.820355
O	-4.960079	3.074198	2.244618
P	-2.666433	2.351855	-0.962017
O	-3.634323	-1.925112	1.573838
C	-4.364911	-1.346980	0.515908
C	-3.966115	-2.093794	-0.772148
H	-4.472911	-3.094760	-0.755764
H	-4.345905	-1.552175	-1.663619
O	-2.559425	-2.211661	-0.870978
H	-2.292890	-2.359514	0.067930
H	-3.154904	-1.148732	2.117399
N	-5.802358	-1.325483	0.632910
H	-6.138757	-2.269191	0.860633

C	-6.443638	-0.311045	1.470335
H	-6.196799	0.687403	1.047247
H	-7.542839	-0.430125	1.339501
C	-6.106448	-0.298727	2.970620
H	-5.037719	-0.028397	3.090586
H	-6.682076	0.527927	3.445611
C	-6.371576	-1.617390	3.704009
H	-7.406533	-1.973542	3.485265
H	-5.682785	-2.391090	3.296093
C	-6.176205	-1.506799	5.222436
H	-6.915356	-0.784562	5.641011
H	-5.175639	-1.064655	5.427541
C	-6.283218	-2.842313	5.969390
H	-7.293518	-3.282344	5.802599
H	-5.562047	-3.561059	5.518484
C	-6.002634	-2.714448	7.471124
H	-6.712734	-2.010193	7.956325
H	-6.088068	-3.690483	7.993673
H	-4.975576	-2.327825	7.644867
H	-4.047517	-0.254915	0.373360
C	-1.507623	3.891574	-1.081810
C	-4.247626	2.616003	-2.025061
C	-5.180834	1.430085	-1.703393
H	-6.111862	1.519084	-2.303840
H	-4.725417	0.450055	-1.949236
H	-5.465200	1.406343	-0.634908
C	-1.418759	4.518394	-2.485780
H	-1.116062	3.782826	-3.260077
H	-2.370803	4.988402	-2.801958
H	-0.647748	5.320124	-2.479270
C	-3.991364	2.636400	-3.546987
H	-3.343008	3.470341	-3.870226
H	-3.543432	1.688227	-3.908501
H	-4.963939	2.752913	-4.073827
C	-1.989928	4.945676	-0.060320
H	-2.988325	5.354201	-0.308197
H	-2.041215	4.519967	0.961624
H	-1.274867	5.796970	-0.045955
C	-4.938099	3.918766	-1.570501
H	-5.944622	3.983327	-2.038219
H	-5.078988	3.945196	-0.470017
H	-4.376401	4.823921	-1.876022
C	-0.095492	3.413818	-0.665833
H	-0.106034	2.903878	0.318372
H	0.356572	2.725161	-1.408844
H	0.575213	4.296710	-0.585925

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TS-IJ SCF Done: -2039.67830554 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = 290.65 cm^{-1}

C	-0.900062	-0.001155	-0.990203
H	-1.292910	0.984694	-2.897384
N	-2.154128	0.332262	2.824146
C	-0.760054	-0.158042	2.698954
C	-0.445047	-0.523778	1.270460
N	-1.123483	0.191869	0.337467
C	-1.796049	0.759848	-1.934471
H	-0.557434	-1.013212	3.381768
H	-0.084856	0.677039	2.997591
H	-2.662627	0.101203	-2.163509
C	0.509257	-1.480055	0.895807
H	1.033111	-2.061781	1.668784
C	0.784603	-1.663871	-0.468923
H	1.536997	-2.400386	-0.790413
C	0.077758	-0.911957	-1.419447
H	0.253908	-1.050478	-2.496242
Ru	-2.585087	1.524761	1.060784
C	-2.438401	0.888848	4.165706
H	-1.792313	1.778196	4.319668
H	-3.482540	1.265113	4.135890
C	-2.281358	-0.105023	5.308038
C	-2.764854	-1.428715	5.189553
C	-1.682800	0.290663	6.522237
C	-2.653306	-2.326776	6.264726
C	-1.580028	-0.604813	7.601354
C	-2.065806	-1.918354	7.475429
H	-3.239384	-1.761339	4.252061
H	-1.294922	1.318094	6.624698
H	-3.042158	-3.351775	6.156180
H	-1.113435	-0.275675	8.543665
H	-1.984975	-2.623034	8.318300
H	-1.377091	2.542248	1.553359
C	-3.804215	2.757375	1.688542
O	-4.563182	3.578987	2.069227
P	-2.537267	2.271717	-1.080890
O	-3.762348	-1.648218	2.038931
C	-4.409624	-1.234102	1.011861
C	-4.024389	-1.947371	-0.311032
H	-4.728703	-2.814274	-0.425361
H	-4.172339	-1.280075	-1.189077
O	-2.685009	-2.359102	-0.233053
H	-2.540296	-2.374244	0.749940
H	-2.805065	-0.487166	2.638581
N	-5.745938	-0.848379	1.081740
H	-6.118216	-0.637533	0.149879
C	-6.243307	0.105531	2.077119
H	-5.771856	1.104257	1.901186
H	-7.332508	0.214250	1.884156
C	-6.023241	-0.285803	3.542251
H	-4.956143	-0.141102	3.800974
H	-6.588188	0.446975	4.161988

C	-6.416947	-1.717659	3.919457
H	-7.446256	-1.946710	3.558946
H	-5.736300	-2.409529	3.376768
C	-6.318374	-1.966548	5.432549
H	-7.135704	-1.420174	5.958631
H	-5.371717	-1.520667	5.812752
C	-6.350373	-3.448532	5.830127
H	-7.290412	-3.916623	5.457645
H	-5.524680	-3.977395	5.300082
C	-6.216649	-3.668862	7.342155
H	-7.047232	-3.180061	7.895713
H	-6.224684	-4.746696	7.608437
H	-5.268060	-3.231985	7.723080
H	-3.720049	0.231928	0.658086
C	-1.261734	3.671715	-1.468859
C	-4.168643	2.576551	-2.061059
C	-5.208878	1.569094	-1.523867
H	-6.168369	1.712346	-2.067885
H	-4.885961	0.519619	-1.681153
H	-5.383781	1.705501	-0.439877
C	-1.227878	4.123769	-2.940410
H	-1.045771	3.280442	-3.639476
H	-2.158329	4.640070	-3.249289
H	-0.394523	4.847199	-3.080564
C	-4.029498	2.367004	-3.584274
H	-3.308888	3.059593	-4.055002
H	-3.727389	1.329946	-3.837624
H	-5.016577	2.541819	-4.066569
C	-1.562281	4.870567	-0.542728
H	-2.528136	5.359034	-0.774411
H	-1.583099	4.548799	0.518142
H	-0.764172	5.635592	-0.662190
C	-4.675785	4.001320	-1.752296
H	-5.699290	4.125022	-2.169084
H	-4.734445	4.187794	-0.660136
H	-4.039906	4.784682	-2.209844
C	0.127456	3.104539	-1.091065
H	0.129726	2.706138	-0.055895
H	0.463933	2.304337	-1.782110
H	0.878229	3.922584	-1.146472

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J SCF Done: -2039.69004171 A.U.

Number of imaginary frequencies = 0

C	-0.956296	0.007850	-1.005777
H	-1.328707	0.960259	-2.933804
N	-2.162472	0.455672	2.807489
C	-0.768338	-0.035699	2.679550
C	-0.496132	-0.473184	1.263468
N	-1.151383	0.252196	0.318889
C	-1.825911	0.788804	-1.956781

H	-0.538165	-0.850685	3.401207
H	-0.101291	0.828864	2.905955
H	-2.730474	0.169957	-2.149842
C	0.397192	-1.492327	0.906011
H	0.901555	-2.076679	1.690070
C	0.641210	-1.733192	-0.456951
H	1.346143	-2.520027	-0.766278
C	-0.037608	-0.969931	-1.419175
H	0.113565	-1.149863	-2.493721
Ru	-2.533172	1.675993	1.018958
C	-2.445825	1.058460	4.125886
H	-1.830113	1.977318	4.218702
H	-3.502816	1.399705	4.095520
C	-2.236986	0.139902	5.322555
C	-2.561292	-1.235041	5.265086
C	-1.751181	0.666891	6.537515
C	-2.409396	-2.053794	6.397667
C	-1.606589	-0.148984	7.672958
C	-1.936088	-1.514269	7.606807
H	-2.940567	-1.675684	4.328994
H	-1.484857	1.735655	6.594014
H	-2.668112	-3.122917	6.333331
H	-1.228749	0.283589	8.613212
H	-1.820276	-2.156831	8.494009
H	-1.239552	2.628698	1.572560
C	-3.744543	2.924526	1.624754
O	-4.536804	3.722252	1.993429
P	-2.483335	2.357801	-1.133256
O	-3.718203	-1.734680	2.080398
C	-4.505168	-1.499103	1.134690
C	-4.152032	-2.081133	-0.245719
H	-4.823538	-2.962013	-0.425769
H	-4.379658	-1.324084	-1.031625
O	-2.796702	-2.436985	-0.279938
H	-2.520567	-2.378186	0.668692
H	-2.805282	-0.351415	2.649047
N	-5.719277	-0.908489	1.261344
H	-6.165331	-0.692515	0.365647
C	-6.099254	0.009129	2.346595
H	-5.515978	0.952166	2.218583
H	-7.170019	0.250322	2.178774
C	-5.911277	-0.528006	3.769992
H	-4.835982	-0.525797	4.029828
H	-6.391410	0.205573	4.455748
C	-6.469858	-1.931922	4.025190
H	-7.545165	-1.978507	3.734316
H	-5.938143	-2.650150	3.362447
C	-6.301264	-2.372619	5.486095
H	-6.870924	-1.682825	6.151612
H	-5.233903	-2.249677	5.779836
C	-6.736138	-3.819453	5.758263

H	-7.806546	-3.943826	5.474781
H	-6.167870	-4.501611	5.085007
C	-6.531696	-4.245677	7.217537
H	-7.117747	-3.604011	7.910259
H	-6.842098	-5.297289	7.390588
H	-5.464253	-4.155848	7.514177
H	-3.704950	0.564858	0.558299
C	-1.159697	3.694816	-1.587788
C	-4.117911	2.692674	-2.103251
C	-5.198498	1.734831	-1.551224
H	-6.146125	1.904414	-2.109301
H	-4.913966	0.669753	-1.681383
H	-5.375418	1.898545	-0.471522
C	-1.123373	4.107516	-3.070070
H	-0.984937	3.239570	-3.748973
H	-2.034706	4.655219	-3.382684
H	-0.261875	4.791351	-3.237775
C	-3.995448	2.452578	-3.624077
H	-3.249290	3.106296	-4.109763
H	-3.737767	1.399850	-3.861531
H	-4.976847	2.660458	-4.105143
C	-1.399845	4.925658	-0.686812
H	-2.340335	5.456577	-0.930788
H	-1.437534	4.621943	0.379466
H	-0.564535	5.647800	-0.819626
C	-4.569859	4.141204	-1.819121
H	-5.591958	4.296161	-2.229319
H	-4.609554	4.351056	-0.730467
H	-3.908727	4.890291	-2.297971
C	0.206531	3.076900	-1.206551
H	0.195726	2.706731	-0.160359
H	0.501067	2.245669	-1.880266
H	0.992458	3.859157	-1.287541

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hydroxyacetamide SCF Done: -520.543001097 A.U.

Number of imaginary frequencies = 0

O	-2.210081	-1.371556	5.287048
C	-3.612169	-1.168315	5.148268
C	-4.056702	-1.345920	3.687946
O	-5.251868	-1.367694	3.393073
H	-1.928275	-1.018826	6.149466
H	-4.217250	-1.887915	5.750421
H	-3.933625	-0.141870	5.449992
N	-3.024540	-1.433167	2.797431
H	-2.083860	-1.474248	3.201639
C	-3.233083	-1.690636	1.382598
H	-4.268605	-1.364237	1.150728
H	-2.540236	-1.053705	0.788191
C	-3.055814	-3.169353	0.998322
H	-3.769803	-3.774806	1.599532

H	-2.035786	-3.508348	1.292764
C	-3.277016	-3.429602	-0.497599
H	-4.295811	-3.080443	-0.784261
H	-2.569055	-2.806181	-1.092362
C	-3.113546	-4.902804	-0.897267
H	-3.821125	-5.525559	-0.302187
H	-2.094611	-5.252338	-0.609228
C	-3.337400	-5.168707	-2.393559
H	-4.355716	-4.817348	-2.677485
H	-2.630132	-4.543168	-2.985085
C	-3.172224	-6.643394	-2.781211
H	-3.339402	-6.806321	-3.866296
H	-2.151519	-7.011226	-2.540268
H	-3.891744	-7.287091	-2.230798

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K SCF Done: -2038.48406087 A.U.

Number of imaginary frequencies = 0

C	-2.514881	-0.400324	-0.586321
H	-2.750739	1.172609	-2.078207
N	-2.123311	-0.587905	3.393870
C	-1.477529	-1.715986	2.714434
C	-1.814514	-1.735861	1.249034
N	-2.207484	-0.537896	0.736628
C	-3.016880	0.956104	-1.022908
H	-1.747540	-2.695225	3.177048
H	-0.358034	-1.650799	2.792296
H	-4.128336	0.944536	-0.969201
C	-1.707173	-2.867282	0.421863
H	-1.398854	-3.829417	0.856912
C	-1.991312	-2.741354	-0.944547
H	-1.905734	-3.611969	-1.613334
C	-2.399474	-1.494855	-1.455569
H	-2.642742	-1.371349	-2.521330
Ru	-2.277719	1.073090	2.122815
C	-1.649450	-0.440127	4.786138
H	-0.568511	-0.155580	4.803963
H	-2.230902	0.390166	5.230848
C	-1.855062	-1.698922	5.614378
C	-3.163396	-2.100764	5.967733
C	-0.767710	-2.510695	5.998390
C	-3.370251	-3.287870	6.688951
C	-0.973226	-3.698682	6.723570
C	-2.277999	-4.090834	7.069619
H	-4.011029	-1.467786	5.661541
H	0.256110	-2.203791	5.723586
H	-4.395166	-3.589313	6.960259
H	-0.111752	-4.319842	7.018689
H	-2.444169	-5.020894	7.637184
C	-0.809329	2.922456	-0.568275
C	-3.845631	3.636816	-0.031744

C	-5.061213	3.117133	0.765450
H	-5.900725	3.840417	0.671269
H	-5.426844	2.140317	0.383240
H	-4.830630	2.995164	1.842129
C	-4.282497	3.881999	-1.491284
H	-3.473558	4.287808	-2.124965
H	-4.671095	2.962342	-1.975235
H	-5.110794	4.624669	-1.501729
C	-3.364742	4.950475	0.619257
H	-4.214563	5.665299	0.678008
H	-2.994499	4.784597	1.652015
H	-2.564202	5.442706	0.031980
C	-0.954017	3.699129	-1.889576
H	0.056735	3.908524	-2.304283
H	-1.509306	3.125161	-2.660794
H	-1.455916	4.677208	-1.752238
C	-0.092458	3.795300	0.485358
H	-0.637678	4.733572	0.703243
H	0.034541	3.247092	1.440122
H	0.915590	4.074336	0.108074
C	0.047982	1.659959	-0.826431
H	0.133116	1.029138	0.081299
H	-0.353059	1.033105	-1.649352
H	1.072904	1.972622	-1.122435
H	-0.719187	1.281231	2.053522
C	-2.322693	2.500348	3.294861
O	-2.346129	3.446596	3.995056
P	-2.475611	2.302264	0.188982
O	-4.659341	-1.221409	3.160212
C	-5.172657	0.010246	2.835318
C	-5.360511	0.938632	4.059923
O	-4.664397	0.799569	5.066685
H	-3.651452	-1.033471	3.388608
H	-4.479073	0.625867	2.141878
H	-6.100678	-0.098258	2.230873
N	-6.249168	1.988128	3.945980
H	-6.289984	2.551153	4.803207
C	-7.393049	2.080308	3.043992
H	-7.665183	3.153889	2.945676
H	-7.085913	1.763023	2.027362
C	-8.613730	1.263040	3.498572
H	-8.914200	1.594443	4.518366
H	-8.307803	0.197516	3.603588
C	-9.803983	1.375686	2.537212
H	-10.092743	2.447053	2.426780
H	-9.488598	1.045448	1.519818
C	-11.029763	0.562090	2.976322
H	-11.346058	0.893176	3.992664
H	-10.739353	-0.508094	3.088954
C	-12.221576	0.667828	2.012974
H	-12.506676	1.739145	1.901385

H	-11.900805	0.336845	0.998584
C	-13.440339	-0.147930	2.461947
H	-14.285169	-0.053973	1.748380
H	-13.192305	-1.227705	2.548043
H	-13.803617	0.186104	3.457625

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TS-KL SCF Done: -2038.47724781 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -740.82 cm⁻¹

C	-2.760369	-0.328649	-0.569083
H	-2.934462	1.257631	-2.054866
N	-2.253517	-0.575916	3.392459
C	-1.664922	-1.721337	2.679586
C	-2.085266	-1.715963	1.234474
N	-2.405181	-0.491073	0.737613
C	-3.166728	1.064407	-0.987093
H	-1.938139	-2.691435	3.155926
H	-0.546977	-1.663775	2.707027
H	-4.271046	1.148389	-0.879218
C	-2.108227	-2.852454	0.408991
H	-1.858753	-3.836289	0.832822
C	-2.445410	-2.704232	-0.943773
H	-2.462259	-3.579121	-1.612187
C	-2.773298	-1.429294	-1.439499
H	-3.053618	-1.285689	-2.493558
Ru	-2.300267	1.106542	2.108916
C	-1.732591	-0.441163	4.773702
H	-0.643159	-0.208660	4.746887
H	-2.263727	0.422599	5.217475
C	-1.985200	-1.678733	5.617714
C	-3.311895	-2.031092	5.956533
C	-0.929207	-2.512819	6.038244
C	-3.566888	-3.193646	6.701399
C	-1.183802	-3.675492	6.788647
C	-2.505681	-4.018743	7.121096
H	-4.134955	-1.384718	5.611852
H	0.108048	-2.244400	5.774165
H	-4.604958	-3.458719	6.960076
H	-0.347152	-4.315297	7.113552
H	-2.709780	-4.929129	7.707785
C	-0.777327	2.833734	-0.630822
C	-3.716937	3.800820	0.042635
C	-4.939421	3.381204	0.888033
H	-5.722331	4.167843	0.818370
H	-5.393517	2.434679	0.525523
H	-4.684800	3.244188	1.956945
C	-4.192094	4.088893	-1.397473
H	-3.378521	4.424877	-2.065200
H	-4.680201	3.208707	-1.864224
H	-4.951716	4.901185	-1.371959

C	-3.098363	5.066892	0.671769
H	-3.881349	5.850620	0.767373
H	-2.698246	4.867904	1.687308
H	-2.285259	5.491262	0.049491
C	-0.909367	3.629101	-1.942367
H	0.097795	3.754114	-2.397671
H	-1.543077	3.110020	-2.691823
H	-1.319432	4.645605	-1.781017
C	0.054236	3.633154	0.396687
H	-0.396291	4.615249	0.637664
H	0.166756	3.068117	1.343469
H	1.068004	3.823420	-0.018506
C	-0.044754	1.503257	-0.927572
H	0.020618	0.863472	-0.024428
H	-0.532026	0.919614	-1.735676
H	0.990687	1.727695	-1.264110
H	-0.718506	1.124168	1.993212
C	-2.143202	2.525674	3.285474
O	-2.023522	3.460258	3.988865
P	-2.454832	2.356234	0.193865
O	-4.706574	-0.963694	3.198031
C	-5.082264	0.280545	2.857403
C	-5.293937	1.223267	4.072918
O	-4.574156	1.123347	5.068434
H	-3.525922	-0.838117	3.416648
H	-4.258684	0.893033	2.238345
H	-5.925110	0.310334	2.122408
N	-6.248048	2.215711	3.980865
H	-6.315950	2.762784	4.846881
C	-7.413081	2.233834	3.099801
H	-7.819332	3.268527	3.099092
H	-7.089621	2.043735	2.056077
C	-8.510427	1.231969	3.495910
H	-8.838952	1.446004	4.538144
H	-8.065028	0.211793	3.520872
C	-9.715901	1.254858	2.547579
H	-10.147559	2.282639	2.517311
H	-9.370311	1.045447	1.508142
C	-10.815790	0.252681	2.926104
H	-11.163060	0.462311	3.964411
H	-10.381703	-0.773326	2.958942
C	-12.021194	0.265824	1.974060
H	-12.450663	1.293489	1.942808
H	-11.669298	0.057549	0.937587
C	-13.112786	-0.739638	2.361335
H	-13.970443	-0.709207	1.657528
H	-12.719150	-1.778818	2.366038
H	-13.507073	-0.533251	3.379618

Number of imaginary frequencies = 0

C	-5.327648	2.601295	2.877676
H	-5.020955	3.008479	4.996111
N	-4.399607	-0.314290	0.236083
C	-4.394581	1.051220	-0.345196
C	-5.039289	2.036510	0.597235
N	-4.885294	1.744226	1.915269
C	-5.147568	2.149955	4.304846
H	-4.876192	1.083988	-1.347361
H	-3.326627	1.349588	-0.463151
H	-6.071132	1.611145	4.612805
C	-5.675098	3.215800	0.184285
H	-5.801626	3.421275	-0.889018
C	-6.125547	4.120779	1.159654
H	-6.618392	5.059688	0.863812
C	-5.942281	3.812631	2.518057
H	-6.285507	4.499919	3.305632
Ru	-3.908471	-0.068543	2.365587
C	-3.577794	-1.287897	-0.537309
H	-2.531413	-0.919227	-0.519127
H	-3.600504	-2.237881	0.029540
C	-4.079380	-1.506129	-1.951553
C	-5.106672	-2.442091	-2.202393
C	-3.582781	-0.740079	-3.028214
C	-5.634593	-2.597375	-3.494844
C	-4.107914	-0.894007	-4.323025
C	-5.139494	-1.820591	-4.557934
H	-5.494706	-3.069423	-1.384750
H	-2.769508	-0.017611	-2.847012
H	-6.434227	-3.334570	-3.669161
H	-3.707087	-0.290968	-5.153491
H	-5.551871	-1.943184	-5.572111
C	-2.188734	1.901103	4.781320
C	-4.289952	-0.128677	6.014304
C	-5.501127	-1.007818	5.636252
H	-5.802896	-1.605021	6.524322
H	-6.380270	-0.410737	5.317078
H	-5.261112	-1.697384	4.807878
C	-4.702263	0.760774	7.208123
H	-3.873449	1.370220	7.608381
H	-5.542219	1.440473	6.955945
H	-5.056286	0.106959	8.035298
C	-3.118416	-1.054551	6.406773
H	-3.453008	-1.756798	7.201390
H	-2.771574	-1.663554	5.546806
H	-2.252091	-0.492530	6.809444
C	-2.118436	2.540531	6.179759
H	-1.236777	3.217366	6.225441
H	-3.013030	3.155109	6.413758
H	-1.988738	1.788630	6.983110
C	-0.961033	0.993933	4.547335

H	-0.896326	0.167717	5.282074
H	-0.989194	0.552150	3.531065
H	-0.033506	1.599926	4.642614
C	-2.175001	3.026342	3.719547
H	-2.291726	2.610908	2.697313
H	-2.965800	3.785138	3.894312
H	-1.197888	3.554579	3.766165
H	-2.491068	0.641662	1.796257
C	-2.924481	-1.574777	2.752249
O	-2.256251	-2.515606	3.013901
P	-3.778826	0.854556	4.435657
O	-7.276337	-0.660178	0.206262
C	-7.800000	-1.759740	0.327350
C	-7.046748	-3.051161	0.648507
O	-7.432350	-4.075009	0.063038
H	-5.390917	-0.630204	0.228474
H	-5.448628	-0.692838	2.748991
H	-8.884117	-1.938122	0.077517
N	-5.981549	-2.925440	1.469931
H	-5.757126	-1.993528	1.921954
C	-5.139058	-4.052018	1.853000
H	-5.544950	-4.959710	1.360527
H	-4.110711	-3.888637	1.456418
C	-5.065113	-4.205163	3.377457
H	-4.803945	-3.214697	3.805467
H	-6.074598	-4.458512	3.771414
C	-4.024493	-5.226037	3.847877
H	-3.046015	-4.978441	3.379809
H	-4.297041	-6.246526	3.492093
C	-3.857006	-5.230060	5.373936
H	-3.590700	-4.199527	5.705784
H	-4.835677	-5.457878	5.857824
C	-2.794411	-6.214294	5.883088
H	-1.822538	-5.984435	5.390139
H	-3.061326	-7.244906	5.554615
C	-2.621656	-6.184359	7.406857
H	-1.846504	-6.900879	7.750334
H	-2.321238	-5.172778	7.756168
H	-3.570343	-6.442641	7.925394

26

oxoacetamide SCF Done: -519.324406671 A.U.

Number of imaginary frequencies = 0

O	-2.294945	-1.123816	5.407675
C	-3.463919	-1.016044	5.086215
C	-3.978130	-1.180660	3.643256
O	-5.181677	-1.093732	3.394353
H	-4.297252	-0.792735	5.814537
N	-2.974248	-1.412388	2.751246
H	-2.033389	-1.499774	3.152426
C	-3.202503	-1.681222	1.341297

H	-4.239196	-1.350052	1.122364
H	-2.515160	-1.052694	0.731678
C	-3.031041	-3.164407	0.971707
H	-3.735641	-3.766603	1.587054
H	-2.006719	-3.499734	1.254630
C	-3.271247	-3.436175	-0.519546
H	-4.293641	-3.089830	-0.796141
H	-2.570653	-2.817668	-1.127500
C	-3.111752	-4.913054	-0.907246
H	-3.811849	-5.530834	-0.298392
H	-2.089175	-5.259273	-0.628759
C	-3.353865	-5.191240	-2.398515
H	-4.375745	-4.842700	-2.672786
H	-2.654012	-4.570547	-3.003655
C	-3.192629	-6.669171	-2.775043
H	-3.373034	-6.840887	-3.856511
H	-2.168856	-7.034408	-2.543751
H	-3.905195	-7.308391	-2.210666

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M SCF Done: -2037.27422683 A.U.

Number of imaginary frequencies = 0

C	-1.908639	-0.533288	-1.034325
H	-2.594313	0.885418	-2.537876
N	-1.083091	-0.511821	2.853994
C	-0.254172	-1.473983	2.136627
C	-0.760359	-1.637609	0.721463
N	-1.450876	-0.567121	0.248029
C	-2.630248	0.726810	-1.440790
H	-0.230726	-2.471918	2.646371
H	0.824308	-1.156718	2.055759
H	-3.701353	0.632094	-1.154834
C	-0.524714	-2.756552	-0.094175
H	0.025476	-3.619064	0.310221
C	-0.996454	-2.748165	-1.415461
H	-0.833062	-3.617802	-2.070317
C	-1.691576	-1.623323	-1.893463
H	-2.072213	-1.588383	-2.924696
Ru	-1.479018	1.163837	1.552480
C	-0.664789	-0.355911	4.250273
H	-0.362165	-1.353423	4.658934
H	0.229862	0.309066	4.354733
C	-1.813791	0.173244	5.088703
C	-1.934007	1.542195	5.394068
C	-2.849303	-0.698784	5.488139
C	-3.075880	2.038176	6.049728
C	-3.992149	-0.211476	6.144796
C	-4.111907	1.165163	6.420079
H	-1.131317	2.234620	5.100615
H	-2.769729	-1.772558	5.256003
H	-3.155863	3.115807	6.263641

H	-4.796110	-0.906529	6.435174
H	-5.010446	1.551459	6.927263
C	-0.455391	2.794604	-1.465005
C	-3.424795	3.472170	-0.607154
C	-4.502596	3.026032	0.404206
H	-5.377822	3.707180	0.323652
H	-4.867790	1.995363	0.212010
H	-4.130609	3.053277	1.445320
C	-4.062881	3.533002	-2.011360
H	-3.359286	3.851904	-2.801029
H	-4.505542	2.561431	-2.312490
H	-4.894704	4.271314	-1.995237
C	-2.907229	4.862669	-0.181981
H	-3.768519	5.559004	-0.084505
H	-2.394424	4.826037	0.801453
H	-2.213210	5.303203	-0.925239
C	-0.805707	3.465481	-2.806462
H	0.133563	3.679501	-3.362525
H	-1.426468	2.814078	-3.456651
H	-1.330937	4.431560	-2.674286
C	0.365020	3.762964	-0.583879
H	-0.192275	4.682649	-0.322829
H	0.676546	3.276273	0.361099
H	1.281117	4.070783	-1.133636
C	0.411613	1.546458	-1.755377
H	0.639817	0.979183	-0.830759
H	-0.065073	0.856579	-2.481265
H	1.376061	1.874494	-2.200498
H	0.053599	1.256401	1.197372
C	-1.224344	2.728398	2.483232
O	-1.011159	3.770751	2.993788
P	-1.986883	2.202500	-0.443687
O	-3.769553	1.103017	2.650896
C	-4.612398	0.336539	3.108481
H	-5.474725	0.720078	3.715741
C	-4.718921	-1.148046	2.778823
O	-5.857704	-1.640568	2.716644
N	-3.548947	-1.766720	2.520212
H	-2.618746	-1.231992	2.680141
C	-3.529566	-3.149276	2.071530
H	-2.492450	-3.528000	2.193412
H	-4.190717	-3.764263	2.723996
C	-3.976453	-3.296298	0.606584
H	-3.453799	-2.523331	0.004554
H	-5.060661	-3.059688	0.549867
C	-3.689426	-4.679007	0.014166
H	-2.599012	-4.895068	0.109379
H	-4.206081	-5.465818	0.610729
C	-4.095615	-4.801191	-1.460654
H	-3.612159	-3.978433	-2.037794
H	-5.191843	-4.626006	-1.557658

C	-3.731082	-6.149216	-2.098837
H	-2.633236	-6.314073	-1.997116
H	-4.209282	-6.970502	-1.517908
C	-4.135226	-6.254592	-3.574556
H	-3.644358	-5.464884	-4.183931
H	-3.856575	-7.236096	-4.011490
H	-5.232255	-6.130689	-3.700633

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N SCF Done: -2329.87294870 A.U.

Number of imaginary frequencies = 0

C	-0.842256	0.357359	-1.143829
H	-1.209675	2.157499	-2.328813
N	-1.792105	-1.004765	2.560492
C	-0.537869	-1.567539	2.004605
C	-0.348985	-1.224592	0.546239
N	-0.906254	-0.054446	0.150066
C	-1.675507	1.559971	-1.518260
H	-0.465036	-2.666832	2.161451
H	0.306575	-1.109608	2.570089
H	-2.643947	1.173224	-1.905180
C	0.379857	-2.016716	-0.354368
H	0.821347	-2.966531	-0.017671
C	0.529327	-1.571862	-1.678552
H	1.108742	-2.165913	-2.402326
C	-0.093091	-0.378654	-2.079676
H	-0.027466	-0.027732	-3.120368
Ru	-2.187040	0.878821	1.535315
C	-1.765417	-0.956840	4.040290
H	-0.994870	-0.220180	4.349456
H	-2.741389	-0.537818	4.359224
C	-1.531246	-2.298244	4.715874
C	-2.228540	-3.452129	4.292085
C	-0.629878	-2.412991	5.793859
C	-2.031663	-4.685482	4.934475
C	-0.435788	-3.644902	6.443709
C	-1.136320	-4.785744	6.015167
H	-2.929895	-3.376909	3.445940
H	-0.073929	-1.521836	6.130230
H	-2.584640	-5.574620	4.591369
H	0.270724	-3.714425	7.286283
H	-0.983563	-5.752500	6.520653
C	-0.754427	3.855289	0.176611
C	-3.805586	3.408330	-0.545255
C	-4.931509	2.361576	-0.385771
H	-5.886127	2.806881	-0.741557
H	-4.746113	1.431981	-0.957384
H	-5.061812	2.064497	0.672290
C	-3.784211	3.891466	-2.011639
H	-2.991406	4.633733	-2.218377
H	-3.667896	3.050840	-2.725889

H	-4.758203	4.375353	-2.244615
C	-4.102262	4.586478	0.406911
H	-5.128856	4.963773	0.207298
H	-4.065972	4.271752	1.470308
H	-3.406730	5.437505	0.264704
C	-0.733078	4.921860	-0.933953
H	0.168974	5.560762	-0.809603
H	-0.677310	4.475339	-1.949051
H	-1.613675	5.592867	-0.895409
C	-0.869650	4.523650	1.564298
H	-1.768440	5.162594	1.656464
H	-0.905179	3.758777	2.366190
H	0.018493	5.170800	1.734654
C	0.570673	3.058029	0.128759
H	0.576361	2.241836	0.879164
H	0.768219	2.620657	-0.872009
H	1.414141	3.745064	0.357860
H	-0.958784	1.526477	2.367553
C	-3.313912	1.699934	2.736698
O	-4.029345	2.243250	3.502718
P	-2.170829	2.557893	0.003837
O	-3.508378	-0.349283	0.281437
C	-4.648512	-0.902992	0.777580
C	-5.569798	-1.402687	-0.381936
O	-6.685140	-1.905731	-0.200334
H	-2.654009	-1.546911	2.242454
N	-4.356249	-2.066536	1.700331
H	-4.200198	-2.890612	1.101667
C	-5.440257	-2.369650	2.664334
H	-6.435308	-2.302564	2.168290
H	-5.325973	-3.426114	2.995274
C	-5.384601	-1.447107	3.887858
H	-4.473174	-1.684260	4.479187
H	-5.265615	-0.392931	3.551626
C	-6.616907	-1.553692	4.793829
H	-7.527722	-1.288919	4.209233
H	-6.759844	-2.614056	5.108443
C	-6.527455	-0.659372	6.038315
H	-6.363359	0.395753	5.718859
H	-5.620254	-0.936320	6.624815
C	-7.761965	-0.731659	6.949062
H	-8.665707	-0.452776	6.360276
H	-7.924321	-1.788769	7.261986
C	-7.655951	0.164749	8.189221
H	-7.526387	1.230978	7.903890
H	-8.560774	0.095892	8.828743
H	-6.780827	-0.115660	8.814498
H	-5.275243	-0.195877	1.384323
N	-4.972091	-1.233232	-1.597146
H	-4.019492	-0.842685	-1.489723
C	-5.513927	-1.717607	-2.847098

H	-6.579193	-1.969135	-2.653099
H	-5.499453	-0.903412	-3.608499
C	-4.771907	-2.950497	-3.391375
H	-3.690847	-2.705326	-3.510863
H	-4.821327	-3.757634	-2.626585
C	-5.338216	-3.455164	-4.724890
H	-5.299442	-2.634198	-5.478661
H	-6.419752	-3.691964	-4.598005
C	-4.609320	-4.687031	-5.280095
H	-4.649410	-5.508459	-4.527388
H	-3.526546	-4.450297	-5.404534
C	-5.174581	-5.193904	-6.615478
H	-5.134928	-4.370020	-7.364534
H	-6.256004	-5.428373	-6.487252
C	-4.439535	-6.424721	-7.160778
H	-4.868765	-6.768852	-8.124778
H	-3.362808	-6.208140	-7.331692
H	-4.494208	-7.274959	-6.447171

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O SCF Done: -2329.87033381 A.U.

Number of imaginary frequencies = 0

C	-1.531847	-0.226718	-1.564370
H	-2.117159	0.974055	-3.288306
N	-2.338570	-0.341263	2.406747
C	-1.048016	-0.966741	2.040604
C	-0.890262	-1.102947	0.546656
N	-1.633095	-0.246408	-0.202719
C	-2.490510	0.675327	-2.288422
H	-0.917506	-1.957072	2.532626
H	-0.218170	-0.318750	2.409714
H	-3.423533	0.073250	-2.415794
C	0.021156	-1.983627	-0.058041
H	0.605827	-2.676360	0.564994
C	0.177155	-1.945053	-1.451220
H	0.888579	-2.619911	-1.950551
C	-0.605858	-1.061115	-2.211358
H	-0.524071	-1.031916	-3.307531
Ru	-2.883496	1.126398	0.864205
C	-2.373918	0.050497	3.834754
H	-1.646329	0.872878	4.005968
H	-3.380666	0.481420	4.019158
C	-2.124833	-1.087497	4.813684
C	-2.758172	-2.340700	4.642813
C	-1.285755	-0.897096	5.930307
C	-2.545087	-3.374003	5.569546
C	-1.085839	-1.927382	6.866765
C	-1.713832	-3.171687	6.686656
H	-3.428075	-2.498264	3.781295
H	-0.784705	0.075470	6.071485
H	-3.046611	-4.344256	5.425415

H	-0.432530	-1.757683	7.737612
H	-1.558457	-3.981842	7.416658
H	-1.634541	2.029017	1.228235
C	-3.919038	2.356789	1.766470
O	-4.572142	3.162763	2.323226
P	-3.011159	2.121104	-1.203829
O	-4.157478	-2.012098	1.757714
C	-4.796800	-1.378985	0.750674
C	-4.540538	-2.078541	-0.626093
O	-4.586775	-1.520728	-1.735692
H	-3.143621	-1.117599	2.200258
N	-6.244150	-1.178669	0.883598
H	-6.640058	-2.080667	1.180022
C	-6.706050	-0.098217	1.759548
H	-6.460062	0.868299	1.268987
H	-7.817908	-0.150664	1.778641
C	-6.169356	-0.050093	3.202807
H	-5.077249	0.145963	3.161796
H	-6.616080	0.837341	3.707298
C	-6.412636	-1.313464	4.032703
H	-7.500469	-1.561858	4.039501
H	-5.893905	-2.157464	3.526713
C	-5.900140	-1.191008	5.474061
H	-6.451296	-0.379392	6.004208
H	-4.836522	-0.862654	5.452261
C	-5.987988	-2.488440	6.288154
H	-7.052971	-2.806577	6.368094
H	-5.472830	-3.298244	5.723297
C	-5.364870	-2.365377	7.683637
H	-5.861579	-1.568744	8.278886
H	-5.443184	-3.312193	8.258548
H	-4.286828	-2.106034	7.609981
H	-4.410263	-0.291332	0.539895
C	-1.666050	3.461337	-1.541706
C	-4.699659	2.638409	-1.953256
C	-5.741877	1.652683	-1.381695
H	-6.730133	1.864417	-1.845081
H	-5.494373	0.587859	-1.569816
H	-5.850577	1.781611	-0.288027
C	-1.736767	4.072117	-2.954347
H	-1.677322	3.301277	-3.750877
H	-2.655804	4.669180	-3.114004
H	-0.872945	4.757776	-3.099029
C	-4.731547	2.552873	-3.494656
H	-3.988039	3.205057	-3.989291
H	-4.583667	1.514323	-3.852976
H	-5.736545	2.872856	-3.846975
C	-1.792182	4.569642	-0.473155
H	-2.742761	5.130538	-0.550359
H	-1.727551	4.147545	0.549581
H	-0.962650	5.298962	-0.600802

C	-5.054062	4.062348	-1.476303
H	-6.108109	4.282786	-1.752247
H	-4.974710	4.156143	-0.373307
H	-4.422578	4.843553	-1.944980
C	-0.292239	2.769901	-1.373649
H	-0.205021	2.261026	-0.392520
H	-0.091495	2.025778	-2.171375
H	0.508600	3.538698	-1.432122
N	-4.276943	-3.398921	-0.451555
H	-4.084300	-3.622228	0.538069
C	-3.933786	-4.289290	-1.544503
H	-4.129900	-5.336420	-1.227313
H	-4.617041	-4.064040	-2.392251
C	-2.480084	-4.119978	-2.011960
H	-2.350392	-3.057158	-2.305590
H	-1.795391	-4.285540	-1.149346
C	-2.090581	-5.034373	-3.178075
H	-2.794402	-4.871508	-4.026814
H	-2.219921	-6.101530	-2.881819
C	-0.651498	-4.813748	-3.666012
H	-0.528332	-3.746568	-3.965281
H	0.052295	-4.967325	-2.814311
C	-0.236752	-5.718851	-4.834978
H	-0.942967	-5.565229	-5.682532
H	-0.360056	-6.783827	-4.532682
C	1.201910	-5.477861	-5.308780
H	1.343201	-4.429387	-5.649966
H	1.931456	-5.658703	-4.489865
H	1.476449	-6.143392	-6.153370

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TS-OP SCF Done: -2329.86381614 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -281.36 cm⁻¹

C	-2.077149	-1.169864	-0.984433
H	-2.812966	-0.166018	-2.775425
N	-1.884326	-0.410213	2.955641
C	-0.820222	-1.332119	2.494836
C	-1.098251	-1.794643	1.084836
N	-1.790051	-0.908701	0.322356
C	-2.975912	-0.178589	-1.678384
H	-0.698932	-2.201896	3.178987
H	0.145034	-0.774077	2.491651
H	-4.027899	-0.503404	-1.498198
C	-0.642421	-3.006618	0.544142
H	-0.099218	-3.719971	1.181542
C	-0.868316	-3.268118	-0.817870
H	-0.497510	-4.198324	-1.275398
C	-1.585785	-2.339146	-1.589599
H	-1.793796	-2.529796	-2.652390
Ru	-2.441868	0.840655	1.285354

C	-1.589111	0.219799	4.264898
H	-0.715606	0.894410	4.145778
H	-2.462416	0.862145	4.501106
C	-1.357652	-0.783394	5.382684
C	-2.351186	-1.743397	5.686017
C	-0.155070	-0.790291	6.117658
C	-2.138982	-2.683466	6.707443
C	0.054615	-1.728019	7.145183
C	-0.937897	-2.677662	7.441957
H	-3.286183	-1.761220	5.100221
H	0.627050	-0.048839	5.882660
H	-2.920150	-3.426784	6.934367
H	0.998684	-1.717954	7.713309
H	-0.775970	-3.414735	8.244744
H	-0.922234	1.437562	1.263215
C	-2.966926	2.414377	2.095176
O	-3.285399	3.444531	2.576888
P	-2.860662	1.513657	-0.850655
O	-4.110309	-1.775312	2.882068
C	-4.816579	-1.157971	1.983875
C	-5.067633	-1.910942	0.640650
O	-5.814170	-1.468781	-0.248031
H	-2.785788	-0.999873	3.048065
N	-5.937684	-0.406302	2.372512
H	-6.432822	-0.041815	1.548934
C	-5.707571	0.581246	3.413892
H	-5.508353	0.055046	4.372654
H	-4.768497	1.148663	3.171997
C	-6.866003	1.567533	3.559410
H	-7.088422	2.012299	2.561050
H	-7.788464	1.027345	3.870012
C	-6.545860	2.697882	4.547040
H	-6.304181	2.260237	5.543372
H	-5.620050	3.218198	4.210725
C	-7.679528	3.720577	4.701687
H	-8.608351	3.199561	5.032496
H	-7.920611	4.154612	3.703177
C	-7.356536	4.857452	5.682856
H	-7.116599	4.421230	6.679592
H	-6.425804	5.370806	5.349970
C	-8.490521	5.880272	5.825280
H	-9.424041	5.399064	6.189235
H	-8.230365	6.689285	6.539462
H	-8.726358	6.357728	4.849687
H	-3.979527	-0.121649	1.374027
C	-1.393853	2.364488	-1.776808
C	-4.522438	2.366438	-1.306961
C	-5.578629	1.845600	-0.307234
H	-6.559622	2.310692	-0.550224
H	-5.702443	0.745048	-0.361016
H	-5.316220	2.115276	0.734296

C	-1.700320	2.735193	-3.240007
H	-2.030701	1.859415	-3.837331
H	-2.470315	3.526603	-3.327035
H	-0.775887	3.126150	-3.719735
C	-4.998905	2.040969	-2.738916
H	-4.285814	2.360920	-3.521042
H	-5.201935	0.958863	-2.870329
H	-5.957333	2.572153	-2.929121
C	-0.969489	3.616258	-0.977698
H	-1.740726	4.409571	-0.982446
H	-0.751337	3.352857	0.077130
H	-0.047662	4.044562	-1.428691
C	-4.380399	3.890794	-1.110104
H	-5.383431	4.361018	-1.204665
H	-3.992471	4.138553	-0.100449
H	-3.724956	4.364053	-1.867813
C	-0.218400	1.358784	-1.757406
H	0.000278	1.012615	-0.726825
H	-0.405230	0.472640	-2.398169
H	0.692201	1.860619	-2.151010
N	-4.336509	-3.049006	0.609151
H	-3.861400	-3.188143	1.518065
C	-4.321187	-4.107321	-0.389588
H	-3.289111	-4.524603	-0.399301
H	-4.989671	-4.942017	-0.067047
C	-4.697986	-3.679147	-1.813647
H	-4.160750	-2.743382	-2.068514
H	-5.773108	-3.412914	-1.857094
C	-4.356660	-4.761774	-2.844228
H	-3.266984	-4.996967	-2.786848
H	-4.879930	-5.711429	-2.584784
C	-4.711578	-4.359428	-4.282149
H	-4.189450	-3.406336	-4.534405
H	-5.799114	-4.123563	-4.339657
C	-4.362468	-5.423531	-5.333041
H	-3.274948	-5.658080	-5.268299
H	-4.887465	-6.372491	-5.078426
C	-4.717097	-5.003811	-6.764974
H	-4.179128	-4.076361	-7.057773
H	-4.454829	-5.790200	-7.502908
H	-5.804416	-4.798143	-6.865992

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P SCF Done: -2329.87624854 A.U.

Number of imaginary frequencies = 0

C	-1.069674	0.052743	-1.188524
H	-1.606109	1.079386	-3.035939
N	-2.164452	0.155298	2.683888
C	-0.783751	-0.343652	2.475765
C	-0.524714	-0.620204	1.016689
N	-1.242582	0.155384	0.161254

C	-2.022589	0.854856	-2.032850
H	-0.558762	-1.237576	3.100209
H	-0.094822	0.475219	2.789461
H	-2.939587	0.235328	-2.174496
C	0.436444	-1.525511	0.543397
H	0.999594	-2.146592	1.256049
C	0.681666	-1.595352	-0.839368
H	1.446995	-2.279205	-1.237372
C	-0.080105	-0.798177	-1.710480
H	0.073911	-0.844604	-2.798744
Ru	-2.596451	1.508843	1.017159
C	-2.382532	0.653597	4.060916
H	-1.722292	1.532337	4.213371
H	-3.422778	1.039943	4.095046
C	-2.179764	-0.384587	5.154625
C	-2.705376	-1.690694	5.021876
C	-1.491146	-0.049924	6.338990
C	-2.543904	-2.632258	6.052345
C	-1.340328	-0.987874	7.375641
C	-1.866571	-2.284073	7.234777
H	-3.253445	-1.973874	4.109141
H	-1.070582	0.963373	6.451606
H	-2.965161	-3.643172	5.934162
H	-0.804153	-0.705678	8.295868
H	-1.748130	-3.022146	8.043912
H	-1.290753	2.430167	1.589725
C	-3.790541	2.695106	1.770239
O	-4.573358	3.446947	2.237754
P	-2.634535	2.368489	-1.077596
O	-3.939656	-1.836728	1.941231
C	-4.645425	-1.488190	0.963219
C	-4.224982	-1.880559	-0.474903
O	-4.882660	-1.565433	-1.479172
H	-2.833376	-0.627955	2.490773
N	-5.881092	-0.938744	0.987702
H	-6.210044	-0.777180	0.024360
C	-6.414795	-0.013939	1.989860
H	-6.035559	1.006709	1.743286
H	-7.518486	-0.002680	1.857715
C	-6.069077	-0.314998	3.449127
H	-4.983052	-0.158217	3.601182
H	-6.576643	0.465935	4.058717
C	-6.442599	-1.708931	3.964794
H	-7.503360	-1.943391	3.716291
H	-5.821444	-2.456783	3.424936
C	-6.213456	-1.844593	5.478219
H	-6.964912	-1.231735	6.028305
H	-5.224099	-1.403653	5.735941
C	-6.249842	-3.289561	5.993528
H	-7.234618	-3.750090	5.749356
H	-5.494391	-3.886791	5.432316

C	-5.975900	-3.397809	7.498641
H	-6.731651	-2.834334	8.087198
H	-5.994572	-4.450913	7.849771
H	-4.979710	-2.973484	7.749444
H	-3.802346	0.456005	0.508151
C	-1.309947	3.723138	-1.475190
C	-4.295210	2.789931	-1.956698
C	-5.374026	1.823242	-1.418437
H	-6.332067	2.039140	-1.941907
H	-5.124036	0.757983	-1.595565
H	-5.528908	1.957211	-0.331441
C	-1.322833	4.245024	-2.923380
H	-1.208463	3.429042	-3.667916
H	-2.243004	4.812816	-3.165338
H	-0.465824	4.939658	-3.068545
C	-4.229671	2.629276	-3.491779
H	-3.471560	3.275548	-3.969876
H	-4.032030	1.579523	-3.789812
H	-5.216667	2.904138	-3.924793
C	-1.505143	4.885278	-0.476819
H	-2.450788	5.436557	-0.642268
H	-1.501034	4.504728	0.565194
H	-0.670744	5.611802	-0.590518
C	-4.702622	4.229827	-1.577466
H	-5.736098	4.423621	-1.939301
H	-4.701108	4.377384	-0.477679
H	-4.045992	4.994868	-2.037120
C	0.065238	3.073082	-1.193955
H	0.091630	2.620510	-0.180933
H	0.330396	2.298977	-1.943457
H	0.852351	3.857026	-1.240495
N	-3.089011	-2.612635	-0.494496
H	-2.647111	-2.764344	0.420012
C	-2.515281	-3.153097	-1.714570
H	-2.041412	-2.334053	-2.302319
H	-3.341630	-3.543040	-2.348614
C	-1.479913	-4.236709	-1.409001
H	-0.772342	-3.847092	-0.642903
H	-1.983605	-5.116446	-0.949254
C	-0.684039	-4.665932	-2.646929
H	-0.204541	-3.766089	-3.098226
H	-1.380265	-5.056124	-3.424313
C	0.394242	-5.715890	-2.347120
H	1.085144	-5.317968	-1.566974
H	-0.081011	-6.615221	-1.891462
C	1.208342	-6.138213	-3.579134
H	1.677295	-5.235174	-4.033226
H	0.514828	-6.535734	-4.354869
C	2.288710	-7.180914	-3.266599
H	2.860486	-7.466576	-4.173760
H	3.015885	-6.796294	-2.519313

H 1.843610 -8.107788 -2.845200

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oxalamide SCF Done: -810.726579095 A.U.

Number of imaginary frequencies = 0

O	-2.239535	0.650177	-1.494117
C	-3.117597	0.540487	-2.358017
C	-2.959882	1.142870	-3.781380
O	-3.855022	1.070049	-4.631547
N	-1.745889	1.726379	-3.938477
H	-1.157215	1.718252	-3.095916
C	-1.345232	2.440526	-5.137168
H	-0.331504	2.100138	-5.446653
H	-2.055166	2.140231	-5.936352
C	-1.359068	3.968780	-4.964401
H	-2.383961	4.281747	-4.665261
H	-0.689910	4.250732	-4.119281
C	-0.931279	4.715143	-6.235128
H	0.090315	4.383751	-6.534549
H	-1.599778	4.421109	-7.076947
C	-0.945013	6.242913	-6.084347
H	-1.966273	6.573677	-5.783961
H	-0.276842	6.536384	-5.241430
C	-0.520453	6.994864	-7.354755
H	0.499623	6.660405	-7.652861
H	-1.189400	6.697775	-8.194569
C	-0.538414	8.519954	-7.193527
H	-0.227942	9.036854	-8.125279
H	-1.554529	8.884921	-6.930314
H	0.148467	8.847461	-6.383589
N	-4.306753	-0.096756	-2.221041
H	-4.917834	-0.039772	-3.045578
C	-4.764661	-0.688012	-0.976809
H	-5.145492	-1.714998	-1.175776
H	-3.870988	-0.785291	-0.325075
C	-5.845527	0.148253	-0.271157
H	-6.709849	0.290711	-0.959745
H	-5.435403	1.163746	-0.075173
C	-6.327224	-0.486552	1.040258
H	-6.722219	-1.508790	0.834969
H	-5.456040	-0.633411	1.719574
C	-7.402660	0.337064	1.762805
H	-7.007561	1.359134	1.967446
H	-8.273225	0.484936	1.082118
C	-7.886816	-0.293246	3.077319
H	-7.014063	-0.440500	3.753825
H	-8.278988	-1.315064	2.869086
C	-8.960420	0.537525	3.791047
H	-8.582980	1.551952	4.042937
H	-9.858614	0.670781	3.150304
H	-9.291344	0.059175	4.736250

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A-PCH3 SCF Done: -1281.95436156 A.U.

Number of imaginary frequencies = 0

C	-0.537425	-0.108444	-0.633543
H	0.372312	1.660926	-1.432245
N	-0.814353	0.249204	3.323088
C	-0.511124	-1.113782	2.929747
C	-0.429519	-1.266153	1.435949
N	-0.538439	-0.103596	0.736103
C	-0.651336	1.244637	-1.291704
H	-1.278952	-1.834368	3.314488
H	0.459998	-1.466725	3.372726
H	-1.128919	1.183428	-2.292018
C	-0.289997	-2.497519	0.773320
H	-0.202974	-3.423158	1.362075
C	-0.287556	-2.522592	-0.628097
H	-0.192759	-3.476734	-1.169168
C	-0.420584	-1.313731	-1.338631
H	-0.428488	-1.301905	-2.438713
Ru	-0.834999	1.638453	1.887648
C	-1.039478	0.369275	4.760064
H	-0.210049	-0.107814	5.341642
H	-1.033021	1.445825	5.024083
C	-2.366635	-0.250696	5.191709
C	-3.567754	0.206389	4.606209
C	-2.428038	-1.291850	6.138344
C	-4.800463	-0.357151	4.969714
C	-3.662332	-1.862731	6.503754
C	-4.851881	-1.395773	5.920379
H	-3.515137	1.006243	3.848529
H	-1.494178	-1.660203	6.596449
H	-5.730712	0.015231	4.510617
H	-3.692612	-2.677972	7.244757
H	-5.819552	-1.840222	6.203654
H	0.505406	2.346562	1.393469
C	-1.217013	3.159078	2.871811
O	-1.465038	4.152068	3.453665
P	-1.492539	2.454328	-0.115322
C	-1.011377	4.100594	-0.805655
H	-1.516083	4.886743	-0.208289
H	0.082585	4.228424	-0.687451
H	-1.297087	4.211000	-1.872330
C	-3.282479	2.349749	-0.595611
H	-3.450332	2.600473	-1.664646
H	-3.638525	1.320486	-0.389353
H	-3.859503	3.047603	0.044516

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TS-EF-PCH3 SCF Done: -1283.11235866 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -931.12 cm⁻¹

C	-0.568213	0.170474	-0.679704
H	-0.680582	1.458412	-2.438280
N	-1.306615	0.539339	3.263737
C	-0.222841	-0.380669	2.968105
C	-0.146264	-0.687453	1.492016
N	-0.618768	0.291280	0.676210
C	-1.212192	1.280053	-1.479724
H	-2.478624	0.759780	2.411192
H	-0.299716	-1.333060	3.548226
H	0.773285	0.072854	3.246963
H	-2.249781	0.968924	-1.738284
C	0.417405	-1.856029	0.953017
H	0.784764	-2.642985	1.628249
C	0.512062	-1.987978	-0.440734
H	0.963723	-2.888529	-0.885296
C	0.016132	-0.964446	-1.266543
H	0.064309	-1.046668	-2.362575
Ru	-1.375347	2.015298	1.655531
C	-1.342899	0.970318	4.650049
H	-0.403999	1.514292	4.936510
H	-2.164835	1.713763	4.750290
C	-1.585812	-0.166556	5.640200
C	-2.532872	-1.171962	5.347809
C	-0.887725	-0.233949	6.862658
C	-2.781457	-2.212299	6.257835
C	-1.137502	-1.270444	7.780295
C	-2.085769	-2.263971	7.480456
H	-3.063881	-1.129367	4.382603
H	-0.135869	0.538673	7.097031
H	-3.524465	-2.989040	6.013659
H	-0.582853	-1.305794	8.732007
H	-2.279860	-3.079495	8.195516
H	0.172016	2.512834	1.790974
C	-1.846531	3.579053	2.529155
O	-2.101660	4.593077	3.064342
P	-1.393457	2.850110	-0.445523
H	-3.031860	1.207345	1.699622
C	0.001723	3.914248	-1.032387
H	-0.029684	4.870693	-0.472242
H	0.952762	3.404723	-0.781000
H	-0.048516	4.117902	-2.122613
C	-2.859393	3.671097	-1.217791
H	-2.738420	3.806373	-2.313085
H	-3.759842	3.061140	-1.005802
H	-2.994398	4.662572	-0.739946

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A-PiPr SCF Done: -1439.26462664 A.U.

Number of imaginary frequencies = 0

C	-0.622003	-0.013579	-0.739321
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H	-0.587863	1.468004	-2.344337
N	-0.924325	0.251918	3.216892
C	-0.525582	-1.076551	2.802513
C	-0.370813	-1.182653	1.309877
N	-0.600049	-0.024988	0.628743
C	-1.119024	1.253983	-1.393703
H	-1.264533	-1.856056	3.126776
H	0.442629	-1.384155	3.283740
H	-2.183758	1.085379	-1.667090
C	-0.047902	-2.369105	0.629871
H	0.146902	-3.287684	1.203849
C	0.014393	-2.357220	-0.770160
H	0.276280	-3.270883	-1.325758
C	-0.295635	-1.168983	-1.461634
H	-0.305034	-1.141061	-2.561541
Ru	-0.853054	1.691190	1.825961
C	-1.191210	0.336660	4.646519
H	-0.374801	-0.141938	5.245997
H	-1.211888	1.407195	4.934413
C	-2.523372	-0.311689	5.017592
C	-3.712299	0.161543	4.420315
C	-2.600629	-1.396055	5.912848
C	-4.949258	-0.427627	4.722714
C	-3.839152	-1.994321	6.215821
C	-5.016543	-1.510520	5.621995
H	-3.646930	0.996025	3.701674
H	-1.676291	-1.776460	6.380346
H	-5.870048	-0.041829	4.255735
H	-3.882011	-2.843908	6.916551
H	-5.987257	-1.976123	5.856682
H	0.637215	2.182180	1.688495
C	-1.173894	3.205658	2.832916
O	-1.384405	4.202383	3.426978
P	-1.088452	2.717740	-0.201693
C	-2.643786	3.724143	-0.629814
H	-2.306207	4.774810	-0.476206
C	0.341304	3.782718	-0.856622
H	0.443731	4.536258	-0.041866
C	1.630249	2.943799	-0.901387
H	2.509664	3.596849	-1.085225
H	1.797456	2.397735	0.049243
H	1.599227	2.196953	-1.724245
C	0.117499	4.514815	-2.188448
H	1.014232	5.121031	-2.442019
H	-0.033685	3.801834	-3.028043
H	-0.747298	5.207262	-2.163009
C	-3.155134	3.568325	-2.074047
H	-2.364744	3.681216	-2.840583
H	-3.629736	2.574848	-2.222461
H	-3.938269	4.327827	-2.285068
C	-3.766252	3.423246	0.378504

H	-4.053669	2.350020	0.347612
H	-3.462805	3.651637	1.418196
H	-4.669223	4.024635	0.136027

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TS-EF-PiPr SCF Done: -1440.42732225 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -927.70 cm⁻¹

C	-0.468520	0.100507	-0.677149
H	-0.665715	1.261977	-2.513121
N	-1.343315	0.557825	3.222314
C	-0.204283	-0.314808	2.995196
C	-0.061512	-0.663391	1.533085
N	-0.554413	0.264991	0.672535
C	-1.153908	1.146411	-1.524674
H	-2.487699	0.702566	2.322111
H	-0.254740	-1.251429	3.603135
H	0.756706	0.198295	3.293180
H	-2.196279	0.805125	-1.717607
C	0.573720	-1.819123	1.048400
H	0.959648	-2.565475	1.758495
C	0.713596	-1.989977	-0.337440
H	1.222119	-2.880025	-0.739786
C	0.187233	-1.021735	-1.210349
H	0.265668	-1.139092	-2.301406
Ru	-1.409875	1.985451	1.571944
C	-1.452895	1.029140	4.591307
H	-0.553563	1.628894	4.893116
H	-2.313808	1.732867	4.636573
C	-1.676029	-0.086974	5.609379
C	-2.561133	-1.147459	5.317416
C	-1.020216	-0.081290	6.856832
C	-2.790743	-2.170471	6.251748
C	-1.251495	-1.100237	7.798648
C	-2.137965	-2.149252	7.498713
H	-3.058321	-1.161440	4.333515
H	-0.316302	0.735152	7.091620
H	-3.485091	-2.990988	6.007484
H	-0.730539	-1.078167	8.769617
H	-2.317161	-2.951191	8.232786
H	0.108320	2.545390	1.769741
C	-1.978037	3.562569	2.353007
O	-2.294756	4.596006	2.816952
P	-1.347945	2.759395	-0.567246
H	-3.030254	1.100823	1.575205
C	0.166491	3.801405	-1.012933
H	0.909113	3.346902	-0.320697
C	0.725772	3.711813	-2.440976
H	0.970650	2.670649	-2.735435
H	0.034314	4.127738	-3.200723
H	1.669994	4.294860	-2.505749

C	-0.069157	5.251249	-0.556138
H	0.885261	5.819128	-0.568833
H	-0.776356	5.783063	-1.228156
H	-0.472090	5.293216	0.477444
C	-2.843310	3.590988	-1.357001
H	-2.846959	4.584016	-0.852856
C	-4.133230	2.857871	-0.951969
H	-4.197356	1.850788	-1.418881
H	-4.198365	2.722405	0.145576
H	-5.019481	3.433699	-1.293943
C	-2.758227	3.800747	-2.877554
H	-1.925257	4.470040	-3.167445
H	-2.629100	2.839002	-3.418778
H	-3.697205	4.261888	-3.252897

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A-PH SCF Done: -1203.26739703 A.U.

Number of imaginary frequencies = 0

C	-1.060379	-0.200769	-0.727351
H	-0.584329	1.627713	-1.736061
N	-1.256562	0.392126	3.206518
C	-0.637953	-0.881181	2.885559
C	-0.604786	-1.136216	1.404884
N	-1.009846	-0.088755	0.635578
C	-1.491477	1.035123	-1.479932
H	-1.170563	-1.731211	3.383976
H	0.416364	-0.937166	3.271909
H	-2.004307	0.784233	-2.430428
C	-0.216025	-2.353775	0.821003
H	0.106055	-3.185722	1.465180
C	-0.265769	-2.488493	-0.572969
H	0.022239	-3.436631	-1.052690
C	-0.698213	-1.400388	-1.355155
H	-0.750840	-1.477038	-2.451330
Ru	-1.648282	1.623560	1.692769
C	-1.366605	0.598740	4.647729
H	-0.381920	0.438553	5.156205
H	-1.646702	1.655831	4.828312
C	-2.408772	-0.316115	5.286458
C	-3.731751	-0.311531	4.792746
C	-2.083340	-1.185785	6.345626
C	-4.707447	-1.149505	5.354442
C	-3.058665	-2.028896	6.911324
C	-4.373606	-2.012208	6.416884
H	-3.979370	0.355165	3.949932
H	-1.050278	-1.201964	6.732930
H	-5.737670	-1.130598	4.963450
H	-2.787590	-2.704074	7.739069
H	-5.139117	-2.671574	6.856520
H	-0.463989	2.538677	1.155492
C	-2.279563	3.090732	2.636429

O	-2.676654	4.036220	3.209513
P	-2.489036	2.164582	-0.338446
H	-3.844769	1.887094	-0.758169
H	-2.363291	3.404084	-1.059752

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TS-EF-PH SCF Done: -1204.42528828 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -968.52 cm⁻¹

C	-0.562484	0.084554	-0.702558
H	-0.612993	1.348358	-2.477866
N	-1.322187	0.543693	3.227506
C	-0.234382	-0.381161	2.956642
C	-0.157193	-0.724905	1.489376
N	-0.625554	0.235231	0.649053
C	-1.184936	1.177766	-1.542932
H	-2.490800	0.712139	2.385449
H	-0.312714	-1.315738	3.563434
H	0.758672	0.083334	3.224959
H	-2.206340	0.853655	-1.843220
C	0.404991	-1.907544	0.981637
H	0.767434	-2.678878	1.677136
C	0.505048	-2.073145	-0.408164
H	0.954958	-2.985677	-0.829286
C	0.020018	-1.066412	-1.259820
H	0.077488	-1.172486	-2.353317
Ru	-1.401938	1.971893	1.595158
C	-1.364760	1.005964	4.606004
H	-0.434126	1.569812	4.877022
H	-2.199656	1.736277	4.690398
C	-1.586525	-0.118360	5.613415
C	-2.572151	-1.100267	5.371952
C	-0.826001	-0.202828	6.796657
C	-2.796897	-2.134641	6.294560
C	-1.051412	-1.233942	7.726858
C	-2.037938	-2.203757	7.478266
H	-3.154625	-1.046076	4.437560
H	-0.044764	0.551559	6.990226
H	-3.571042	-2.892460	6.091557
H	-0.448099	-1.283205	8.647752
H	-2.213709	-3.014566	8.203282
H	0.138762	2.486792	1.723226
C	-1.889185	3.527584	2.482977
O	-2.153148	4.521633	3.045487
P	-1.421474	2.756632	-0.525091
H	-3.050303	1.141581	1.662184
H	-0.401361	3.611890	-1.071490
H	-2.520970	3.343502	-1.243821

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A-PCF3 SCF Done: -1877.65259171 A.U.

Number of imaginary frequencies = 0

C	-0.643407	-0.156192	-0.644548
H	0.234760	1.543026	-1.634571
N	-0.870523	0.245851	3.310335
C	-0.564298	-1.120519	2.926597
C	-0.511851	-1.290236	1.434578
N	-0.620257	-0.135301	0.723301
C	-0.774287	1.181163	-1.334776
H	-1.319527	-1.835874	3.341094
H	0.418440	-1.456597	3.354554
H	-1.390777	1.129284	-2.254405
C	-0.390891	-2.529811	0.783934
H	-0.304665	-3.449834	1.381200
C	-0.403967	-2.569011	-0.616428
H	-0.322111	-3.529180	-1.148551
C	-0.539892	-1.368161	-1.338637
H	-0.566555	-1.368172	-2.438244
Ru	-0.869347	1.617291	1.878433
C	-1.046531	0.388634	4.753875
H	-0.190433	-0.067813	5.310965
H	-1.045955	1.468901	5.001381
C	-2.350401	-0.242839	5.234628
C	-3.573471	0.172164	4.663983
C	-2.366534	-1.252111	6.216982
C	-4.785460	-0.402616	5.076359
C	-3.580210	-1.832180	6.632461
C	-4.792414	-1.408199	6.062827
H	-3.558986	0.948191	3.880588
H	-1.414991	-1.587313	6.663734
H	-5.733072	-0.064529	4.627001
H	-3.576597	-2.621087	7.401817
H	-5.743775	-1.861007	6.384916
H	0.563052	2.199993	1.526613
C	-1.176076	3.141312	2.902869
O	-1.361591	4.115244	3.526619
P	-1.400732	2.449766	-0.105739
C	-0.746518	4.053087	-0.937943
F	-1.342208	5.140064	-0.404549
F	0.586898	4.142208	-0.719967
F	-0.939287	4.078533	-2.281244
C	-3.242487	2.592389	-0.649429
F	-3.894092	3.527226	0.071381
F	-3.418752	2.872125	-1.965404
F	-3.825120	1.387109	-0.410575

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TS-EF-PCF3 SCF Done: -1878.80821043 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -943.40 cm⁻¹

C	-0.530117	0.158439	-0.653646
H	-0.453225	1.524862	-2.362284

N	-1.335538	0.561735	3.278303
C	-0.259800	-0.375190	3.000503
C	-0.176043	-0.698147	1.529406
N	-0.620097	0.282183	0.699504
C	-1.091186	1.290014	-1.486337
H	-2.515908	0.743104	2.429319
H	-0.358546	-1.315428	3.594424
H	0.739311	0.068073	3.281357
H	-2.087296	0.996865	-1.885759
C	0.375028	-1.879797	1.007505
H	0.717377	-2.668357	1.693655
C	0.490914	-2.022599	-0.383365
H	0.931163	-2.934980	-0.814587
C	0.039409	-0.991307	-1.223851
H	0.117009	-1.075227	-2.317846
Ru	-1.400966	2.006200	1.667266
C	-1.373647	1.012346	4.662582
H	-0.438673	1.566252	4.937433
H	-2.204544	1.746020	4.754821
C	-1.601274	-0.124532	5.653219
C	-2.625924	-1.067976	5.420515
C	-0.804450	-0.263124	6.806882
C	-2.853000	-2.118404	6.323978
C	-1.031865	-1.310938	7.717887
C	-2.056963	-2.242143	7.478636
H	-3.238456	-0.971881	4.509001
H	0.006420	0.461228	6.992692
H	-3.658038	-2.845454	6.129302
H	-0.400342	-1.403153	8.616181
H	-2.234760	-3.065492	8.188776
H	0.136945	2.499858	1.842410
C	-1.888832	3.558719	2.575127
O	-2.149590	4.546386	3.143202
P	-1.383908	2.793953	-0.402115
H	-3.059399	1.188202	1.724656
C	0.013995	3.951919	-1.025672
F	0.026744	5.111080	-0.341158
F	1.197132	3.319575	-0.826670
F	-0.072913	4.241668	-2.349545
C	-2.857965	3.592296	-1.337491
F	-2.993207	4.888928	-0.989540
F	-2.740431	3.523252	-2.687591
F	-3.989550	2.932803	-0.996480

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A-POMe SCF Done: -1432.49038997 A.U.

Number of imaginary frequencies = 0

C	-0.633995	-0.602783	-0.804187
H	0.217589	1.074376	-1.859837
N	-0.801503	0.040456	3.123258
C	-0.555636	-1.356914	2.820593

C	-0.492692	-1.612044	1.340106
N	-0.597173	-0.501418	0.561178
C	-0.784759	0.694223	-1.559010
H	-1.350727	-2.016957	3.254923
H	0.401870	-1.716131	3.285445
H	-1.398424	0.586593	-2.475897
C	-0.377891	-2.888738	0.764946
H	-0.292560	-3.771569	1.416238
C	-0.398247	-3.011849	-0.631042
H	-0.320550	-4.002744	-1.104626
C	-0.538011	-1.856476	-1.422783
H	-0.574703	-1.922064	-2.520136
Ru	-0.815438	1.330369	1.599878
C	-1.016856	0.266090	4.548941
H	-0.207023	-0.207430	5.159249
H	-0.961308	1.356575	4.742011
C	-2.368484	-0.263680	5.025147
C	-3.549452	0.157263	4.375654
C	-2.470742	-1.181502	6.088769
C	-4.802529	-0.320805	4.788827
C	-3.725561	-1.665030	6.505625
C	-4.894924	-1.235127	5.856441
H	-3.466421	0.858330	3.528144
H	-1.553233	-1.522052	6.598406
H	-5.716197	0.021138	4.276114
H	-3.787804	-2.384078	7.338423
H	-5.878472	-1.612791	6.178930
H	0.564075	1.928455	1.076355
C	-1.127335	2.922161	2.496649
O	-1.325692	3.951721	3.029225
P	-1.459899	2.000426	-0.411359
O	-1.062939	3.434155	-1.169116
C	0.072639	4.185995	-0.729055
H	0.034918	4.397023	0.361649
H	1.029216	3.660485	-0.950336
H	0.055336	5.143731	-1.286696
O	-3.053705	1.939382	-0.889089
C	-3.991921	2.721993	-0.138053
H	-3.853259	2.573726	0.957963
H	-3.888227	3.804295	-0.372727
H	-5.006882	2.383753	-0.425126

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TS-EF-POMe SCF Done: -1433.64694990 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -816.91 cm⁻¹

C	-0.273145	-0.250652	-0.808566
H	0.467217	1.331170	-2.070453
N	-1.245139	0.352725	3.091215
C	-0.252208	-0.679265	2.872060
C	-0.154643	-1.066110	1.416744

N	-0.452856	-0.077108	0.531240
C	-0.508584	0.947791	-1.698708
H	-2.427560	0.546973	2.171954
H	-0.434682	-1.588159	3.496370
H	0.779943	-0.316784	3.156887
H	-1.123171	0.700382	-2.588621
C	0.280261	-2.322559	0.964496
H	0.496207	-3.116298	1.694772
C	0.435429	-2.536962	-0.413493
H	0.771094	-3.515623	-0.790567
C	0.168731	-1.487906	-1.307931
H	0.302718	-1.617165	-2.392047
Ru	-1.251200	1.708795	1.372086
C	-1.237054	0.890713	4.440071
H	-0.257785	1.384077	4.682371
H	-2.001717	1.697691	4.487647
C	-1.553235	-0.146331	5.515346
C	-2.591697	-1.081542	5.314236
C	-0.832167	-0.190174	6.725332
C	-2.906418	-2.029782	6.301032
C	-1.147416	-1.134177	7.719545
C	-2.186161	-2.057827	7.510235
H	-3.142076	-1.059731	4.359192
H	-0.009954	0.527021	6.888861
H	-3.720453	-2.752481	6.127936
H	-0.573514	-1.152403	8.660224
H	-2.432055	-2.801166	8.285466
H	0.288811	2.213957	1.520383
C	-1.759610	3.324344	2.130981
O	-2.029418	4.368877	2.591858
P	-1.302877	2.347565	-0.749455
H	-2.923521	0.922438	1.424407
O	-0.564054	3.709851	-1.365040
C	0.442126	4.391499	-0.604788
H	0.081741	4.660511	0.411156
H	1.364092	3.778254	-0.494706
H	0.687334	5.315797	-1.164800
O	-2.713571	2.435783	-1.621843
C	-3.726325	3.330443	-1.137877
H	-3.959258	3.130300	-0.067373
H	-3.411930	4.391168	-1.251923
H	-4.633871	3.153998	-1.747414

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A-pyr-F SCF Done: -1617.20716478 A.U.

Number of imaginary frequencies = 0

C	-0.482112	-0.319178	-0.648840
H	-0.328096	1.025904	-2.361843
N	-1.001458	0.247749	3.250457
C	-0.629456	-1.120731	2.959273
C	-0.394244	-1.342186	1.489741

N	-0.539215	-0.231480	0.714400
C	-0.900294	0.909103	-1.419385
H	-1.413025	-1.850153	3.294787
H	0.299335	-1.423760	3.515538
H	-1.959260	0.752782	-1.720920
C	-0.078497	-2.588748	0.925395
H	0.051382	-3.485282	1.547748
C	0.062808	-2.657839	-0.463524
C	-0.157013	-1.529577	-1.272921
H	-0.097793	-1.614764	-2.366849
Ru	-0.774600	1.581428	1.770075
C	-1.323522	0.448531	4.656735
H	-0.539268	0.010161	5.326469
H	-1.339219	1.538818	4.857948
C	-2.679418	-0.151064	5.024381
C	-3.831724	0.262815	4.320706
C	-2.813975	-1.132177	6.025679
C	-5.089208	-0.282243	4.621388
C	-4.073139	-1.685510	6.328550
C	-5.213917	-1.260959	5.627479
H	-3.719985	1.014491	3.521203
H	-1.918428	-1.467069	6.576552
H	-5.981011	0.056625	4.069485
H	-4.160796	-2.454302	7.113330
H	-6.200501	-1.692228	5.861467
C	0.678402	3.408020	-1.006488
C	-2.494625	3.360375	-0.881976
C	-3.634349	2.593711	-0.170446
H	-3.682051	1.525935	-0.473550
H	-3.514554	2.620776	0.931512
H	-4.610134	3.058522	-0.432847
C	-2.771237	3.363026	-2.399951
H	-2.023909	3.938618	-2.975410
H	-2.819598	2.339591	-2.826418
H	-3.761939	3.833152	-2.587005
C	-2.460687	4.806137	-0.344525
H	-3.463235	5.270801	-0.469478
H	-2.208299	4.840076	0.735044
H	-1.736368	5.440253	-0.894383
C	0.527421	3.982589	-2.426426
H	1.504634	4.393348	-2.764075
H	0.224224	3.212675	-3.166967
H	-0.204730	4.813134	-2.467850
C	1.013214	4.536670	-0.007031
H	0.220913	5.308204	0.045185
H	1.162215	4.135139	1.014978
H	1.952647	5.041746	-0.321426
C	1.838711	2.384807	-0.998536
H	1.923774	1.873290	-0.017421
H	1.732234	1.611126	-1.786835
H	2.795855	2.916575	-1.190453

H	0.748491	1.968930	1.679974
C	-1.057620	3.173606	2.656735
O	-1.234616	4.216284	3.180072
P	-0.871760	2.464332	-0.344411
F	0.380039	-3.827420	-1.042964

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TS-EF-pyr-F SCF Done: -1618.40877790 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -941.16 cm⁻¹

C	-0.964714	-0.163005	-0.874552
H	-0.514145	1.124548	-2.574710
N	-2.374478	0.240586	2.892632
C	-1.387944	-0.858417	2.729707
C	-1.144921	-1.149931	1.269682
N	-1.245963	-0.064187	0.457218
C	-1.180456	1.085307	-1.688621
H	-3.303916	-0.097574	2.600862
H	-1.672149	-1.778165	3.287864
H	-0.431236	-0.473366	3.154977
H	-2.229890	1.067900	-2.059021
C	-0.758369	-2.404497	0.780150
H	-0.681846	-3.284092	1.434504
C	-0.445866	-2.499423	-0.583498
C	-0.540967	-1.382604	-1.425836
H	-0.303260	-1.475958	-2.494602
Ru	-1.842512	1.739488	1.357278
C	-2.469093	0.736213	4.295291
H	-1.484837	1.184546	4.540393
H	-3.209402	1.560617	4.286474
C	-2.864021	-0.341712	5.286104
C	-4.205678	-0.777085	5.359130
C	-1.900406	-0.978157	6.096432
C	-4.575164	-1.825317	6.218007
C	-2.266283	-2.025668	6.959850
C	-3.604430	-2.452982	7.020380
H	-4.971503	-0.279156	4.739933
H	-0.850747	-0.643771	6.048963
H	-5.626755	-2.149726	6.268462
H	-1.503067	-2.509756	7.589818
H	-3.893105	-3.272527	7.697424
C	0.762146	3.124353	-0.645483
C	-2.164464	3.896809	-1.576250
C	-3.651601	3.562513	-1.323164
H	-3.915851	2.534050	-1.644299
H	-3.915463	3.641161	-0.252303
H	-4.279211	4.273384	-1.905044
C	-1.913179	3.860010	-3.100177
H	-0.871702	4.098950	-3.380141
H	-2.174181	2.877393	-3.544198
H	-2.566294	4.615426	-3.590244

C	-1.881707	5.308269	-1.017707
H	-2.606991	6.027513	-1.457319
H	-2.002480	5.344521	0.084405
H	-0.866103	5.670586	-1.273504
C	1.246675	3.683807	-1.995180
H	2.347645	3.838352	-1.951055
H	1.051087	2.988259	-2.838511
H	0.793144	4.665091	-2.237805
C	1.016311	4.144837	0.485125
H	0.503018	5.110404	0.311566
H	0.672443	3.736941	1.457589
H	2.106695	4.352992	0.554341
C	1.560693	1.838771	-0.325707
H	1.195149	1.368599	0.610808
H	1.516604	1.094745	-1.148126
H	2.630960	2.103930	-0.182460
H	-0.339730	1.798423	2.162325
C	-2.349822	3.336817	2.128446
O	-2.666429	4.371585	2.600151
P	-1.108944	2.623113	-0.586707
H	-3.375110	1.468336	0.696022
F	-0.054547	-3.680489	-1.092232

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A-pyr-OMe SCF Done: -1632.50320703 A.U.

Number of imaginary frequencies = 0

C	-0.617246	-0.239347	-0.778105
H	-0.401091	1.086724	-2.504318
N	-1.287273	0.343132	3.088287
C	-0.852404	-1.017566	2.823841
C	-0.604748	-1.254567	1.357341
N	-0.710283	-0.140395	0.577255
C	-0.981986	0.998297	-1.563697
H	-1.597070	-1.774149	3.182221
H	0.093484	-1.260190	3.381906
H	-2.046522	0.886763	-1.866022
C	-0.307540	-2.502042	0.802939
H	-0.214776	-3.397921	1.433318
C	-0.122588	-2.610305	-0.591794
C	-0.302630	-1.457839	-1.395322
H	-0.229510	-1.495982	-2.490005
Ru	-0.948554	1.678656	1.623913
C	-1.533585	0.566399	4.504604
H	-0.640324	0.295806	5.127635
H	-1.701864	1.652171	4.660676
C	-2.745778	-0.197421	5.038957
C	-3.931485	-0.259916	4.275177
C	-2.717712	-0.836128	6.294849
C	-5.062561	-0.936070	4.760259
C	-3.849704	-1.511575	6.786630
C	-5.026748	-1.563725	6.020024

H	-3.940303	0.223473	3.284277
H	-1.792651	-0.804352	6.895609
H	-5.981267	-0.974295	4.152284
H	-3.809165	-2.005816	7.770948
H	-5.913347	-2.095965	6.400627
C	0.746231	3.381248	-1.088637
C	-2.422247	3.561360	-1.117762
C	-3.647627	2.893756	-0.450349
H	-3.761210	1.828000	-0.742986
H	-3.576688	2.929052	0.655502
H	-4.572913	3.425794	-0.763605
C	-2.628895	3.560732	-2.646795
H	-1.811741	4.064399	-3.194204
H	-2.739862	2.536864	-3.060259
H	-3.568786	4.105592	-2.886708
C	-2.303153	5.008396	-0.596027
H	-3.261128	5.545447	-0.771199
H	-2.096515	5.038643	0.493476
H	-1.509027	5.577739	-1.119801
C	0.706291	3.953462	-2.516894
H	1.725323	4.292749	-2.807656
H	0.387291	3.200192	-3.267972
H	0.036684	4.832564	-2.599120
C	1.115360	4.490868	-0.080183
H	0.380370	5.318727	-0.071011
H	1.183547	4.088122	0.950024
H	2.103895	4.922779	-0.350491
C	1.826266	2.275659	-1.019422
H	1.827984	1.770813	-0.031259
H	1.697011	1.502245	-1.804660
H	2.828142	2.732948	-1.172012
H	0.591834	1.998183	1.629435
C	-1.204915	3.282169	2.497009
O	-1.358151	4.333934	3.010678
P	-0.897905	2.555346	-0.494924
O	0.193318	-3.840068	-1.066041
C	0.380721	-4.010420	-2.467425
H	0.644449	-5.074222	-2.616624
H	-0.548053	-3.784545	-3.038985
H	1.208800	-3.373753	-2.853407

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TS-EF-pyr-OMe SCF Done: -1633.66046326 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -924.70 cm⁻¹

C	-0.508335	0.024909	-0.621261
H	-0.678364	1.162041	-2.476135
N	-1.266567	0.607483	3.275688
C	-0.191950	-0.343648	3.049506
C	-0.099557	-0.726260	1.592340
N	-0.546748	0.219265	0.725649

C	-1.141343	1.100680	-1.469920
H	-2.411117	0.815841	2.388090
H	-0.296025	-1.262282	3.677333
H	0.805968	0.109463	3.323110
H	-2.209595	0.828570	-1.621561
C	0.445158	-1.930198	1.115501
H	0.797782	-2.688151	1.830580
C	0.538045	-2.134452	-0.270015
H	0.975883	-3.063561	-0.667217
C	0.054588	-1.149301	-1.148401
H	0.096822	-1.290491	-2.238604
Ru	-1.250186	2.013376	1.611179
C	-1.329011	1.101401	4.642005
H	-0.390203	1.648654	4.922321
H	-2.144992	1.856537	4.685916
C	-1.596519	0.005463	5.668478
C	-2.611823	-0.944849	5.446842
C	-0.845464	-0.098493	6.859010
C	-2.887867	-1.963249	6.375904
C	-1.106321	-1.101605	7.800947
C	-2.132775	-2.043994	7.567844
H	-3.191371	-0.889545	4.510500
H	-0.035489	0.625367	7.051071
H	-3.690349	-2.683727	6.162530
H	-0.523071	-1.185239	8.730674
C	0.454079	3.606071	-1.122341
C	-2.710448	3.627366	-1.330496
C	-3.954963	3.003165	-0.659693
H	-4.868895	3.465041	-1.093351
H	-4.023253	1.907380	-0.824903
H	-3.957703	3.170467	0.434485
C	-2.834277	3.450542	-2.859228
H	-1.989512	3.890952	-3.418818
H	-2.925396	2.384776	-3.153507
H	-3.759947	3.959316	-3.207931
C	-2.657040	5.125373	-0.962235
H	-3.620428	5.606876	-1.238555
H	-2.508646	5.274964	0.127171
H	-1.854355	5.664723	-1.503619
C	0.461059	4.063624	-2.592707
H	1.475350	4.439066	-2.852672
H	0.231179	3.236018	-3.296350
H	-0.249209	4.892520	-2.782798
C	0.722228	4.805782	-0.187320
H	-0.040032	5.602596	-0.286070
H	0.747236	4.482386	0.872332
H	1.708530	5.253508	-0.438823
C	1.580591	2.564866	-0.919299
H	1.566896	2.151066	0.109672
H	1.519643	1.724780	-1.641673
H	2.563127	3.060703	-1.076477

H	0.302857	2.451408	1.808275
C	-1.695402	3.631543	2.385643
O	-1.941118	4.686083	2.846550
P	-1.181069	2.752500	-0.554501
H	-2.932294	1.241099	1.645472
O	-2.311774	-2.988725	8.541634
C	-3.331223	-3.957273	8.363892
H	-4.342562	-3.493396	8.287525
H	-3.161181	-4.585134	7.457703
H	-3.304557	-4.608830	9.258645

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A-pyr-CF3 SCF Done: -1855.12052564 A.U.

Number of imaginary frequencies = 0

C	-0.497379	-0.335437	-0.645385
H	-0.406190	1.006705	-2.365303
N	-0.923268	0.222682	3.271752
C	-0.579110	-1.146870	2.963187
C	-0.358543	-1.358609	1.491749
N	-0.532831	-0.246125	0.721816
C	-0.949045	0.886363	-1.406113
H	-1.375496	-1.865311	3.293720
H	0.344414	-1.473549	3.513583
H	-2.015631	0.720840	-1.674751
C	-0.027998	-2.594653	0.915781
H	0.123474	-3.478288	1.551950
C	0.099111	-2.680745	-0.477529
C	-0.162734	-1.540374	-1.268591
H	-0.129780	-1.603369	-2.365563
Ru	-0.776632	1.550893	1.779517
C	-1.247837	0.422501	4.678463
H	-0.492600	-0.065951	5.345169
H	-1.209195	1.509474	4.893169
C	-2.635366	-0.114749	5.021763
C	-3.765154	0.414211	4.360115
C	-2.820666	-1.156436	5.951179
C	-5.050272	-0.078680	4.631906
C	-4.108090	-1.658417	6.223698
C	-5.225702	-1.119867	5.565183
H	-3.616784	1.215220	3.616153
H	-1.943606	-1.579304	6.470292
H	-5.923783	0.350043	4.114477
H	-4.236032	-2.475567	6.951938
H	-6.234226	-1.510186	5.776100
C	0.640492	3.381939	-1.008610
C	-2.532088	3.340190	-0.851549
C	-3.665611	2.579824	-0.123521
H	-3.721542	1.511456	-0.422862
H	-3.533485	2.610026	0.976840
H	-4.642505	3.047629	-0.375878
C	-2.825614	3.336355	-2.366484
H	-2.081563	3.904782	-2.953216
H	-2.884681	2.311042	-2.786759
H	-3.815667	3.811110	-2.544360

C	-2.487229	4.788415	-0.321481
H	-3.489493	5.255470	-0.438797
H	-2.224247	4.827522	0.755246
H	-1.766725	5.417329	-0.882081
C	0.476425	3.956761	-2.427150
H	1.451087	4.365791	-2.773721
H	0.165520	3.187183	-3.164720
H	-0.254809	4.788405	-2.461681
C	0.988129	4.509868	-0.012772
H	0.199215	5.284362	0.045984
H	1.145622	4.108879	1.008224
H	1.926421	5.011161	-0.336113
C	1.797380	2.354483	-1.012928
H	1.893869	1.843531	-0.032652
H	1.678985	1.580175	-1.798718
H	2.753715	2.882958	-1.217028
H	0.736552	1.969537	1.687577
C	-1.089780	3.142254	2.664271
O	-1.285954	4.183410	3.182320
P	-0.905279	2.441738	-0.336400
C	0.536896	-3.967977	-1.139976
F	0.308961	-5.047705	-0.352954
F	-0.111362	-4.167780	-2.316751
F	1.867542	-3.946381	-1.420338

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TS-EF-pyr-CF3 SCF Done: -1856.28194912 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -947.48 cm⁻¹

C	-0.503552	0.028299	-0.627246
H	-0.678461	1.164333	-2.480677
N	-1.258675	0.596229	3.273088
C	-0.184901	-0.354837	3.043269
C	-0.093005	-0.729596	1.584811
N	-0.544433	0.217584	0.721475
C	-1.138698	1.102826	-1.473469
H	-2.402953	0.807581	2.392232
H	-0.288492	-1.277525	3.665210
H	0.813768	0.095900	3.317312
H	-2.206715	0.827660	-1.621497
C	0.458586	-1.927990	1.106422
H	0.823912	-2.689123	1.810040
C	0.552154	-2.123347	-0.280464
C	0.066261	-1.137806	-1.158612
H	0.122958	-1.280176	-2.246961
Ru	-1.244215	2.003169	1.608678
C	-1.315777	1.091042	4.638322
H	-0.375632	1.636575	4.916187
H	-2.130659	1.847159	4.686798
C	-1.589546	0.000831	5.671072
C	-2.567345	-0.985697	5.417673
C	-0.886393	-0.044767	6.891480
C	-2.840658	-1.986532	6.364048
C	-1.160778	-1.041716	7.845309
H	-3.103445	-0.961646	4.454640

H	-0.111021	0.713014	7.095532
H	-3.607274	-2.749112	6.150506
H	-0.601677	-1.060964	8.794797
C	0.453809	3.608884	-1.121216
C	-2.712831	3.625235	-1.324846
C	-3.954680	2.997164	-0.652724
H	-4.870009	3.457307	-1.084872
H	-4.021375	1.901466	-0.819162
H	-3.957293	3.163804	0.441533
C	-2.838360	3.450416	-2.853735
H	-1.994787	3.892111	-3.414009
H	-2.930227	2.385256	-3.149880
H	-3.764684	3.959440	-3.199827
C	-2.660808	5.122804	-0.954255
H	-3.625323	5.602809	-1.228675
H	-2.511590	5.271670	0.135109
H	-1.859883	5.664191	-1.496077
C	0.456972	4.071170	-2.590231
H	1.470232	4.448681	-2.850500
H	0.227295	3.245715	-3.296369
H	-0.254641	4.899765	-2.776174
C	0.721968	4.805963	-0.182713
H	-0.043258	5.600648	-0.275149
H	0.753826	4.479598	0.875785
H	1.705449	5.257706	-0.437377
C	1.581684	2.567921	-0.924107
H	1.571475	2.149911	0.103212
H	1.521812	1.731550	-1.650881
H	2.563268	3.065497	-1.080545
H	0.308055	2.444339	1.808880
C	-1.682952	3.624579	2.385330
O	-1.923074	4.678620	2.847571
P	-1.179738	2.753248	-0.555478
H	-2.926693	1.236894	1.650054
C	-2.139191	-2.016593	7.584162
H	-2.352488	-2.801366	8.327520
C	1.107222	-3.419315	-0.838182
F	1.753035	-3.216983	-2.014085
F	0.111037	-4.311520	-1.076296
F	1.977519	-4.004319	0.018949

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A-NCH3 SCF Done: -1286.78086265 A.U.

Number of imaginary frequencies = 0

C	-0.813932	-0.176787	-0.804392
H	-0.146786	1.109877	-2.438917
N	-2.246008	0.482353	2.847528
C	-1.834253	-0.895744	2.677105
C	-1.319952	-1.170771	1.289524
N	-1.182174	-0.064272	0.508131
C	-0.909553	1.080389	-1.634332
H	-2.665231	-1.618180	2.895668
H	-1.019997	-1.175461	3.403083
H	-1.897784	1.057713	-2.144830

C	-1.004665	-2.447744	0.795339
H	-1.114496	-3.325990	1.449448
C	-0.551710	-2.574638	-0.525216
H	-0.283987	-3.562241	-0.931567
C	-0.470833	-1.426249	-1.337968
H	-0.162910	-1.499517	-2.391733
Ru	-1.505773	1.771786	1.491537
C	-2.668780	0.750622	4.209875
H	-1.841792	0.605872	4.953934
H	-3.028199	1.792631	4.303540
C	0.889408	3.292729	-0.759599
C	-2.161907	3.773006	-1.486655
C	-3.562822	3.234019	-1.113567
H	-3.716897	2.185720	-1.447521
H	-3.731147	3.262849	-0.018103
H	-4.340120	3.857505	-1.607894
C	-2.025684	3.777537	-3.023530
H	-1.064706	4.197431	-3.371896
H	-2.138028	2.764819	-3.463144
H	-2.834626	4.405790	-3.457947
C	-2.021610	5.206506	-0.933517
H	-2.859831	5.832532	-1.310683
H	-2.060767	5.226660	0.174900
H	-1.079484	5.690927	-1.260328
C	1.218647	3.856606	-2.153374
H	2.303905	4.095650	-2.208066
H	1.003286	3.131934	-2.966676
H	0.668978	4.794562	-2.367827
C	1.131381	4.368742	0.321196
H	0.496268	5.264390	0.179392
H	0.930897	3.968944	1.335213
H	2.192242	4.700143	0.282164
C	1.818485	2.089554	-0.471511
H	1.559650	1.596328	0.488106
H	1.789010	1.324773	-1.274872
H	2.868456	2.447966	-0.399077
H	0.013781	1.957325	1.855368
C	-1.812240	3.402383	2.299454
O	-1.984045	4.469282	2.773447
P	-0.915083	2.631544	-0.557375
H	-3.503103	0.073162	4.522250

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TS-EF-NCH3 SCF Done: -1287.94217617 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -923.53 cm⁻¹

C	-0.605645	0.053586	-0.716372
H	-0.850683	1.224219	-2.541785
N	-1.301938	0.525178	3.207375
C	-0.203209	-0.379340	2.937663
C	-0.128130	-0.732837	1.470582

N	-0.621943	0.217412	0.635077
C	-1.289946	1.126582	-1.527796
H	-2.472629	0.719076	2.346206
H	-0.260277	-1.316109	3.549844
H	0.788454	0.098740	3.196440
H	-2.351902	0.823042	-1.663265
C	0.443540	-1.908276	0.956509
H	0.834853	-2.670719	1.646295
C	0.513721	-2.079381	-0.434988
H	0.971545	-2.985488	-0.861659
C	-0.017915	-1.090799	-1.280887
H	0.005732	-1.206844	-2.374608
Ru	-1.362725	1.967676	1.575584
C	-1.339918	0.984788	4.579411
H	-0.434685	1.585132	4.859202
H	-2.227452	1.631289	4.735487
C	0.231087	3.674089	-1.157504
C	-2.936488	3.596454	-1.301895
C	-4.146196	2.916767	-0.621382
H	-5.083187	3.359955	-1.024281
H	-4.184052	1.823795	-0.813069
H	-4.130646	3.056554	0.476581
C	-3.085590	3.449657	-2.831521
H	-2.267153	3.929857	-3.397478
H	-3.147994	2.388210	-3.148125
H	-4.034270	3.935147	-3.150379
C	-2.924073	5.086715	-0.900364
H	-3.907528	5.542940	-1.147422
H	-2.759332	5.216465	0.189228
H	-2.149680	5.663734	-1.444116
C	0.192987	4.164035	-2.616841
H	1.189252	4.577493	-2.888672
H	-0.025422	3.345373	-3.334491
H	-0.546917	4.973783	-2.773601
C	0.481251	4.860749	-0.201045
H	-0.306738	5.635665	-0.267085
H	0.537289	4.514854	0.850330
H	1.448216	5.344246	-0.461421
C	1.393957	2.665280	-1.000977
H	1.414868	2.228842	0.018491
H	1.344466	1.839762	-1.740838
H	2.356847	3.195676	-1.166810
H	0.179933	2.450956	1.754195
C	-1.842322	3.553134	2.396133
O	-2.111874	4.588760	2.885741
P	-1.363811	2.756252	-0.575110
H	-3.018510	1.146370	1.624159
H	-1.411098	0.129028	5.297401

Number of imaginary frequencies = 0

C	-0.406373	-0.351637	-0.663938
H	-0.330072	1.002138	-2.377528
N	-1.205144	0.098265	3.198415
C	-0.608259	-1.195207	2.931743
C	-0.310933	-1.388223	1.468823
N	-0.528240	-0.287932	0.696992
C	-0.887357	0.856881	-1.429812
H	-1.250989	-2.049435	3.264036
H	0.354468	-1.327412	3.497718
H	-1.943867	0.659155	-1.717123
C	0.137449	-2.591855	0.898328
H	0.319755	-3.464487	1.543785
C	0.341183	-2.654986	-0.486973
H	0.701609	-3.583180	-0.956737
C	0.048663	-1.525394	-1.278377
H	0.153949	-1.558980	-2.373065
Ru	-0.946809	1.480705	1.761390
C	-1.633891	0.290967	4.573763
H	-1.139727	-0.453552	5.247907
H	-1.309110	1.295763	4.924825
C	0.665820	3.345718	-0.897977
C	-2.507524	3.308416	-0.965726
C	-3.692523	2.557663	-0.313791
H	-3.728094	1.486031	-0.604487
H	-3.641102	2.600084	0.792706
H	-4.647934	3.023928	-0.640943
C	-2.698436	3.305203	-2.496722
H	-1.904906	3.857011	-3.032432
H	-2.747406	2.279123	-2.916413
H	-3.664873	3.797877	-2.743651
C	-2.489693	4.756165	-0.432313
H	-3.479504	5.229310	-0.614453
H	-2.298018	4.791204	0.659788
H	-1.729936	5.381747	-0.942680
C	0.606987	3.935214	-2.318653
H	1.603999	4.349110	-2.588144
H	0.353164	3.172947	-3.085209
H	-0.121166	4.766529	-2.399405
C	0.945558	4.462295	0.131392
H	0.159943	5.242405	0.136920
H	1.020664	4.050396	1.157524
H	1.909562	4.959102	-0.114692
C	1.816792	2.313855	-0.828824
H	1.840818	1.796169	0.152353
H	1.749767	1.544970	-1.625969
H	2.787364	2.839542	-0.961619
H	0.567107	1.906897	1.821380
C	-1.328381	3.050949	2.650026
O	-1.554909	4.086002	3.170684
P	-0.924990	2.400955	-0.342584

C	-3.179222	0.184068	4.810266
C	-3.698185	-1.182845	4.322379
C	-3.917422	1.306349	4.056365
H	-3.572649	2.309354	4.383744
H	-3.735495	1.233514	2.963278
H	-5.012927	1.242649	4.229151
H	-3.523682	-1.298539	3.231837
H	-4.789844	-1.281477	4.503529
H	-3.193495	-2.021568	4.849957
C	-3.428950	0.329686	6.325214
H	-3.048228	1.303046	6.702462
H	-4.514055	0.279861	6.557355
H	-2.923498	-0.477610	6.898590

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TS-EF-NCH2tBu SCF Done: -1445.26657258 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -945.51 cm⁻¹

C	-0.386837	0.026875	-0.752343
H	-0.867197	1.186288	-2.537924
N	-0.787728	0.425585	3.233629
C	0.345215	-0.399664	2.853099
C	0.324318	-0.732042	1.380305
N	-0.303200	0.183043	0.597640
C	-1.214292	1.048750	-1.493246
H	-2.034852	0.540974	2.452281
H	0.413097	-1.348854	3.437928
H	1.319166	0.143338	3.034871
H	-2.257347	0.664903	-1.547235
C	0.936029	-1.860093	0.808079
H	1.436019	-2.595433	1.455816
C	0.904927	-2.018707	-0.586025
H	1.391006	-2.886731	-1.058197
C	0.234483	-1.068143	-1.375280
H	0.175959	-1.177341	-2.468380
Ru	-1.095775	1.864279	1.614191
C	-0.807945	0.818064	4.640340
H	0.224142	0.750208	5.069207
H	-1.094744	1.887261	4.728332
C	0.130375	3.704466	-1.217665
C	-3.022287	3.381859	-1.102056
C	-4.115573	2.608870	-0.330119
H	-5.114202	2.974863	-0.654870
H	-4.080502	1.516038	-0.522758
H	-4.023937	2.751344	0.763703
C	-3.286947	3.227946	-2.615418
H	-2.556575	3.769112	-3.243474
H	-3.297215	2.165612	-2.935006
H	-4.292230	3.642278	-2.850075
C	-3.091407	4.867868	-0.690281
H	-4.125413	5.245315	-0.847461

H	-2.843560	5.008891	0.382057
H	-2.415136	5.505382	-1.294154
C	-0.065103	4.194169	-2.664413
H	0.870238	4.685449	-3.012446
H	-0.276737	3.362850	-3.369399
H	-0.876297	4.943657	-2.752822
C	0.363546	4.903998	-0.273233
H	-0.484869	5.615158	-0.269781
H	0.529559	4.560158	0.767119
H	1.266315	5.462143	-0.604860
C	1.377060	2.789452	-1.165005
H	1.513009	2.351944	-0.154854
H	1.332487	1.965577	-1.906989
H	2.279359	3.394257	-1.401583
H	0.413881	2.469711	1.674579
C	-1.641091	3.398446	2.487476
O	-1.961668	4.397809	3.020032
P	-1.334731	2.661805	-0.517731
H	-2.668821	0.917062	1.773168
C	-1.780925	0.004058	5.548022
C	-3.232861	0.247384	5.085509
H	-3.486689	1.328437	5.113709
H	-3.384847	-0.105527	4.044611
H	-3.954853	-0.292182	5.735217
C	-1.609420	0.505095	6.996484
H	-2.304513	-0.019734	7.686048
H	-0.574774	0.332887	7.364277
H	-1.817519	1.594082	7.072301
C	-1.468018	-1.503303	5.477663
H	-1.595557	-1.880910	4.441497
H	-0.426666	-1.716604	5.803257
H	-2.151355	-2.083242	6.134478

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A-NCH₂CF₃ SCF Done: -1623.98744262 A.U.

Number of imaginary frequencies = 0

C	-0.663946	-0.240725	-0.748999
H	-0.201386	1.086198	-2.421717
N	-1.762040	0.328852	3.025555
C	-1.404739	-1.054220	2.786012
C	-0.959332	-1.276473	1.365448
N	-0.932331	-0.156978	0.590071
C	-0.888204	1.016245	-1.553909
H	-2.253599	-1.755194	2.987518
H	-0.577592	-1.393543	3.468250
H	-1.915156	0.950518	-1.976441
C	-0.615011	-2.531177	0.833224
H	-0.630992	-3.419533	1.482643
C	-0.260539	-2.623745	-0.518996
H	0.023826	-3.593163	-0.956523
C	-0.303094	-1.466604	-1.322832

H	-0.076974	-1.516425	-2.398391
Ru	-1.223065	1.662828	1.613120
C	-2.316776	0.583070	4.329402
H	-1.971974	-0.139903	5.109429
H	-2.053034	1.600946	4.684141
C	0.867762	3.318599	-0.834767
C	-2.266282	3.634387	-1.245872
C	-3.587210	3.010548	-0.736350
H	-3.707168	1.952450	-1.052908
H	-3.650984	3.035669	0.370213
H	-4.446869	3.580854	-1.151862
C	-2.286750	3.654738	-2.788462
H	-1.389436	4.128012	-3.226724
H	-2.389511	2.640238	-3.226171
H	-3.167660	4.241090	-3.131403
C	-2.153218	5.071345	-0.695278
H	-3.061512	5.647077	-0.978164
H	-2.079823	5.086262	0.411342
H	-1.280580	5.612912	-1.112793
C	1.027382	3.906598	-2.248451
H	2.087645	4.204200	-2.406434
H	0.772238	3.175590	-3.044379
H	0.410287	4.814526	-2.398368
C	1.154663	4.400879	0.228609
H	0.458663	5.259114	0.160670
H	1.079823	3.985263	1.253094
H	2.185659	4.793036	0.088004
C	1.884121	2.166488	-0.651296
H	1.746084	1.651623	0.321870
H	1.819940	1.407280	-1.457892
H	2.915008	2.581997	-0.674169
H	0.313601	1.902526	1.823555
C	-1.507216	3.274813	2.466293
O	-1.662978	4.328995	2.971433
P	-0.868636	2.560434	-0.466949
C	-3.846803	0.514518	4.335921
F	-4.338772	0.735574	5.584115
F	-4.402748	1.434025	3.509689
F	-4.297856	-0.709653	3.933000

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TS-EF-NCH2CF3 SCF Done: -1625.14786799 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -988.58 cm⁻¹

C	-0.557639	0.051883	-0.745462
H	-0.840388	1.235309	-2.557630
N	-1.219986	0.478302	3.195568
C	-0.124023	-0.436273	2.904229
C	-0.054795	-0.752268	1.428624
N	-0.562532	0.202667	0.607856
C	-1.265270	1.122440	-1.539214

H	-2.375540	0.661670	2.365290
H	-0.186069	-1.387866	3.480248
H	0.863381	0.034365	3.180280
H	-2.324714	0.805812	-1.663814
C	0.523216	-1.917173	0.897544
H	0.923196	-2.684576	1.576696
C	0.586348	-2.071673	-0.495923
H	1.049642	-2.968636	-0.935579
C	0.037497	-1.079874	-1.326816
H	0.052240	-1.184646	-2.421780
Ru	-1.307066	1.939338	1.564415
C	-1.289205	0.949784	4.554584
H	-0.310808	1.338715	4.938658
H	-2.014177	1.785698	4.620279
C	0.225798	3.688616	-1.165616
C	-2.943395	3.567986	-1.264263
C	-4.133786	2.867987	-0.570347
H	-5.081847	3.298009	-0.961061
H	-4.157699	1.774995	-0.763567
H	-4.108096	3.005895	0.527487
C	-3.113032	3.427795	-2.792632
H	-2.307823	3.918702	-3.368201
H	-3.171277	2.367714	-3.114340
H	-4.070671	3.906461	-3.093961
C	-2.944792	5.056356	-0.855124
H	-3.938086	5.499354	-1.085829
H	-2.766958	5.184214	0.232458
H	-2.187018	5.647082	-1.407401
C	0.158102	4.192180	-2.619392
H	1.143910	4.623319	-2.901070
H	-0.058120	3.377618	-3.342269
H	-0.595995	4.992033	-2.757067
C	0.472978	4.869384	-0.201174
H	-0.329228	5.631130	-0.243953
H	0.555537	4.513787	0.845084
H	1.426279	5.372104	-0.474614
C	1.405058	2.695022	-1.037216
H	1.448362	2.249067	-0.022633
H	1.356166	1.876379	-1.784663
H	2.357323	3.241125	-1.212410
H	0.234997	2.437506	1.716979
C	-1.796431	3.522293	2.383460
O	-2.073416	4.554719	2.875412
P	-1.347761	2.742913	-0.573579
H	-2.942000	1.094194	1.636187
C	-1.783216	-0.093531	5.560751
F	-1.932243	0.466680	6.789769
F	-2.978805	-0.617223	5.197893
F	-0.914776	-1.139156	5.704176

A-NCH2PhOMe SCF Done: -1632.49896728 A.U.

Number of imaginary frequencies = 0

C	-1.204412	-0.212188	-0.919547
H	-1.529178	1.077746	-2.652671
N	-1.182314	0.412474	3.006989
C	-0.654178	-0.893537	2.673722
C	-0.628416	-1.133315	1.189288
N	-1.058188	-0.083521	0.434584
C	-1.915771	0.916473	-1.625967
H	-1.248011	-1.719001	3.147341
H	0.388366	-1.028620	3.072845
H	-2.977193	0.605287	-1.743196
C	-0.226453	-2.338213	0.588129
H	0.129647	-3.166657	1.219049
C	-0.290517	-2.459221	-0.806642
H	0.030615	-3.388259	-1.302477
C	-0.803514	-1.388562	-1.566252
H	-0.914284	-1.471491	-2.657819
Ru	-1.395279	1.708271	1.493510
C	-1.287262	0.620359	4.446279
H	-0.330388	0.360867	4.969233
H	-1.464188	1.700048	4.626435
C	-2.421302	-0.192985	5.061616
C	-3.740389	-0.029489	4.576219
C	-2.205571	-1.135476	6.080077
C	-4.801672	-0.770072	5.101109
C	-3.261796	-1.895480	6.623671
C	-4.571199	-1.712462	6.133095
H	-3.917451	0.690202	3.759459
H	-1.183727	-1.286219	6.468420
H	-5.831744	-0.643327	4.734077
H	-3.048081	-2.622995	7.419431
C	-0.640870	3.612328	-1.496540
C	-3.724206	3.159457	-0.888893
C	-4.634377	2.281296	0.001768
H	-4.590274	1.206448	-0.275635
H	-4.353065	2.360242	1.071380
H	-5.690258	2.611755	-0.112900
C	-4.222214	3.070143	-2.346513
H	-3.650059	3.713042	-3.039585
H	-4.199472	2.033306	-2.741487
H	-5.282496	3.404339	-2.388799
C	-3.800659	4.616664	-0.388005
H	-4.862969	4.944900	-0.365276
H	-3.395685	4.722179	0.639206
H	-3.256983	5.317267	-1.053375
C	-1.077561	4.114689	-2.884377
H	-0.225445	4.637367	-3.372834
H	-1.382442	3.287322	-3.559362
H	-1.911962	4.841234	-2.824796
C	-0.312151	4.807627	-0.575937

H	-1.183138	5.471329	-0.413138
H	0.040478	4.463085	0.416548
H	0.493951	5.419102	-1.037437
C	0.632396	2.747541	-1.653008
H	0.931713	2.285880	-0.689358
H	0.510411	1.938833	-2.402924
H	1.470620	3.390800	-1.998786
H	0.024743	2.307425	1.173595
C	-1.777556	3.274157	2.391859
O	-2.028525	4.299387	2.919878
P	-1.935229	2.497343	-0.592916
O	-5.673619	-2.389556	6.578376
C	-5.507557	-3.339670	7.616889
H	-4.827157	-4.172104	7.319619
H	-5.111029	-2.875609	8.550365
H	-6.511785	-3.756998	7.824553

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TS-EF-NCH2PhOMe SCF Done: -1633.66074346 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -944.69 cm⁻¹

C	-0.397646	0.218540	-0.568775
H	-0.591099	1.399448	-2.394001
N	-1.198673	0.672464	3.335517
C	-0.095325	-0.240701	3.093113
C	0.018446	-0.580295	1.626692
N	-0.449890	0.375366	0.782539
C	-1.057634	1.297345	-1.392697
H	-2.342720	0.870510	2.444796
H	-0.177676	-1.178859	3.694677
H	0.887211	0.233119	3.387066
H	-2.116224	0.997225	-1.558501
C	0.600196	-1.754981	1.121601
H	0.968722	-2.522230	1.818498
C	0.707986	-1.918821	-0.268196
H	1.174353	-2.824232	-0.687050
C	0.202286	-0.924358	-1.123227
H	0.255181	-1.034919	-2.216497
Ru	-1.211893	2.123263	1.711021
C	-1.290926	1.123409	4.715349
H	-0.374587	1.693965	5.022209
H	-2.134484	1.846547	4.772609
C	-1.529040	-0.014735	5.700729
C	-2.557225	-0.956934	5.461864
C	-0.743553	-0.178772	6.853949
C	-2.795644	-2.011815	6.346783
C	-0.969417	-1.231540	7.763010
C	-2.003684	-2.157247	7.510910
H	-3.167851	-0.854842	4.549708
H	0.073313	0.534895	7.055302
H	-3.595633	-2.746513	6.167433

H	-0.330923	-1.320062	8.653357
C	0.457527	3.840190	-0.969605
C	-2.705113	3.769552	-1.195524
C	-3.933081	3.089595	-0.548894
H	-4.858641	3.535251	-0.974782
H	-3.967129	1.997253	-0.744698
H	-3.946009	3.226263	0.549488
C	-2.815665	3.629532	-2.729094
H	-1.981606	4.109357	-3.272091
H	-2.873297	2.569595	-3.051546
H	-3.754406	4.119395	-3.069834
C	-2.699785	5.258061	-0.787454
H	-3.675997	5.717194	-1.056757
H	-2.561824	5.382839	0.306429
H	-1.911130	5.835818	-1.309483
C	0.458309	4.335723	-2.427622
H	1.462051	4.748361	-2.671704
H	0.257356	3.520046	-3.153703
H	-0.275874	5.147406	-2.600591
C	0.683930	5.022825	-0.002343
H	-0.100039	5.799907	-0.087298
H	0.710058	4.673076	1.048883
H	1.658851	5.504806	-0.234173
C	1.614434	2.829098	-0.786155
H	1.607698	2.389215	0.232009
H	1.583181	2.006064	-1.529727
H	2.582089	3.358598	-0.924779
H	0.326346	2.601462	1.931720
C	-1.709924	3.705312	2.526766
O	-1.989667	4.738706	3.015428
P	-1.153111	2.922244	-0.433819
H	-2.871055	1.301887	1.711648
O	-2.314752	-3.219380	8.315491
C	-1.561867	-3.410798	9.501166
H	-1.646227	-2.542733	10.196277
H	-1.980375	-4.307539	9.997635
H	-0.481583	-3.589403	9.288468

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A-NCH2PhF SCF Done: -1617.20787468 A.U.

Number of imaginary frequencies = 0

C	-1.299110	-0.230434	-0.908367
H	-1.401666	1.092656	-2.643539
N	-1.561887	0.357249	3.015195
C	-1.103582	-0.980481	2.708303
C	-0.959675	-1.204586	1.227622
N	-1.261650	-0.123711	0.455024
C	-1.883115	0.943894	-1.655862
H	-1.799934	-1.765055	3.107006
H	-0.116363	-1.199836	3.199260
H	-2.946051	0.694125	-1.867730

C	-0.576382	-2.424570	0.645174
H	-0.323466	-3.278743	1.291381
C	-0.527508	-2.527600	-0.751630
H	-0.218350	-3.468645	-1.232122
C	-0.912265	-1.421713	-1.536046
H	-0.934101	-1.487532	-2.634138
Ru	-1.579765	1.676562	1.505742
C	-1.806283	0.555577	4.437093
H	-0.962274	0.161522	5.059543
H	-1.862322	1.645686	4.632112
C	-3.105184	-0.107305	4.889923
C	-4.321258	0.262929	4.273780
C	-3.129795	-1.108733	5.879685
C	-5.533485	-0.337264	4.642423
C	-4.334954	-1.728095	6.261945
C	-5.522170	-1.330423	5.635602
H	-4.301624	1.029782	3.481405
H	-2.187607	-1.412835	6.365979
H	-6.489481	-0.053020	4.177478
H	-4.367696	-2.513790	7.031504
C	-0.483069	3.566984	-1.385964
C	-3.624637	3.273265	-1.032690
C	-4.647281	2.436682	-0.228076
H	-4.630641	1.361718	-0.507940
H	-4.453041	2.498457	0.861734
H	-5.672881	2.817911	-0.427828
C	-4.009413	3.223925	-2.526126
H	-3.351725	3.842720	-3.162902
H	-4.009056	2.191246	-2.932418
H	-5.044172	3.613981	-2.647144
C	-3.664121	4.728299	-0.521081
H	-4.705776	5.113111	-0.580390
H	-3.338930	4.804169	0.536653
H	-3.031423	5.403430	-1.131756
C	-0.779376	4.107492	-2.796539
H	0.135783	4.589585	-3.206213
H	-1.070723	3.305549	-3.507260
H	-1.576706	4.877000	-2.793156
C	-0.167532	4.733228	-0.424185
H	-1.013524	5.439780	-0.320225
H	0.087673	4.360118	0.587559
H	0.702802	5.306643	-0.811814
C	0.751148	2.636426	-1.452764
H	0.945111	2.146382	-0.476160
H	0.648843	1.845542	-2.224291
H	1.647993	3.237616	-1.717435
H	-0.109252	2.199415	1.305985
C	-1.946874	3.253664	2.390451
O	-2.183650	4.286363	2.910355
P	-1.902853	2.514042	-0.606716
F	-6.687150	-1.918387	5.991364

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TS-EF-NCH2PhF SCF Done: -1618.36962336 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -945.93 cm⁻¹

C	-0.416421	0.215357	-0.613793
H	-0.619072	1.423502	-2.420034
N	-1.176798	0.618277	3.306077
C	-0.081971	-0.299326	3.038212
C	0.014542	-0.618336	1.565501
N	-0.454072	0.353319	0.740102
C	-1.076159	1.310666	-1.415561
H	-2.318475	0.836616	2.435275
H	-0.164167	-1.246854	3.625235
H	0.905270	0.164558	3.329907
H	-2.138662	1.020965	-1.574718
C	0.582110	-1.790105	1.038465
H	0.951755	-2.570118	1.720452
C	0.675276	-1.934690	-0.354636
H	1.130703	-2.837408	-0.790875
C	0.169067	-0.924217	-1.190198
H	0.210513	-1.019532	-2.285375
Ru	-1.192590	2.093958	1.699275
C	-1.247371	1.056697	4.688734
H	-0.316521	1.603734	4.994218
H	-2.072725	1.799185	4.763071
C	-1.509349	-0.078690	5.674898
C	-2.473792	-1.066336	5.377251
C	-0.811679	-0.169674	6.896001
C	-2.745086	-2.112170	6.272830
C	-1.071861	-1.205620	7.810582
C	-2.038911	-2.165339	7.484158
H	-3.006186	-1.010765	4.413786
H	-0.045892	0.585821	7.138958
H	-3.494196	-2.887703	6.052727
H	-0.533574	-1.286218	8.766842
C	0.463023	3.835801	-0.971895
C	-2.702688	3.792597	-1.165447
C	-3.929346	3.112709	-0.516263
H	-4.855413	3.571864	-0.926290
H	-3.974154	2.023716	-0.727857
H	-3.930488	3.233263	0.584042
C	-2.829745	3.675382	-2.699696
H	-1.997205	4.155852	-3.244376
H	-2.900170	2.620784	-3.036778
H	-3.767572	4.178145	-3.023573
C	-2.681491	5.275178	-0.736584
H	-3.656544	5.745444	-0.990213
H	-2.532325	5.383978	0.357514
H	-1.893346	5.853998	-1.258155
C	0.452347	4.351710	-2.422855

H	1.456770	4.759736	-2.671571
H	0.237334	3.548052	-3.158228
H	-0.276911	5.171597	-2.576657
C	0.708286	5.003230	0.009150
H	-0.071179	5.786706	-0.056225
H	0.744044	4.638970	1.055102
H	1.683803	5.481719	-0.227084
C	1.613942	2.813458	-0.814944
H	1.614860	2.359297	0.196934
H	1.568649	2.001400	-1.569764
H	2.584041	3.337606	-0.956437
H	0.351892	2.557799	1.910162
C	-1.671583	3.669680	2.538411
O	-1.939580	4.698449	3.042852
P	-1.149220	2.922781	-0.433650
H	-2.854350	1.283376	1.707600
F	-2.292960	-3.170734	8.352520

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A-NEt SCF Done: -1326.11246659 A.U.

Number of imaginary frequencies = 0

C	-0.723050	-0.216261	-0.773113
H	-0.213936	1.100116	-2.440929
N	-1.883717	0.384452	2.986498
C	-1.499552	-0.994119	2.758809
C	-1.059062	-1.239085	1.340925
N	-1.001980	-0.122685	0.563220
C	-0.913491	1.043412	-1.582258
H	-2.323151	-1.719912	2.986187
H	-0.658164	-1.300228	3.440095
H	-1.936079	0.996552	-2.017937
C	-0.740354	-2.502779	0.815115
H	-0.781614	-3.388507	1.467139
C	-0.374594	-2.607507	-0.533856
H	-0.107043	-3.584008	-0.966223
C	-0.383504	-1.451280	-1.340260
H	-0.148201	-1.508383	-2.413565
Ru	-1.289098	1.696635	1.585532
C	-2.327821	0.633866	4.354576
H	-1.655264	0.115643	5.088163
H	-2.233084	1.718979	4.559654
C	0.882862	3.301292	-0.829482
C	-2.228352	3.696668	-1.314113
C	-3.580219	3.113630	-0.839817
H	-3.725172	2.061080	-1.164367
H	-3.667339	3.135569	0.265156
H	-4.411115	3.712864	-1.273223
C	-2.210073	3.714218	-2.856844
H	-1.291107	4.164517	-3.273663
H	-2.326128	2.701284	-3.294948
H	-3.067692	4.320867	-3.223225

C	-2.088786	5.130799	-0.762198
H	-2.972292	5.732662	-1.068779
H	-2.042857	5.144253	0.346036
H	-1.190148	5.646203	-1.157063
C	1.088340	3.881711	-2.240207
H	2.159242	4.151393	-2.375806
H	0.831682	3.155661	-3.040233
H	0.498621	4.805146	-2.405181
C	1.176052	4.378189	0.237476
H	0.506605	5.255692	0.150942
H	1.064965	3.967414	1.260738
H	2.220961	4.740405	0.120359
C	1.865615	2.124151	-0.623192
H	1.694513	1.616481	0.348477
H	1.797721	1.364512	-1.429103
H	2.907190	2.513024	-0.626752
H	0.248376	1.927670	1.827555
C	-1.581842	3.315075	2.422539
O	-1.746984	4.376237	2.912117
P	-0.880932	2.586126	-0.494031
C	-3.782535	0.201770	4.612146
H	-4.467905	0.748090	3.931267
H	-3.929912	-0.885983	4.440658
H	-4.081490	0.416361	5.660481

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TS-EF-NEt SCF Done: -1327.27419446 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -910.23 cm⁻¹

C	-0.604818	0.047208	-0.747063
H	-0.859329	1.234974	-2.560154
N	-1.286918	0.479335	3.192138
C	-0.189490	-0.425633	2.903149
C	-0.118091	-0.758035	1.431227
N	-0.617273	0.197854	0.606084
C	-1.293720	1.127129	-1.545093
H	-2.463663	0.686564	2.331476
H	-0.240416	-1.378335	3.485447
H	0.802091	0.048709	3.168872
H	-2.356279	0.824740	-1.678314
C	0.455579	-1.926845	0.903466
H	0.851043	-2.694817	1.584743
C	0.522177	-2.084512	-0.489612
H	0.981550	-2.985057	-0.926262
C	-0.015529	-1.089687	-1.324488
H	0.004911	-1.195194	-2.419335
Ru	-1.352326	1.935893	1.566550
C	-1.322548	0.962800	4.565476
H	-0.377135	1.517492	4.813198
H	-2.139129	1.712506	4.631696
C	0.230170	3.669905	-1.155259

C	-2.938094	3.595485	-1.286153
C	-4.145280	2.910200	-0.606772
H	-5.083696	3.357443	-1.001784
H	-4.184464	1.819018	-0.808120
H	-4.125218	3.040139	0.492311
C	-3.094293	3.463313	-2.816421
H	-2.277387	3.947076	-3.381532
H	-3.160422	2.405017	-3.142666
H	-4.043359	3.953734	-3.126453
C	-2.922896	5.081919	-0.870678
H	-3.907145	5.540959	-1.109213
H	-2.753391	5.201479	0.219336
H	-2.150567	5.663597	-1.412396
C	0.185728	4.174509	-2.609434
H	1.180963	4.590258	-2.881519
H	-0.036235	3.363211	-3.334317
H	-0.554472	4.986086	-2.754768
C	0.485318	4.846759	-0.188088
H	-0.303224	5.622071	-0.241643
H	0.547583	4.490162	0.859331
H	1.450674	5.333181	-0.448956
C	1.393342	2.659158	-1.014205
H	1.418575	2.212400	0.000687
H	1.340313	1.841220	-1.762169
H	2.355653	3.190962	-1.178868
H	0.192338	2.413591	1.742985
C	-1.822990	3.517392	2.400208
O	-2.086005	4.551238	2.897225
P	-1.362659	2.746930	-0.575383
H	-3.008653	1.117960	1.614526
C	-1.565361	-0.133664	5.617042
H	-2.491324	-0.701324	5.384728
H	-0.726031	-0.859030	5.672879
H	-1.675783	0.314383	6.626989

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A-NCF3 SCF Done: -1584.67566566 A.U.

Number of imaginary frequencies = 0

C	-0.852368	-0.168248	-0.817048
H	-0.252086	1.112439	-2.480615
N	-2.294397	0.436306	2.836987
C	-1.756176	-0.913179	2.699370
C	-1.284045	-1.164283	1.293734
N	-1.215839	-0.064003	0.496881
C	-0.982895	1.085166	-1.646938
H	-2.504896	-1.692434	2.976015
H	-0.883181	-1.079714	3.382984
H	-1.991779	1.068651	-2.115338
C	-0.920678	-2.431336	0.803133
H	-0.978606	-3.307605	1.466076
C	-0.486052	-2.548456	-0.523329

H	-0.183769	-3.527607	-0.926028
C	-0.461868	-1.405872	-1.346412
H	-0.158784	-1.474479	-2.401687
Ru	-1.574677	1.780366	1.457926
C	0.876800	3.238759	-0.745605
C	-2.161444	3.810875	-1.479980
C	-3.573289	3.312997	-1.088713
H	-3.757899	2.264318	-1.405717
H	-3.737328	3.368010	0.006727
H	-4.338383	3.947796	-1.586922
C	-2.036261	3.802239	-3.017779
H	-1.058559	4.175045	-3.373771
H	-2.199876	2.794578	-3.452331
H	-2.817456	4.466813	-3.448223
C	-1.973481	5.242791	-0.936744
H	-2.795800	5.889760	-1.312840
H	-2.004582	5.273682	0.171351
H	-1.020397	5.697053	-1.274500
C	1.227888	3.798954	-2.135988
H	2.318731	4.011312	-2.182211
H	1.000659	3.082240	-2.952962
H	0.702600	4.750591	-2.350705
C	1.141975	4.303073	0.341676
H	0.528640	5.214305	0.204786
H	0.933858	3.904978	1.354540
H	2.210155	4.609199	0.303905
C	1.767522	2.006613	-0.457809
H	1.494229	1.518264	0.500059
H	1.716772	1.244649	-1.262746
H	2.827305	2.333379	-0.382486
H	-0.074243	1.910600	1.869555
C	-1.815058	3.425623	2.269197
O	-1.916048	4.501824	2.730988
P	-0.943011	2.633940	-0.567019
C	-2.642496	0.756816	4.143292
F	-3.381739	1.890867	4.207687
F	-3.376544	-0.238347	4.753127
F	-1.559338	0.954865	4.987678

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TS-EF-NCF3 SCF Done: -1585.82950499 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -1131.09 cm⁻¹

C	-0.631241	0.034523	-0.768544
H	-0.771470	1.264701	-2.566184
N	-1.550717	0.373586	3.130743
C	-0.460001	-0.571936	2.886682
C	-0.303207	-0.840949	1.407609
N	-0.722012	0.155026	0.585604
C	-1.264440	1.135998	-1.580932
H	-2.550174	0.573926	2.315328

H	-0.612691	-1.529229	3.433899
H	0.503144	-0.130191	3.249444
H	-2.318187	0.839975	-1.781373
C	0.275158	-2.009537	0.887897
H	0.601979	-2.807356	1.571153
C	0.434007	-2.128894	-0.501845
H	0.902115	-3.027104	-0.933360
C	-0.028521	-1.099330	-1.338431
H	0.057236	-1.176126	-2.432448
Ru	-1.492187	1.897359	1.515772
C	0.224506	3.680652	-1.058077
C	-2.933484	3.594707	-1.350466
C	-4.173878	2.899687	-0.745161
H	-5.088658	3.349000	-1.189800
H	-4.197344	1.810293	-0.956854
H	-4.217184	3.017848	0.354126
C	-3.009504	3.482136	-2.889108
H	-2.162455	3.967640	-3.406154
H	-3.066853	2.428791	-3.232338
H	-3.938496	3.983085	-3.239452
C	-2.941104	5.076609	-0.918068
H	-3.912914	5.535238	-1.203034
H	-2.830356	5.186722	0.179972
H	-2.143782	5.665694	-1.413373
C	0.249393	4.213108	-2.503109
H	1.253964	4.641020	-2.714234
H	0.072790	3.414691	-3.254257
H	-0.488546	5.022201	-2.671104
C	0.419899	4.839729	-0.056359
H	-0.368629	5.612308	-0.138036
H	0.428218	4.463497	0.985826
H	1.395141	5.334756	-0.256123
C	1.384907	2.673324	-0.877811
H	1.359876	2.208570	0.129061
H	1.375284	1.870307	-1.643684
H	2.350809	3.213353	-0.982378
H	0.049993	2.374401	1.785238
C	-2.031581	3.479485	2.310515
O	-2.340326	4.512443	2.775370
P	-1.389603	2.735513	-0.586773
H	-3.104229	1.081382	1.468103
C	-1.731920	0.746410	4.464075
F	-2.844661	1.502266	4.603330
F	-1.866796	-0.343684	5.290304
F	-0.682225	1.460417	4.984823

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A-NtBu SCF Done: -1404.77509875 A.U.

Number of imaginary frequencies = 0

C	-0.224705	-5.097090	-0.749954
H	0.159706	-5.045892	-2.900480

N	-0.897844	-2.338863	2.062142
C	-0.570100	-3.637341	2.629858
C	-0.353917	-4.692525	1.582760
N	-0.320029	-4.232259	0.305582
C	-0.392887	-4.486295	-2.118688
H	-1.359554	-4.028868	3.317610
H	0.362026	-3.603381	3.258572
H	-1.471374	-4.559948	-2.381741
C	-0.210594	-6.064310	1.859691
H	-0.229974	-6.412936	2.903456
C	-0.042728	-6.959670	0.795518
H	0.084306	-8.036571	0.986207
C	-0.065912	-6.470281	-0.526873
H	0.021721	-7.153124	-1.385057
Ru	-0.273029	-2.132855	0.131715
C	1.805682	-2.593449	-2.796672
C	-1.243516	-1.929655	-3.372700
C	-2.592418	-1.850584	-2.619663
H	-2.942772	-2.845646	-2.271592
H	-2.523523	-1.191774	-1.730465
H	-3.371204	-1.443537	-3.301577
C	-1.432313	-2.786293	-4.642274
H	-0.514593	-2.862132	-5.253479
H	-1.779349	-3.814932	-4.413017
H	-2.214497	-2.320131	-5.281493
C	-0.807106	-0.499815	-3.755144
H	-1.618711	-0.010148	-4.336788
H	-0.610202	0.127002	-2.861726
H	0.099334	-0.495567	-4.393247
C	1.921187	-2.945750	-4.290626
H	2.995605	-3.006286	-4.573135
H	1.465426	-3.929200	-4.531880
H	1.457714	-2.177792	-4.941134
C	2.389178	-1.188425	-2.532567
H	1.853167	-0.392871	-3.084976
H	2.350219	-0.935370	-1.454541
H	3.452874	-1.163799	-2.856056
C	2.614192	-3.623685	-1.972646
H	2.489770	-3.460129	-0.882331
H	2.330659	-4.671562	-2.201675
H	3.694306	-3.516269	-2.213134
H	1.296131	-2.113237	0.226080
C	-0.147742	-0.316171	-0.148855
O	-0.009586	0.827473	-0.414045
P	0.008741	-2.643584	-2.093019
C	-1.059582	-1.255430	3.075808
C	0.312953	-0.605841	3.383021
C	-1.671461	-1.779767	4.401953
H	-2.625400	-2.318303	4.218514
H	-0.986078	-2.451776	4.958139
H	-1.893983	-0.923831	5.071056

H	1.033260	-1.368072	3.749633
H	0.225687	0.182584	4.160715
H	0.735135	-0.155695	2.463235
C	-2.033189	-0.193408	2.521275
H	-1.646508	0.262913	1.591766
H	-3.013679	-0.659051	2.290950
H	-2.189326	0.620178	3.260523

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TS-EF-NtBu SCF Done: -1405.93767813 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -893.84 cm⁻¹

C	-0.828807	0.029756	-0.890952
H	-0.812730	1.345944	-2.631461
N	-1.878573	0.237559	2.996245
C	-0.801686	-0.704045	2.737227
C	-0.615119	-0.944469	1.259582
N	-0.958766	0.096754	0.462576
C	-1.348893	1.212707	-1.669473
H	-2.922846	0.616461	2.004294
H	-0.956659	-1.692315	3.231823
H	0.193918	-0.324210	3.110667
H	-2.415601	1.015824	-1.917266
C	-0.083021	-2.122039	0.706260
H	0.187281	-2.960039	1.365812
C	0.102375	-2.198956	-0.682384
H	0.530878	-3.105653	-1.137390
C	-0.277082	-1.113619	-1.491389
H	-0.161437	-1.152097	-2.584700
Ru	-1.647216	1.830042	1.477284
C	0.342036	3.572106	-0.949769
C	-2.790929	3.800190	-1.380844
C	-4.115005	3.196854	-0.859694
H	-4.966454	3.748343	-1.315246
H	-4.229063	2.125133	-1.126162
H	-4.193790	3.270642	0.241828
C	-2.810510	3.769839	-2.924535
H	-1.897344	4.192933	-3.380518
H	-2.953138	2.744710	-3.323884
H	-3.669747	4.376484	-3.286425
C	-2.683074	5.253848	-0.872584
H	-3.595899	5.814730	-1.170116
H	-2.608455	5.299531	0.233237
H	-1.815010	5.789212	-1.306208
C	0.487956	4.167720	-2.362392
H	1.536492	4.509721	-2.506977
H	0.275909	3.425619	-3.160624
H	-0.164573	5.048891	-2.521271
C	0.596079	4.658612	0.118186
H	-0.113360	5.505152	0.043936
H	0.520194	4.233874	1.138895

H	1.621182	5.068823	-0.013462
C	1.395654	2.453210	-0.769422
H	1.280714	1.945537	0.210033
H	1.349372	1.690093	-1.573621
H	2.410968	2.904600	-0.804851
H	-0.097282	2.159751	1.839554
C	-2.061685	3.418205	2.319673
O	-2.278686	4.468082	2.809149
P	-1.372897	2.763011	-0.593657
H	-3.351110	1.149862	1.283859
C	-2.155490	0.516961	4.427167
C	-1.037651	1.369167	5.074245
C	-2.302720	-0.811433	5.216508
H	-3.029733	-1.484512	4.714788
H	-1.338834	-1.351056	5.322425
H	-2.671292	-0.607324	6.242677
H	-0.052568	0.861195	5.005071
H	-1.243095	1.551254	6.150111
H	-0.948806	2.345684	4.558849
C	-3.501503	1.264588	4.528576
H	-4.317843	0.659924	4.080649
H	-3.755443	1.461179	5.590258
H	-3.468239	2.237291	4.002053

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A-NCH2OCH3 SCF Done: -1401.35640193 A.U.

Number of imaginary frequencies = 0

C	-0.475962	-0.336539	-0.664578
H	-0.287496	1.010774	-2.374453
N	-1.375090	0.147927	3.176898
C	-0.814942	-1.168688	2.924233
C	-0.488782	-1.370242	1.471736
N	-0.642792	-0.264687	0.691162
C	-0.891974	0.880912	-1.453690
H	-1.505222	-1.981576	3.257111
H	0.127074	-1.329334	3.518556
H	-1.937646	0.706637	-1.791037
C	-0.068091	-2.591364	0.915754
H	0.057228	-3.468898	1.567867
C	0.184599	-2.663393	-0.460281
H	0.529899	-3.604206	-0.916228
C	-0.037718	-1.525604	-1.261846
H	0.106167	-1.564277	-2.351940
Ru	-1.077032	1.520533	1.728733
C	-1.641310	0.365648	4.564744
H	-0.718537	0.203402	5.201559
H	-1.978479	1.417146	4.718972
C	0.688131	3.338068	-0.854443
C	-2.478166	3.367025	-1.075410
C	-3.707864	2.640049	-0.482016
H	-3.758517	1.572967	-0.786716
H	-3.703469	2.670016	0.626139
H	-4.636404	3.133307	-0.844821

C	-2.594839	3.364987	-2.614051
H	-1.770593	3.907206	-3.111872
H	-2.636696	2.339597	-3.036085
H	-3.542493	3.869258	-2.906056
C	-2.456974	4.815617	-0.544328
H	-3.425476	5.309050	-0.779214
H	-2.322052	4.850805	0.556046
H	-1.658254	5.422884	-1.015852
C	0.705455	3.923577	-2.277916
H	1.721964	4.315595	-2.503304
H	0.470133	3.163876	-3.052788
H	-0.001012	4.769431	-2.393053
C	0.942473	4.453100	0.183225
H	0.169663	5.245374	0.154820
H	0.969105	4.043271	1.212568
H	1.923594	4.933841	-0.024003
C	1.814399	2.284458	-0.730247
H	1.787938	1.773075	0.254054
H	1.766076	1.511350	-1.524615
H	2.799701	2.790612	-0.825256
H	0.431005	1.940332	1.842960
C	-1.499015	3.099669	2.586278
O	-1.753525	4.136955	3.087256
P	-0.946722	2.428879	-0.374808
O	-2.650389	-0.552783	5.009476
C	-2.872152	-0.486844	6.399218
H	-3.653857	-1.230925	6.654203
H	-1.950793	-0.724544	6.992124
H	-3.228628	0.522498	6.728764

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TS-EF-NCH2OCH3 SCF Done: -1402.51843932 A.U.

Number of imaginary frequencies = 1

Imaginary frequency = -944.69 cm⁻¹

C	-0.435905	0.014817	-0.739177
H	-0.859123	1.186486	-2.531540
N	-0.928394	0.407257	3.219993
C	0.200254	-0.445428	2.880079
C	0.212105	-0.765962	1.405602
N	-0.383998	0.162899	0.613197
C	-1.230845	1.051371	-1.495099
H	-2.154040	0.530149	2.440217
H	0.211693	-1.383997	3.480254
H	1.172537	0.084539	3.101717
H	-2.278540	0.684591	-1.572389
C	0.821884	-1.899012	0.841761
H	1.293365	-2.645069	1.498398
C	0.823712	-2.048979	-0.553524
H	1.309414	-2.920913	-1.018793
C	0.186113	-1.084822	-1.353274
H	0.153275	-1.186888	-2.448134
Ru	-1.175497	1.859906	1.613205
C	-0.913401	0.875222	4.566014
H	0.044143	1.429803	4.805051
H	-1.760382	1.590344	4.713435

C	0.154838	3.682150	-1.176324
C	-3.005620	3.416790	-1.139447
C	-4.131090	2.663257	-0.394968
H	-5.114535	3.045472	-0.746100
H	-4.109636	1.569608	-0.584592
H	-4.066094	2.806709	0.700534
C	-3.236639	3.269016	-2.659010
H	-2.480666	3.795440	-3.269023
H	-3.261358	2.207305	-2.979733
H	-4.227257	3.704132	-2.916927
C	-3.057262	4.903505	-0.727409
H	-4.079936	5.299703	-0.910298
H	-2.834576	5.039220	0.350998
H	-2.354640	5.529218	-1.313226
C	0.001612	4.181714	-2.624897
H	0.953040	4.658637	-2.948180
H	-0.207144	3.357463	-3.338949
H	-0.794524	4.945101	-2.728479
C	0.387746	4.873251	-0.221097
H	-0.450811	5.595943	-0.227402
H	0.532173	4.522015	0.819991
H	1.303437	5.420659	-0.534598
C	1.383850	2.745098	-1.100221
H	1.491308	2.301411	-0.089423
H	1.341297	1.924872	-1.846300
H	2.301167	3.335282	-1.314867
H	0.342633	2.436147	1.706766
C	-1.709662	3.410293	2.465165
O	-2.018216	4.426594	2.971961
P	-1.346148	2.663778	-0.519007
H	-2.765606	0.929207	1.747805
O	-1.033896	-0.236731	5.461477
C	-0.868596	0.129593	6.811825
H	-0.966937	-0.787586	7.427343
H	0.135838	0.584063	7.013501
H	-1.641110	0.865065	7.154086