Influence of Geometry on Reductive Elimination of Hydrocarbyl-Palladium-Carbene Complexes

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Supporting Information

1. Bite-Angle Complexes

CX-A80
B3lyp/lanl2dz optimized geometry
Energy = -723.746185 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428429
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.808902

Atom	x-coord	y-coord	z-coord
C	-4.195066	-0.121414	0.738586
N	-2.846847	-0.242027	1.118123
C	-2.028350	-0.303674	0.012599
N	-2.886638	-0.223940	-1.061827
C	-4.220249	-0.110231	-0.631253
Pd	-0.004683	-0.536365	-0.024718
C	-0.388965	-2.588908	-0.119125
C	-2.478394	-0.293894	-2.473262
C	-2.386938	-0.328094	2.512322
P	0.710532	1.838125	0.001153
C	2.054275	2.619512	1.089499
P	2.457815	-0.828665	0.007880
C	3.011795	-2.584519	-0.427561
C	1.102128	2.526052	-1.719902
C	-0.725247	2.982157	0.482771
C	3.201787	-0.661557	1.737322
C	3.652021	0.128919	-1.105574
H	0.137050	-2.973130	-1.001764
H	0.026863	-3.031741	0.796072
H	-1.453022	-2.828439	-0.189909
H	-1.390632	-0.380380	-2.515675
H	-2.922484	-1.172350	-2.953287
H	-2.796076	0.607425	-3.008731
H	-1.300587	-0.438226	2.512366
H	-2.663574	0.577123	3.063773
H	-2.831900	-1.199062	3.004758
H	-5.049713	-0.036506	-1.315659
H	-4.998827	-0.059018	1.454064
H	-0.450761	4.033805	0.343724
H	-1.598168	2.752582	-0.135215
H	-0.988206	2.818681	1.532746
H	3.053978	2.248778	0.856448
H	2.040772	3.704221	0.935377
H	1.835234	2.414706	2.142413
H	3.666752	1.198857	-0.893704
H	4.661554	-0.269402	-0.956354
H	3.368445	-0.023264	-2.151704
H	2.797200	-2.790047	-1.480994
H	4.087370	-2.697909	-0.252298
H	2.469016	-3.309180	0.184502
H	2.961497	0.302038	2.188411
H	2.783021	-1.453220	2.366977
H	4.290404	-0.780783	1.696590

H	1.389050	3.581590	-1.652531
H	0.202796	2.443807	-2.339065
H	1.904790	1.965603	-2.202399

CX-A90

B3lyp/lanl2dz optimized geometry
Energy = -723.757461 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428167
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.820183

Atom	x-coord	y-coord	z-coord
C	4.141772	-0.427646	-0.661557
N	2.799110	-0.417015	-1.079636
C	1.947237	-0.418764	0.002616
N	2.778159	-0.431303	1.100340
C	4.128383	-0.436162	0.708390
Pd	-0.093000	-0.488783	-0.016332
C	0.152929	-2.571295	-0.043435
C	2.324587	-0.474429	2.498587
C	2.372398	-0.454440	-2.486820
P	-0.405061	1.971441	0.001469
C	-0.806062	2.746990	-1.676312
P	-2.553243	-0.800940	-0.003542
C	-3.172997	-2.510498	-0.504496
C	-1.667328	2.793862	1.147997
C	1.154185	2.930777	0.478984
C	-3.643131	0.290941	-1.095197
C	-3.321955	-0.599637	1.709149
H	-0.344143	-2.971565	0.850304
H	-0.335714	-2.945979	-0.951004
H	1.202842	-2.875153	-0.040344
H	1.232804	-0.489775	2.508141
H	2.696374	-1.379897	2.989399
H	2.683987	0.404029	3.045667
H	1.281055	-0.434904	-2.518694
H	2.771205	0.408584	-3.030826
H	2.724264	-1.374506	-2.965138
H	4.941057	-0.448294	1.416396
H	4.968084	-0.432138	-1.353676
H	1.000264	4.008381	0.352294
H	1.405553	2.729195	1.525410
H	1.990889	2.609914	-0.148686
H	-1.722018	2.317329	-2.089588
H	-0.929151	3.831501	-1.578180
H	0.015013	2.545904	-2.372062
H	-3.103865	0.391742	2.114522
H	-4.408034	-0.738015	1.661394
H	-2.897320	-1.351356	2.382008
H	-2.699547	-3.278949	0.111620
H	-4.259701	-2.566846	-0.377702
H	-2.924395	-2.703621	-1.552640
H	-3.568535	1.342625	-0.807302
H	-3.337141	0.186158	-2.140840

H	-4.688694	-0.022545	-1.001135
H	-1.577426	3.883586	1.078551
H	-1.477138	2.489557	2.182249
H	-2.688997	2.511579	0.879872

CX-A100

B3lyp/lanl2dz optimized geometry
Energy = -723.758963 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428079
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.822104

Atom	x-coord	y-coord	z-coord
C	4.018474	-0.808657	-0.687551
N	2.679872	-0.657180	-1.091730
C	1.845152	-0.558584	-0.001208
N	2.681753	-0.653097	1.088143
C	4.019649	-0.805941	0.682414
Pd	-0.198411	-0.401408	-0.002800
C	-0.138539	-2.509656	0.005907
C	2.239703	-0.638846	2.490759
C	2.236731	-0.650622	-2.494228
P	-0.059787	2.074713	-0.005849
C	-0.741133	2.971357	-1.524246
P	-2.660985	-0.694868	-0.006057
C	-3.287682	-1.980297	-1.233206
C	-0.917469	2.983522	1.413820
C	1.683850	2.793260	0.102543
C	-3.815009	0.756036	-0.367963
C	-3.321129	-1.316175	1.647330
H	-0.917015	-2.908716	0.667167
H	-0.315498	-2.834970	-1.027577
H	0.833148	-2.881120	0.342256
H	1.149521	-0.579433	2.508774
H	2.553382	-1.558520	2.995322
H	2.663156	0.222097	3.019882
H	1.147775	-0.572252	-2.512585
H	2.674767	0.197271	-3.032309
H	2.534027	-1.581014	-2.988989
H	4.834073	-0.902017	1.381960
H	4.831501	-0.908535	-1.388190
H	1.647805	3.888343	0.091558
H	2.165230	2.462056	1.027926
H	2.283620	2.447386	-0.744691
H	-1.809732	2.764860	-1.631499
H	-0.595207	4.053378	-1.429900
H	-0.226248	2.619709	-2.424062
H	-3.141034	-0.564413	2.422320
H	-4.397078	-1.513132	1.581893
H	-2.805971	-2.238197	1.930966
H	-2.774090	-2.931570	-1.075361
H	-4.365983	-2.128886	-1.107630
H	-3.089846	-1.640331	-2.254684
H	-3.673999	1.549782	0.371712

H	-3.611113	1.156859	-1.365861
H	-4.858163	0.423255	-0.329771
H	-0.758600	4.064653	1.330068
H	-0.514350	2.637991	2.371173
H	-1.992535	2.782106	1.396408

CX-A110

B3lyp/lanl2dz optimized geometry
Energy = -723.754521 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428087
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.817863

Atom	x-coord	y-coord	z-coord
C	3.826528	-1.223305	-0.700175
N	2.522288	-0.877632	-1.097195
C	1.713669	-0.666151	-0.001853
N	2.533906	-0.885999	1.083145
C	3.833903	-1.228162	0.669815
Pd	-0.313425	-0.296429	0.006972
C	-0.406639	-2.413433	0.013811
C	2.097277	-0.850446	2.487819
C	2.070123	-0.839531	-2.497016
P	0.302268	2.105921	0.001056
C	-1.001442	3.472589	0.106032
P	-2.781439	-0.539566	-0.006987
C	-3.448688	-1.774391	-1.263672
C	1.463447	2.597614	1.407640
C	1.286827	2.646536	-1.518188
C	-3.861091	0.971170	-0.352549
C	-3.484864	-1.156561	1.629902
H	-1.214319	-2.773082	0.660519
H	-0.584248	-2.721448	-1.024360
H	0.535233	-2.843575	0.364689
H	1.048379	-0.548905	2.516649
H	2.193229	-1.843918	2.938529
H	2.699516	-0.136745	3.059594
H	1.047490	-0.458378	-2.521800
H	2.718504	-0.186242	-3.090046
H	2.084631	-1.846503	-2.927408
H	4.629565	-1.441974	1.364911
H	4.614169	-1.433457	-1.405424
H	1.593191	3.694028	-1.419917
H	2.180080	2.024392	-1.623771
H	0.671148	2.540219	-2.417120
H	-1.557597	3.381624	1.044760
H	-0.529035	4.460770	0.067975
H	-1.702937	3.380434	-0.728622
H	-3.291840	-0.416979	2.413414
H	-4.566039	-1.313186	1.544491

H	-3.009889	-2.099116	1.915541
H	-2.987945	-2.753691	-1.116148
H	-4.534884	-1.868553	-1.154520
H	-3.220394	-1.426854	-2.276141
H	-3.660959	1.749699	0.389498
H	-3.634605	1.366769	-1.347982
H	-4.922633	0.702648	-0.310380
H	1.723895	3.659164	1.331191
H	2.379858	2.002774	1.357589
H	0.975906	2.420333	2.371485

CX-A120

B3lyp/lanl2dz optimized geometry
Energy = -723.744473 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428404
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.808203

Atom	x-coord	y-coord	z-coord
C	3.619176	-1.612840	-0.642995
N	2.383183	-1.093426	-1.069200
C	1.591418	-0.760159	0.007935
N	2.352752	-1.079934	1.111339
C	3.599996	-1.604313	0.726748
Pd	-0.390956	-0.163561	-0.012185
C	-0.621207	-2.286705	-0.087799
C	1.891029	-0.990532	2.505814
C	1.965739	-1.018041	-2.478451
P	0.644813	2.089787	-0.009964
C	-0.424787	3.653091	-0.010367
P	-2.860251	-0.393269	0.002397
C	-3.579279	-1.515827	-1.329481
C	1.795702	2.440201	1.446444
C	1.779677	2.429452	-1.481412
C	-3.929472	1.153375	-0.195887
C	-3.540466	-1.111878	1.608639
H	-1.463761	-2.644567	0.510159
H	-0.776043	-2.528466	-1.146709
H	0.282532	-2.785470	0.270871
H	0.906131	-0.519672	2.515849
H	1.809083	-1.992326	2.940844
H	2.588264	-0.395029	3.103987
H	0.997915	-0.515886	-2.529659
H	2.700106	-0.456733	-3.065163
H	1.866053	-2.025209	-2.896874
H	4.344986	-1.918754	1.439565
H	4.383586	-1.936215	-1.330785
H	2.221014	3.428076	-1.389310
H	2.583038	1.689024	-1.516524
H	1.206316	2.380602	-2.412431

H	-1.054129	3.666526	0.885380
H	0.196664	4.555945	-0.024134
H	-1.073595	3.652004	-0.892158
H	-3.316585	-0.428902	2.434198
H	-4.626532	-1.237039	1.533731
H	-3.084812	-2.081784	1.824571
H	-3.143960	-2.515406	-1.268570
H	-4.665095	-1.589887	-1.203369
H	-3.363061	-1.095576	-2.316721
H	-3.698790	1.863486	0.604512
H	-3.713279	1.628618	-1.158077
H	-4.995157	0.900971	-0.153858
H	2.231655	3.440282	1.345160
H	2.602662	1.703250	1.475065
H	1.233626	2.392754	2.384371

CX-A130

B3lyp/lanl2dz optimized geometry
Energy = -723.728431 a.u.
Enthalpy Correction (inc. ZPVE) = 0.427513
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.792304

Atom	x-coord	y-coord	z-coord
Pd	0.450524	-0.016401	0.000639
P	-0.961162	2.022536	-0.016109
P	2.919906	-0.245609	0.004632
C	0.790933	-2.152655	-0.052638
H	1.691464	-2.479412	0.470976
H	-0.054740	-2.683166	0.390114
H	0.861843	-2.398749	-1.118786
C	-1.467654	-0.833522	0.008805
N	-2.194265	-1.275868	-1.075021
C	-1.768436	-1.166873	-2.479631
H	-0.871438	-0.546871	-2.526461
H	-1.536184	-2.159162	-2.880735
H	-2.558824	-0.711514	-3.084762
N	-2.196387	-1.240342	1.105878
C	-1.760186	-1.099068	2.504351
H	-0.851926	-0.493999	2.526744
H	-2.538214	-0.614502	3.102642
H	-1.539840	-2.083576	2.931029
C	-3.358854	-1.947233	-0.659227
H	-4.065929	-2.371405	-1.353563
C	-3.359932	-1.925146	0.710405
H	-4.068243	-2.326856	1.416768
C	3.991273	1.302875	-0.197464
C	-2.134432	2.176247	-1.490125
C	-2.158633	2.202582	1.435232
H	-2.723023	3.135593	1.328930

H	-2.861486	1.366443	1.459527
H	-1.601016	2.233170	2.376303
C	-0.172535	3.747859	-0.024728
H	0.465966	3.851393	-0.908058
H	-0.936422	4.534108	-0.039029
H	0.449593	3.868104	0.868178
C	3.642436	-1.345965	-1.345697
H	3.400915	-0.920749	-2.324939
H	4.731701	-1.389156	-1.235849
H	3.238848	-2.358527	-1.290535
C	3.623995	-0.953479	1.606355
H	3.154880	-1.907123	1.859744
H	4.704720	-1.102771	1.504317
H	3.438678	-0.245148	2.420070
H	3.775211	1.773238	-1.162215
H	3.755728	2.016905	0.598123
H	5.057824	1.053769	-0.151967
H	-2.702116	3.109838	-1.409413
H	-2.835580	1.338596	-1.512237
H	-1.560917	2.191806	-2.421984

2. Bite-Angle Transition Structures

TS-A80
B3lyp/lanl2dz optimized geometry
Energy = -723.705201 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426404
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.764385

Atom	x-coord	y-coord	z-coord
N	-2.854214	-0.123629	-1.083319
C	-4.098054	0.334693	-0.613946
C	-4.075285	0.255195	0.752255
N	-2.817701	-0.250635	1.124054
C	-2.040817	-0.523047	-0.011869
C	-2.405496	-0.532318	2.503072
Pd	-0.017634	-0.471964	-0.036427
P	0.890224	1.834297	0.049338
C	1.445918	2.486736	-1.639758
C	-2.495550	-0.236386	-2.501666
P	2.412709	-0.965736	-0.031368
C	3.167467	-1.007906	1.708494
C	-1.481665	-2.265903	-0.136613

C	3.774010	-0.110489	-1.044012
C	2.777138	-2.757112	-0.560376
C	-0.421655	3.137478	0.479833
C	2.269489	2.418354	1.212799
H	-1.079672	-2.585420	-1.103058
H	-0.922505	-2.715912	0.691650
H	-2.514170	-2.623039	-0.065685
H	-1.408767	-0.301182	-2.595870
H	-2.951272	-1.123982	-2.958488
H	-2.837791	0.651804	-3.042932
H	-1.318147	-0.448481	2.580778
H	-2.860604	0.198238	3.178854
H	-2.712969	-1.538657	2.815679
H	-4.869375	0.691892	-1.276768
H	-4.823897	0.531824	1.476776
H	-0.033723	4.152383	0.332896
H	-1.299904	2.989670	-0.156036
H	-0.725771	3.019546	1.525132
H	3.224741	1.932467	1.007015
H	2.395191	3.500362	1.092667
H	1.981995	2.211805	2.248485
H	3.902847	0.939670	-0.774112
H	4.721659	-0.632642	-0.871780
H	3.528775	-0.175633	-2.109126
H	2.552731	-2.879332	-1.625413
H	3.828085	-3.016111	-0.385935
H	2.141662	-3.442538	0.010048
H	1.873613	3.490925	-1.538792
H	2.181671	1.826351	-2.100695
H	0.569247	2.540863	-2.293445
H	4.232055	-1.263146	1.657547
H	3.053144	-0.050140	2.219880
H	2.648714	-1.775576	2.292402

TS-A90

B3lyp/lanl2dz optimized geometry
Energy = -723.718598 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426372
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.777815

Atom	x-coord	y-coord	z-coord
Pd	0.080471	-0.437845	-0.029178
P	0.589518	1.988363	0.040024
P	2.507555	-0.947338	-0.020049
C	-1.233141	-2.347532	-0.122258
H	-0.688347	-2.649859	-1.023157
H	-0.763990	-2.755064	0.778817
H	-2.243901	-2.762765	-0.191515
C	-1.935746	-0.637980	-0.015449
N	-2.772327	-0.304812	-1.090108
C	-2.394320	-0.403536	-2.504124
H	-1.316147	-0.252652	-2.602737
H	-2.660140	-1.383305	-2.921364

H	-2.909681	0.372859	-3.078155
N	-2.738406	-0.435962	1.115360
C	-2.312521	-0.673591	2.499025
H	-1.223288	-0.604325	2.557301
H	-2.744989	0.088275	3.155589
H	-2.631194	-1.663113	2.850526
C	-4.055445	0.040295	-0.628435
H	-4.851173	0.328806	-1.295835
C	-4.033967	-0.039812	0.737567
H	-4.807379	0.169436	1.458635
C	3.334368	-0.881850	1.681672
C	1.140019	2.734036	-1.608831
C	-0.884812	3.094081	0.471316
H	-0.627144	4.153178	0.355601
H	-1.727004	2.852720	-0.184636
H	-1.188412	2.912376	1.507379
C	1.891685	2.652994	1.240908
H	2.886125	2.275461	0.987494
H	1.912240	3.747944	1.197192
H	1.644929	2.343377	2.261203
C	3.735286	0.025131	-1.085874
H	3.791107	1.070086	-0.767032
H	4.733809	-0.418143	-1.001064
H	3.422316	-0.008766	-2.134536
C	2.939753	-2.715469	-0.551829
H	2.679904	-2.857583	-1.606249
H	4.009142	-2.916196	-0.419135
H	2.366404	-3.430539	0.047321
H	1.386543	3.795087	-1.486533
H	2.014330	2.204167	-1.994851
H	0.327213	2.640672	-2.336186
H	4.401135	-1.119779	1.601773
H	3.221188	0.110991	2.125622
H	2.856809	-1.613025	2.342188

TS-A100

B3lyp/lanl2dz optimized geometry
Energy = -723.722673 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426119
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.782477

Atom	x-coord	y-coord	z-coord
Pd	0.186126	-0.368390	-0.005964
P	0.242718	2.110934	0.006208
P	2.617984	-0.854669	-0.005137
C	-0.903294	-2.418113	-0.011385
H	-0.334782	-2.716045	-0.898240
H	-0.394704	-2.723751	0.908256
H	-1.871501	-2.927576	-0.047499
C	-1.803260	-0.772092	-0.001328
N	-2.650735	-0.592107	-1.101225
C	-2.240193	-0.717965	-2.504380
H	-1.160774	-0.564692	-2.578536

H	-2.491808	-1.708376	-2.904289
H	-2.743496	0.043331	-3.109298
N	-2.642785	-0.607958	1.106316
C	-2.218313	-0.736426	2.505039
H	-1.144426	-0.545345	2.574541
H	-2.744564	-0.000410	3.121401
H	-2.432300	-1.739370	2.895334
C	-3.973598	-0.371891	-0.675107
H	-4.784331	-0.211035	-1.367041
C	-3.968374	-0.381277	0.693200
H	-4.773611	-0.228483	1.393291
C	3.474650	-0.734437	1.676954
C	0.683718	2.915517	-1.645946
C	-1.388797	2.962632	0.435264
H	-1.301406	4.049849	0.326889
H	-2.179193	2.595603	-0.226763
H	-1.664762	2.728972	1.468599
C	1.445858	2.955553	1.194118
H	2.473923	2.667597	0.952867
H	1.357694	4.045518	1.120863
H	1.228181	2.648653	2.221936
C	3.762668	0.185861	-1.094902
H	3.735208	1.233675	-0.777871
H	4.794975	-0.175228	-1.024859
H	3.435418	0.125929	-2.138039
C	3.095117	-2.605438	-0.545014
H	2.808210	-2.761690	-1.590334
H	4.175109	-2.763729	-0.446164
H	2.571471	-3.341334	0.074256
H	0.724116	4.006236	-1.545211
H	1.656062	2.550465	-1.989566
H	-0.070465	2.655263	-2.395390
H	4.545162	-0.949848	1.584256
H	3.345890	0.270705	2.090561
H	3.025928	-1.453995	2.369623

TS-A110

B3lyp/lanl2dz optimized geometry
Energy = -723.721832 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426106
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.781736

Atom	x-coord	y-coord	z-coord
Pd	0.294466	-0.261683	-0.003857
P	-0.165642	2.175176	0.016611
P	2.741811	-0.662801	-0.006308
C	-0.494278	-2.448357	-0.030914
H	0.097811	-2.666441	-0.924721
H	0.051550	-2.697805	0.884095

H	-1.399125	-3.063361	-0.065941
C	-1.629361	-0.917708	-0.003931
N	-2.493484	-0.852952	-1.101240
C	-2.069864	-0.905547	-2.505499
H	-1.029670	-0.579166	-2.580699
H	-2.157926	-1.922488	-2.907925
H	-2.692312	-0.234877	-3.106626
N	-2.480660	-0.890135	1.103975
C	-2.039682	-0.973051	2.501306
H	-1.011012	-0.611761	2.577169
H	-2.679086	-0.344352	3.129171
H	-2.087666	-2.004547	2.872210
C	-3.834769	-0.835034	-0.674234
H	-4.660722	-0.789763	-1.365400
C	-3.826463	-0.857779	0.693844
H	-4.644095	-0.834116	1.395836
C	3.568785	-0.660445	1.694301
C	-0.156824	2.988103	-1.689007
C	-1.859269	2.677031	0.686248
H	-2.009245	3.757596	0.579997
H	-2.646182	2.148945	0.139692
H	-1.930072	2.411588	1.745913
C	0.990622	3.302328	0.998025
H	2.006475	3.228647	0.596695
H	0.659292	4.345455	0.937682
H	1.005798	2.992369	2.047688
C	3.883242	0.477916	-0.991957
H	3.819040	1.497093	-0.596606
H	4.923306	0.138311	-0.929130
H	3.575095	0.489980	-2.042479
C	3.248091	-2.359247	-0.673707
H	2.982699	-2.435056	-1.733556
H	4.328513	-2.508793	-0.567769
H	2.727365	-3.150718	-0.124814
H	-0.367302	4.060663	-1.606809
H	0.822189	2.849907	-2.158114
H	-0.917209	2.523524	-2.324664
H	4.637835	-0.885546	1.607345
H	3.446627	0.321319	2.162888
H	3.097682	-1.412489	2.335743

TS-A120

B3lyp/lanl2dz optimized geometry
Energy = -723.718025 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426281
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.777831

Atom	x-coord	y-coord	z-coord
C	-3.604744	-1.336305	0.722751

N	-2.265108	-1.147612	1.112670
C	-1.439911	-1.028500	-0.006198
N	-2.318051	-1.095758	-1.089834
C	-3.637576	-1.304655	-0.644869
Pd	0.384675	-0.121699	-0.017313
C	-0.075054	-2.405896	-0.076411
C	-1.907564	-1.092647	-2.499665
C	-1.791141	-1.180904	2.501723
P	-0.580336	2.162580	0.017632
C	0.525200	3.645707	0.400825
P	2.845630	-0.428394	-0.010783
C	3.433168	-1.916413	-1.019984
C	-1.380218	2.677666	-1.614205
C	-1.997733	2.406025	1.241481
C	3.568333	-0.814701	1.694293
C	4.017659	0.921445	-0.626270
H	0.486332	-2.536866	-1.005127
H	0.544488	-2.595891	0.805190
H	-0.902528	-3.122202	-0.070075
H	-0.963525	-0.552111	-2.600228
H	-1.778776	-2.115217	-2.875852
H	-2.667565	-0.589495	-3.105513
H	-0.820112	-0.683539	2.560861
H	-2.497426	-0.650066	3.147791
H	-1.691080	-2.212836	2.860475
H	-4.469861	-1.391195	-1.324381
H	-4.403622	-1.454330	1.436739
H	-2.414043	3.415225	1.144874
H	-2.786395	1.673513	1.046949
H	-1.631222	2.270952	2.264132
H	1.331539	3.700072	-0.337362
H	-0.049477	4.578775	0.373866
H	0.967829	3.526250	1.394898
H	3.881633	1.825699	-0.024277
H	5.062093	0.597128	-0.553818
H	3.788678	1.158824	-1.670421
H	3.208798	-1.758350	-2.080053
H	4.513993	-2.052825	-0.903426
H	2.927466	-2.827686	-0.685200
H	-1.836617	3.669907	-1.521447
H	-0.623525	2.705618	-2.404512
H	-2.153964	1.954859	-1.889671
H	4.641920	-1.023220	1.622426
H	3.414231	0.039992	2.360757
H	3.065859	-1.686963	2.125407

TS-A130
B3lyp/lanl2dz optimized geometry
Energy = -723.710921 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426382
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point

Energy = -1393.770922

Atom	x-coord	y-coord	z-coord
Pd	0.440728	0.032165	-0.010472
P	-0.962367	2.076983	0.010542
P	2.909119	-0.207500	-0.007625
C	0.313735	-2.304454	-0.067968
H	0.847550	-2.384583	-1.017351
H	0.976331	-2.418576	0.793590
H	-0.442746	-3.093683	-0.024221
C	-1.266828	-1.088885	-0.003772
N	-2.110641	-1.301118	-1.091208
C	-1.689638	-1.247350	-2.497550
H	-0.815667	-0.597801	-2.585272
H	-1.434759	-2.247337	-2.869090
H	-2.496909	-0.838086	-3.112759
N	-2.067292	-1.332230	1.108970
C	-1.590142	-1.310590	2.497774
H	-0.723665	-0.648761	2.567838
H	-2.378059	-0.932260	3.156146
H	-1.303741	-2.316030	2.829845
C	-3.384691	-1.715023	-0.655414
H	-4.186561	-1.936874	-1.340782
C	-3.357614	-1.734359	0.712713
H	-4.131745	-1.976286	1.422721
C	3.571453	-1.045908	1.553988
C	-2.074171	2.274803	-1.503352
C	-2.214754	2.162492	1.421330
H	-2.835482	3.059723	1.318589
H	-2.858723	1.279122	1.401929
H	-1.689675	2.202839	2.380755
C	-0.146520	3.778703	0.116286
H	0.532190	3.910461	-0.732218
H	-0.898052	4.576772	0.104823
H	0.436174	3.846748	1.040386
C	4.083745	1.266890	-0.162948
H	3.898833	1.967984	0.657332
H	5.130501	0.943463	-0.130425
H	3.897253	1.783473	-1.110102
C	3.572603	-1.346741	-1.364876
H	3.366262	-0.910050	-2.347309
H	4.655121	-1.474909	-1.253324
H	3.097468	-2.330914	-1.308396
H	-2.693348	3.173193	-1.400662
H	-1.460772	2.367066	-2.404939
H	-2.727079	1.403302	-1.601611
H	4.650024	-1.218710	1.466286
H	3.382713	-0.406715	2.422368
H	3.074257	-2.008443	1.712234

3. Bite-Angle Products

PR-A80
B3lyp/lanl2dz optimized geometry
Energy = -723.716690 a.u.
Enthalpy Correction (inc. ZPVE) = 0.427632
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.775015

Atom	x-coord	y-coord	z-coord
Pd	-0.055109	-0.607489	-0.102683
P	-0.639668	1.794249	0.098177
P	-2.527858	-0.772459	-0.009414
C	1.753668	-2.290855	-0.538509
H	2.218736	-3.045661	0.103221
H	0.644000	-2.475743	-0.443715
H	2.006322	-2.500766	-1.579522
C	2.206393	-0.891320	-0.148222
N	2.767114	-0.612061	1.114689
C	2.375067	-1.239031	2.381600
H	1.545663	-0.697577	2.852778
H	2.062692	-2.273812	2.215069
H	3.231509	-1.245999	3.062564
N	2.903964	-0.050727	-1.036909
C	2.660788	0.016281	-2.479277
H	1.616952	0.289063	-2.680533
H	3.317156	0.771805	-2.917798
H	2.878565	-0.943228	-2.962947
C	3.636204	0.483860	1.011542
H	4.131670	0.908066	1.869483
C	3.720730	0.826740	-0.312435
H	4.301209	1.598529	-0.790648
C	-3.089671	-2.548033	0.398539
H	-4.172680	-2.661356	0.268033
H	-2.828526	-2.787564	1.434855
C	-1.134356	2.244588	1.873234
H	-0.227296	2.251488	2.486795
H	-1.588662	3.241837	1.905364
C	0.688254	3.136803	-0.173873
H	0.302253	4.130638	0.084503
H	1.561310	2.913285	0.446230
H	0.996184	3.138382	-1.225160
C	-2.011265	2.592067	-0.946209
H	-2.985761	2.127046	-0.796129
H	-2.084894	3.651442	-0.675190
H	-1.744288	2.517771	-2.005227
C	-3.312115	-0.622308	-1.734931
H	-2.906035	-1.419605	-2.366402
H	-4.400395	-0.739077	-1.674777

H	-3.078540	0.337045	-2.201446
C	-3.802524	0.130028	1.083354
H	-3.779903	1.214116	0.957658
H	-4.804425	-0.232899	0.826872
H	-3.605003	-0.107256	2.134021
H	-2.574906	-3.252800	-0.262790
H	-1.829590	1.517073	2.293482

PR-A90

B3lyp/lanl2dz optimized geometry
Energy = -723.732252 a.u.
Enthalpy Correction (inc. ZPVE) = 0.427612
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.789998

Atom	x-coord	y-coord	z-coord
Pd	-0.148272	-0.497964	-0.270081
P	-0.377020	1.927943	0.191491
P	-2.602722	-0.772297	-0.044655
C	1.612240	-2.146185	-1.131198
H	0.495526	-2.271201	-1.109308
H	1.891513	-2.011627	-2.177600
H	2.014517	-3.101605	-0.775793
C	2.123284	-0.990547	-0.292249
N	2.507084	-1.137381	1.051008
C	1.959821	-2.104414	2.012404
H	1.275012	-1.614060	2.713458
H	1.409087	-2.887164	1.485898
H	2.777514	-2.568677	2.574120
N	2.978332	-0.002891	-0.803847
C	2.964251	0.467425	-2.191020
H	1.949479	0.769371	-2.477420
H	3.629206	1.329116	-2.283380
H	3.316234	-0.311517	-2.877811
C	3.442436	-0.147145	1.381393
H	3.831301	-0.032377	2.379893
C	3.731591	0.550455	0.237318
H	4.416791	1.367300	0.080255
C	-3.618200	-0.281541	-1.569820
C	-0.695398	2.329301	2.017047
C	1.017376	3.173455	-0.163151
H	0.741817	4.176131	0.185615
H	1.928545	2.851727	0.349528
H	1.209919	3.214657	-1.240689
C	-1.807986	2.835728	-0.658521
H	-2.774030	2.448740	-0.325411
H	-1.759434	3.903899	-0.417879
H	-1.733088	2.711660	-1.743260
C	-3.589057	0.048717	1.355257
H	-3.565217	1.139045	1.279870
H	-4.633952	-0.279251	1.307582
H	-3.171344	-0.250781	2.321914
C	-3.215771	-2.557577	0.179690
H	-2.832700	-2.961909	1.122689

H	-4.311477	-2.599383	0.192026
H	-2.844233	-3.177816	-0.642685
H	-0.962531	3.385958	2.137135
H	-1.500222	1.707446	2.415507
H	0.216240	2.127118	2.588979
H	-4.690394	-0.401140	-1.374704
H	-3.417746	0.753974	-1.854853
H	-3.335112	-0.930107	-2.405497

PR-A100

B3lyp/lanl2dz optimized geometry
Energy = -723.740792 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428455
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.800975

Atom	x-coord	y-coord	z-coord
Pd	-0.335996	-0.360131	-0.216394
P	-0.567446	2.071872	0.210447
P	-2.709195	-1.056923	-0.035270
C	1.719458	-2.134875	-0.837591
H	0.608806	-1.972190	-0.607806
H	1.803669	-2.193252	-1.924896
H	1.938520	-3.122077	-0.415278
C	2.623108	-1.102061	-0.279232
N	3.110737	-1.067682	1.003551
C	2.702112	-1.980774	2.084834
H	1.611156	-1.990111	2.171501
H	3.065877	-2.996349	1.895152
H	3.127132	-1.627321	3.026543
N	3.243575	-0.088995	-0.967527
C	2.930126	0.296166	-2.351749
H	1.873606	0.585623	-2.417146
H	3.556688	1.143973	-2.635863
H	3.128988	-0.530381	-3.040869
C	3.999009	0.008739	1.133149
H	4.496544	0.239022	2.060371
C	4.077677	0.620512	-0.092914
H	4.653963	1.473354	-0.410398
C	-3.764950	-0.604991	-1.543102
C	-0.954309	2.485658	2.019809
C	0.761251	3.388586	-0.144722
H	0.424632	4.383726	0.170995
H	1.679709	3.133247	0.394641
H	0.975965	3.412060	-1.219044
C	-2.041387	2.874028	-0.671528
H	-2.972387	2.375947	-0.385194
H	-2.113788	3.935241	-0.405434
H	-1.916254	2.784394	-1.755353
C	-3.706434	-0.262819	1.368408
H	-3.713597	0.826395	1.263793
H	-4.741368	-0.624597	1.352544
H	-3.253114	-0.519780	2.331294
C	-3.214641	-2.872749	0.197361

H	-2.792247	-3.253582	1.133394
H	-4.305731	-2.980204	0.227306
H	-2.818770	-3.469408	-0.631197
H	-1.227348	3.542398	2.126513
H	-1.777938	1.862596	2.378780
H	-0.072550	2.280493	2.635784
H	-4.823647	-0.822117	-1.357137
H	-3.650532	0.456884	-1.778992
H	-3.426881	-1.187978	-2.406038

PR-A110
B3lyp/lanl2dz optimized geometry
Energy = -723.746450 a.u.
Enthalpy Correction (inc. ZPVE) = 0.427518
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.806983

Atom	x-coord	y-coord	z-coord
Pd	0.447089	-0.233382	-0.056525
P	0.607745	2.239785	0.033112
P	2.716296	-1.232952	-0.012247
C	-1.722166	-2.283749	-0.198929
H	-1.813021	-2.796443	-1.160255
H	-0.661471	-1.880431	-0.148447
H	-1.803168	-3.024002	0.602774
C	-2.740678	-1.217940	-0.055218
N	-3.364662	-0.542636	-1.069089
C	-3.056666	-0.697809	-2.502107
H	-2.003727	-0.456269	-2.683098
H	-3.263729	-1.719860	-2.834005
H	-3.683993	-0.011616	-3.074391
N	-3.256181	-0.741185	1.119664
C	-2.810756	-1.152055	2.463547
H	-1.742150	-0.941804	2.579664
H	-3.370206	-0.584862	3.210059
H	-2.996687	-2.218747	2.623120
C	-4.257612	0.389572	-0.524182
H	-4.857612	1.041661	-1.136470
C	-4.190127	0.265454	0.841551
H	-4.722378	0.790693	1.616792
C	3.107751	-3.048710	0.381062
H	4.188150	-3.235246	0.350379
H	2.612473	-3.696616	-0.349984
C	2.015579	2.873541	-1.065326
H	1.792609	2.652963	-2.114107
H	2.145228	3.955754	-0.944336
C	-0.740435	3.509966	-0.398309
H	-0.372235	4.535072	-0.268397
H	-1.050794	3.372889	-1.439889
H	-1.609456	3.356269	0.250331

C	1.153201	2.886172	1.729045
H	2.015431	2.311945	2.081342
H	1.423306	3.947739	1.674979
H	0.337980	2.760385	2.449246
C	3.868906	-0.366704	1.216872
H	3.495379	-0.511660	2.235677
H	4.885649	-0.771481	1.146241
H	3.898532	0.707054	1.005641
C	3.676047	-1.013269	-1.630790
H	3.644533	0.036175	-1.939514
H	4.721184	-1.323304	-1.510810
H	3.210627	-1.617810	-2.416039
H	2.730613	-3.296596	1.378992
H	2.949876	2.371146	-0.795642

PR-A120

B3lyp/lanl2dz optimized geometry
Energy = -723.753195 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428595
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.813311

Atom	x-coord	y-coord	z-coord
Pd	0.668837	-0.091827	-0.048411
P	0.957849	2.368762	0.062808
P	2.649969	-1.579393	0.064151
C	-2.020114	-1.588083	1.024544
H	-1.854720	-2.624571	0.706221
H	-1.045229	-1.052760	0.900598
H	-2.273096	-1.588053	2.087147
C	-3.082005	-0.936279	0.213330
N	-3.030199	-0.709147	-1.131077
C	-1.891487	-1.061988	-2.004847
H	-0.954077	-0.648820	-1.583125
H	-1.803728	-2.149146	-2.095310
H	-2.060054	-0.628805	-2.992906
N	-4.274747	-0.439775	0.660009
C	-4.750432	-0.467528	2.058773
H	-4.097059	0.133729	2.697873
H	-5.758075	-0.049013	2.093199
H	-4.785534	-1.495643	2.430053
C	-4.201890	-0.060300	-1.538281
H	-4.381838	0.218452	-2.562985
C	-4.980538	0.109610	-0.419298
H	-5.951624	0.561595	-0.306055
C	2.706796	-3.448945	-0.265306
H	3.726259	-3.837969	-0.153844
H	2.356708	-3.651993	-1.283066
C	2.202358	2.830006	1.413832
H	3.129824	2.268690	1.263175

H	2.424583	3.903691	1.389610
C	1.806904	3.082215	-1.473024
H	2.106212	4.124205	-1.306741
H	2.693168	2.485710	-1.710797
H	1.122530	3.036730	-2.326487
C	-0.376365	3.687733	0.366231
H	-0.866860	3.495700	1.326768
H	0.059967	4.693988	0.383246
H	-1.128730	3.637997	-0.428398
C	3.534437	-1.494773	1.736849
H	2.911691	-1.963323	2.505883
H	4.501945	-2.009621	1.694059
H	3.694195	-0.448032	2.013625
C	4.017522	-0.985313	-1.103741
H	4.231611	0.070632	-0.910239
H	4.934303	-1.569931	-0.959947
H	3.684752	-1.087138	-2.141640
H	2.048235	-3.966363	0.440588
H	1.794367	2.567892	2.395129

PR-A130
B3lyp/lanl2dz optimized geometry
Energy = -723.757702 a.u.
Enthalpy Correction (inc. ZPVE) = 0.429011
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.817739

Atom	x-coord	y-coord	z-coord
Pd	0.784191	-0.002428	0.004659
P	0.717520	2.476629	-0.010490
P	2.723605	-1.545532	-0.084248
C	-1.902601	-1.531810	-1.166903
H	-2.183755	-1.422766	-2.216815
H	-0.956954	-0.959997	-0.996902
H	-1.674191	-2.587607	-0.975658
C	-2.976356	-1.040113	-0.263293
N	-4.210568	-0.575654	-0.623185
C	-4.729034	-0.486474	-2.004201
H	-4.135069	0.219262	-2.592380
H	-4.713171	-1.469976	-2.482247
H	-5.760951	-0.132297	-1.967133
N	-2.895746	-0.953749	1.095869
C	-1.715093	-1.334607	1.900976
H	-0.807267	-0.860169	1.481094
H	-1.861283	-0.983408	2.924607
H	-1.593085	-2.422510	1.904294
C	-4.914343	-0.191052	0.526475
H	-5.914359	0.207139	0.486948
C	-4.091774	-0.429640	1.600428
H	-4.255909	-0.275071	2.653662

C	2.674352	-3.442462	-0.019343
H	3.684404	-3.862614	-0.097716
H	2.065011	-3.823312	-0.846026
C	2.057591	3.155965	-1.161779
H	1.857219	2.834909	-2.188771
H	2.087447	4.251707	-1.123266
C	-0.757891	3.557985	-0.521846
H	-0.497141	4.622722	-0.484902
H	-1.060869	3.300985	-1.542749
H	-1.600730	3.373736	0.153367
C	1.199265	3.287620	1.631299
H	2.127299	2.838338	1.998176
H	1.344524	4.367561	1.507176
H	0.414489	3.113817	2.374877
C	3.981497	-1.182920	1.283268
H	3.541779	-1.413711	2.258841
H	4.890383	-1.781287	1.146141
H	4.243328	-0.120373	1.265183
C	3.777108	-1.278333	-1.634630
H	4.019067	-0.215521	-1.732597
H	4.706822	-1.857494	-1.578148
H	3.213224	-1.586982	-2.520774
H	2.226428	-3.767885	0.925845
H	3.031535	2.758889	-0.858880

4. Bite-Angle Separated Products

Pdbis(TMP)-A80
B3lyp/lanl2dz optimized geometry
Energy = -379.186759 a.u.
Enthalpy Correction (inc. ZPVE) = 0.248611
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.095200

Atom	x-coord	y-coord	z-coord
Pd	0.000255	-1.519454	0.000134
P	-1.593660	0.379591	0.059018
P	1.592373	0.381082	-0.059225
C	1.802593	1.040302	1.719420
C	-1.800078	1.041372	-1.719014
C	-3.458023	0.069391	0.400458
H	-4.074630	0.945248	0.154892
H	-3.785115	-0.786747	-0.199358
H	-3.590586	-0.181343	1.458959

C	-1.500737	2.021330	1.044936
H	-0.547887	2.537811	0.917592
H	-2.311521	2.685101	0.718979
H	-1.635072	1.794938	2.108463
C	1.501456	2.024771	-1.042229
H	0.550459	2.543660	-0.910748
H	2.315149	2.685569	-0.717506
H	1.631815	1.800149	-2.106622
C	3.455395	0.067129	-0.403952
H	3.585853	-0.182234	-1.463034
H	4.074474	0.941115	-0.157927
H	3.781288	-0.790743	0.194028
H	-2.387533	1.968531	-1.733106
H	-0.830786	1.212555	-2.190774
H	-2.328057	0.274507	-2.296340
H	2.387820	1.968865	1.733489
H	0.834183	1.208248	2.194243
H	2.334078	0.273795	2.293998

Pdbis(TMP)-A90
B3lyp/lanl2dz optimized geometry
Energy = -379.205401 a.u.
Enthalpy Correction (inc. ZPVE) = 0.248733
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.114106

Atom	x-coord	y-coord	z-coord
Pd	-0.000016	-1.428733	-0.000148
P	1.753652	0.324661	-0.025831
P	-1.753219	0.325123	0.025659
C	-2.024912	1.137023	-1.676205
C	2.023717	1.136381	1.676381
C	3.590687	-0.024570	-0.439363
H	4.219353	0.865386	-0.297791
H	3.950683	-0.831803	0.207596
H	3.665240	-0.359126	-1.480166
C	1.562466	1.877075	-1.118301
H	0.639393	2.415098	-0.888757
H	2.413853	2.550951	-0.959818
H	1.538746	1.572994	-2.170284
C	-1.562803	1.877459	1.118360
H	-0.639834	2.415867	0.889306
H	-2.414386	2.551063	0.959782
H	-1.539321	1.573142	2.170291
C	-3.589684	-0.025882	0.440073
H	-3.663323	-0.361571	1.480561
H	-4.219132	0.863714	0.299745
H	-3.949437	-0.832741	-0.207503
H	2.686323	2.008303	1.599434
H	1.069205	1.439703	2.112891
H	2.482201	0.394439	2.339269
H	-2.689386	2.007495	-1.598868
H	-1.071044	1.442701	-2.112502
H	-2.481744	0.394421	-2.339484

Pdbis(TMP)-A100
B3lyp/lanl2dz optimized geometry
Energy = -379.217496 a.u.
Enthalpy Correction (inc. ZPVE) = 0.248486
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.126868

Atom	x-coord	y-coord	z-coord
Pd	-0.000002	-1.323811	-0.000095
P	1.899801	0.270232	-0.013346
P	-1.899687	0.270373	0.013262
C	-2.183568	1.137504	-1.656321
C	2.182788	1.137345	1.656394
C	3.719956	-0.111996	-0.453108
H	4.355128	0.779775	-0.364148
H	4.091896	-0.892350	0.219701
H	3.768018	-0.491249	-1.479892
C	1.660800	1.785564	-1.139645
H	0.724175	2.295603	-0.895046
H	2.493306	2.490581	-1.019968
H	1.615451	1.455591	-2.183001
C	-1.660612	1.785771	1.139457
H	-0.723994	2.295780	0.894791
H	-2.493131	2.490775	1.019796
H	-1.615207	1.455859	2.182833
C	-3.719521	-0.112425	0.453790
H	-3.766971	-0.491991	1.480480
H	-4.354987	0.779188	0.365367
H	-4.091562	-0.892687	-0.219073
H	2.912890	1.951957	1.562756
H	1.237267	1.537593	2.033952
H	2.554605	0.400556	2.376497
H	-2.914266	1.951551	-1.562433
H	-1.238395	1.538576	-2.033897
H	-2.554893	0.400562	-2.376512

Pdbis(TMP)-A110
B3lyp/lanl2dz optimized geometry
Energy = -379.225550 a.u.
Enthalpy Correction (inc. ZPVE) = 0.248434
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.135368

Atom	x-coord	y-coord	z-coord
Pd	0.000003	-1.196911	-0.000034
P	2.031494	0.225557	0.005607

P	-2.031485	0.225561	-0.005631
C	-1.881215	1.692975	-1.204148
C	1.881476	1.692528	1.204702
C	3.830555	-0.284769	0.384808
H	4.515216	0.571877	0.324717
H	3.875505	-0.715445	1.391186
H	4.143674	-1.051579	-0.332102
C	2.311364	1.159472	-1.625897
H	1.384880	1.661518	-1.922975
H	3.113350	1.902594	-1.526560
H	2.577911	0.441393	-2.408561
C	-2.311747	1.158853	1.626158
H	-1.385267	1.660573	1.923792
H	-3.113554	1.902175	1.526864
H	-2.578719	0.440480	2.408412
C	-3.830461	-0.284630	-0.385431
H	-4.143709	-1.051803	0.331030
H	-4.515145	0.571978	-0.325046
H	-3.875198	-0.714793	-1.392037
H	2.740819	2.368511	1.107576
H	0.961476	2.247680	0.994083
H	1.830961	1.315804	2.231685
H	-2.740516	2.368987	-1.106868
H	-0.961203	2.247963	-0.993172
H	-1.830592	1.316645	-2.231268

Pdbis(TMP)-A120

B3lyp/lanl2dz optimized geometry
Energy = -379.231155 a.u.
Enthalpy Correction (inc. ZPVE) = 0.248689
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.141237

Atom	x-coord	y-coord	z-coord
Pd	0.000007	-1.055024	-0.000118
P	-2.147692	0.185038	-0.006118
P	2.147777	0.184913	0.005979
C	2.054518	1.702355	1.143510
C	-2.051868	1.706782	-1.137677
C	-3.882549	-0.447886	-0.476325
H	-4.633520	0.350851	-0.412944
H	-3.856473	-0.840882	-1.498564
H	-4.162248	-1.263502	0.199317
C	-2.547168	1.023377	1.650222
H	-1.666798	1.576015	1.994198
H	-3.397723	1.710869	1.554671
H	-2.783021	0.255917	2.394932
C	2.542866	1.029437	-1.648263
H	1.661825	1.583906	-1.987513
H	3.394097	1.716062	-1.552517
H	2.776104	0.264748	-2.396635
C	3.884036	-0.449264	0.469276
H	4.162900	-1.261121	-0.211228
H	4.634333	0.350313	0.408511

H	3.860370	-0.847651	1.489480
H	-2.953533	2.326568	-1.048031
H	-1.173712	2.301998	-0.866084
H	-1.938230	1.378199	-2.175987
H	2.954367	2.324426	1.051480
H	1.173627	2.296602	0.878777
H	1.947035	1.369717	2.181197

Pdbis(TMP)-A130
B3lyp/lanl2dz optimized geometry
Energy = -379.235477 a.u.
Enthalpy Correction (inc. ZPVE) = 0.248643
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.145644

Atom	x-coord	y-coord	z-coord
Pd	-0.000049	-0.894352	-0.003252
P	2.247624	0.153664	0.001727
P	-2.247659	0.153812	-0.003250
C	-2.264396	1.741908	-1.041395
C	2.407123	1.509046	1.319721
C	3.920345	-0.725719	0.235645
H	4.756110	-0.013993	0.207791
H	3.920202	-1.247652	1.198760
H	4.049762	-1.468658	-0.558867
C	2.621948	1.156717	-1.564959
H	1.792621	1.845336	-1.756372
H	3.554460	1.726509	-1.459983
H	2.706409	0.475743	-2.418338
C	-2.815743	0.838005	1.673254
H	-2.017882	1.457091	2.096237
H	-3.729669	1.437771	1.571251
H	-3.003145	0.004799	2.358764
C	-3.868950	-0.642020	-0.604592
H	-4.090340	-1.518957	0.013368
H	-4.707884	0.064136	-0.548087
H	-3.743249	-0.973897	-1.640927
H	3.365898	2.037005	1.234570
H	1.586008	2.223236	1.199804
H	2.327794	1.057297	2.313957
H	-3.231494	2.256405	-0.968050
H	-1.469960	2.407950	-0.689351
H	-2.064810	1.490327	-2.088168

2-Methyl-Imidazolium NN_2Me^{+}
B3lyp/LANL2DZ optimized geometry
Energy = -344.496943 a.u.
Enthalpy Correction (inc. ZPVE) = 0.179209
NIMAG = 0

B3lyp/6-311+G(2d,p) single point
Energy = -344.649607

Atom	x-coord	y-coord	z-coord

C	2.505902	0.207988	0.008655
N	1.098118	-0.250047	-0.002010
C	0.000000	0.559101	0.002976
N	-1.098161	-0.249933	-0.001937
C	-2.505926	0.208186	0.008616
C	0.686893	-1.589047	-0.004264
C	-0.687057	-1.588977	-0.004227
H	-2.666113	0.960020	-0.768401
H	-2.764998	0.624458	0.986963
H	-3.153497	-0.646469	-0.195478
H	2.665623	0.961403	-0.766919
H	3.153345	-0.646250	-0.197591
H	2.765542	0.622307	0.987686
H	1.384976	-2.409570	-0.006886
H	-1.385221	-2.409430	-0.006823
C	0.000180	2.052857	-0.007486
H	0.882684	2.448964	0.503037
H	0.001920	2.444640	-1.033683
H	-0.883916	2.449135	0.500100

5. Twist-Angle Complexes

CX-D15
B3lyp/lanl2dz optimized geometry
Energy = -723.725866 a.u.
Enthalpy Correction (inc. ZPVE) = 0.427997
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.787559

Atom	x-coord	y-coord	z-coord
N	3.067887	0.585634	0.058436
C	2.050904	-0.351621	-0.059066
C	2.956097	1.980064	0.499654
N	2.742138	-1.531600	-0.314378
C	2.171740	-2.827374	-0.724783
C	4.332845	0.009920	-0.146361
C	4.131220	-1.332375	-0.293588
H	2.309068	-3.578036	0.059727
H	1.109585	-2.700484	-0.923557
H	2.669373	-3.164620	-1.639793
H	5.244968	0.581109	-0.083883
H	4.832556	-2.130046	-0.478152
H	1.927665	2.193411	0.767700
H	3.583979	2.137539	1.383162
H	3.283708	2.662137	-0.291621
Pd	-0.065399	-0.295124	0.103348
P	-0.656882	2.099957	-0.149902
P	-2.404562	-1.098229	-0.080331
C	0.157534	-1.941559	1.402693
C	-3.664515	-0.596896	1.234114
C	-0.544736	2.850894	1.591098
C	0.242931	3.355592	-1.257099

C	-2.421211	2.658977	-0.581210
C	-2.609360	-2.974756	-0.073901
C	-3.243385	-0.674378	-1.717182
H	-0.120240	-2.902090	0.964106
H	1.183623	-1.973984	1.772266
H	-0.521310	-1.687196	2.228027
H	-0.031693	3.149964	-2.297242
H	-0.065475	4.376695	-1.004814
H	-3.166622	2.114984	0.003946
H	-2.523587	3.728692	-0.366406
H	-2.612586	2.500944	-1.646753
H	-2.331152	-3.388338	0.898373
H	-3.655145	-3.228015	-0.280390
H	-1.975159	-3.422018	-0.845310
H	-2.635275	-1.063544	-2.540017
H	-4.237389	-1.133381	-1.760946
H	-3.343646	0.404951	-1.837293
H	-0.669120	3.938812	1.544594
H	0.404297	2.616874	2.078628
H	-1.348201	2.430058	2.204685
H	-3.326219	-0.955262	2.211587
H	-3.770913	0.489770	1.281804
H	-4.641549	-1.040700	1.012404
H	1.325935	3.274392	-1.169973

CX-D30

B3lyp/lanl2dz optimized geometry
Energy = -723.734319 a.u.
Enthalpy Correction (inc. ZPVE) = 0.429128
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.796764

Atom	x-coord	y-coord	z-coord
N	2.888713	0.520414	0.532439
C	1.999181	-0.403081	0.001689
C	2.575036	1.550869	1.535737
N	2.822549	-1.408142	-0.477362
C	2.421194	-2.548082	-1.321518
C	4.224099	0.126217	0.314305
C	4.175942	-1.139262	-0.197426
H	1.363392	-2.457719	-1.561047
H	2.999586	-2.533475	-2.251161
H	2.596961	-3.494519	-0.800565
H	5.060377	0.707760	0.668202
H	4.969192	-1.800491	-0.507868
H	1.495104	1.649381	1.627556
H	2.972313	1.241321	2.509019
H	3.021610	2.509167	1.258653
Pd	-0.090327	-0.395448	-0.026268
P	-0.447395	2.040018	-0.328607
P	-2.513561	-0.901406	0.123207
C	0.065229	-2.370781	0.707764
C	-3.089649	-0.960603	1.920483
C	-1.395144	2.862913	1.087510

C	0.954751	3.295195	-0.611831
C	-1.484070	2.501422	-1.848750
C	-3.005794	-2.601230	-0.533325
C	-3.879649	0.149967	-0.656728
H	-0.605002	-2.453011	1.571602
H	-0.225728	-3.090292	-0.065069
H	1.083559	-2.571912	1.043044
H	1.312134	3.704789	0.335337
H	1.785752	2.816614	-1.137322
H	-2.387440	1.897598	-1.921751
H	-1.760371	3.561525	-1.811299
H	-0.877062	2.326800	-2.743498
H	-2.449430	-3.385395	-0.016204
H	-4.078208	-2.761597	-0.376079
H	-2.787741	-2.660035	-1.604256
H	-3.776844	0.157169	-1.745895
H	-4.851506	-0.287220	-0.401887
H	-3.852956	1.177545	-0.284390
H	-1.514892	3.934394	0.892155
H	-0.853877	2.731676	2.030103
H	-2.386337	2.412546	1.194313
H	-2.470615	-1.658384	2.490291
H	-2.998605	0.032138	2.372206
H	-4.135101	-1.283911	1.973621
H	0.575523	4.121783	-1.221482

CX-D45

B3lyp/lanl2dz optimized geometry
Energy = -723.746639 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428938
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.809317

Atom	x-coord	y-coord	z-coord
N	2.789090	0.321700	0.797522
C	1.932532	-0.468099	0.048634
C	2.392851	1.206204	1.903875
N	2.773941	-1.353961	-0.595057
C	2.377975	-2.339087	-1.615970
C	4.132398	-0.033120	0.573240
C	4.114827	-1.142294	-0.226527
H	1.311854	-2.234264	-1.813194
H	2.933833	-2.155491	-2.541405
H	2.582851	-3.355948	-1.266089
H	4.952272	0.456163	1.074057
H	4.925269	-1.724832	-0.634223
H	1.310776	1.331854	1.889928
H	2.671864	0.749734	2.859983
H	2.887237	2.179362	1.821277
Pd	-0.139595	-0.417745	-0.023480
P	-0.278285	2.031817	-0.385163
P	-2.584188	-0.793576	0.158493
C	-0.042576	-2.457804	0.504374
C	-3.097998	-1.006891	1.962154

C	-0.937118	3.083883	1.043584
C	1.296102	2.958549	-0.883705
C	-1.379445	2.601799	-1.817657
C	-3.211650	-2.377212	-0.651330
C	-3.883736	0.438094	-0.446890
H	-0.710112	-2.633329	1.356264
H	-0.362993	-3.059006	-0.355148
H	0.971143	-2.738381	0.796782
H	2.083489	2.850673	-0.138061
H	1.658176	2.548886	-1.832078
H	-2.428273	2.378539	-1.619323
H	-1.270794	3.682071	-1.965663
H	-1.075670	2.085007	-2.733540
H	-2.667251	-3.241322	-0.264625
H	-4.279634	-2.505163	-0.442700
H	-3.062165	-2.321968	-1.734161
H	-3.803697	0.569417	-1.529746
H	-4.882356	0.052502	-0.213544
H	-3.761358	1.407163	0.045988
H	-1.007250	4.134152	0.739076
H	-0.276317	3.013231	1.912804
H	-1.931323	2.734005	1.338731
H	-2.508359	-1.800572	2.428250
H	-2.921431	-0.076261	2.510714
H	-4.160877	-1.264974	2.027291
H	1.073366	4.023104	-1.017465

CX-D60

B3lyp/lanl2dz optimized geometry
Energy = -723.754596 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428453
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.816780

Atom	x-coord	y-coord	z-coord
N	2.745103	0.110374	0.971503
C	1.898513	-0.499259	0.066710
C	2.319254	0.845860	2.171081
N	2.738249	-1.223983	-0.751371
C	2.315939	-2.024999	-1.911667
C	4.088070	-0.203826	0.697081
C	4.079074	-1.080584	-0.354333
H	1.232974	-1.948642	-2.013029
H	2.792162	-1.648367	-2.823176
H	2.590842	-3.074999	-1.767916
H	4.906186	0.165347	1.294098
H	4.893119	-1.561710	-0.871902
H	1.234494	0.962469	2.145381
H	2.585446	0.281280	3.071164
H	2.800879	1.828488	2.214604
Pd	-0.156386	-0.423127	0.006032
P	-0.200863	2.025907	-0.382112
P	-2.611866	-0.742090	0.144877
C	-0.068900	-2.482205	0.446568

C	-3.164601	-0.942888	1.937639
C	-0.962854	3.104396	0.973176
C	1.459648	2.886690	-0.663517
C	-1.124273	2.611162	-1.926579
C	-3.269470	-2.307470	-0.674827
C	-3.846006	0.535883	-0.498273
H	-0.719886	-2.686498	1.305735
H	-0.419627	-3.034955	-0.434069
H	0.947637	-2.795515	0.696020
H	2.085627	2.824482	0.229181
H	1.984885	2.403902	-1.493299
H	-2.180346	2.340146	-1.869951
H	-1.040761	3.699046	-2.029364
H	-0.687767	2.135474	-2.810637
H	-2.757779	-3.185612	-0.274601
H	-4.344766	-2.404506	-0.488299
H	-3.095441	-2.260382	-1.754348
H	-3.745351	0.640131	-1.582783
H	-4.866005	0.205766	-0.272184
H	-3.681890	1.508666	-0.025624
H	-0.902809	4.163353	0.697564
H	-0.430434	2.954228	1.917783
H	-2.013671	2.838323	1.123488
H	-2.610053	-1.760986	2.405977
H	-2.962506	-0.022643	2.494705
H	-4.236895	-1.163096	1.985625
H	1.296597	3.942112	-0.908361

CX-D75

B3lyp/lanl2dz optimized geometry
Energy = -723.758229 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428099
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.820975

Atom	x-coord	y-coord	z-coord
N	2.724719	-0.174238	1.091623
C	1.882840	-0.512022	0.054354
C	2.286864	0.298146	2.413100
N	2.719692	-0.982778	-0.932702
C	2.279321	-1.476909	-2.246635
C	4.066748	-0.419520	0.750160
C	4.061738	-0.942160	-0.516093
H	1.188957	-1.443460	-2.280736
H	2.688198	-0.851217	-3.047402
H	2.610546	-2.510269	-2.391974
H	4.884782	-0.228972	1.425736
H	4.876618	-1.265501	-1.143235
H	1.203810	0.436085	2.391981
H	2.531326	-0.443098	3.181327
H	2.776164	1.245714	2.663673
Pd	-0.163809	-0.426409	0.012784
P	-0.170609	2.036621	-0.276769
P	-2.623820	-0.729387	0.096152

C	-0.062188	-2.508741	0.313335
C	-3.230509	-0.921901	1.871821
C	-1.067542	3.060628	1.037077
C	1.524440	2.872777	-0.292464
C	-0.908240	2.699525	-1.886664
C	-3.277762	-2.286484	-0.740994
C	-3.811008	0.568425	-0.593509
H	-0.727461	-2.778979	1.143268
H	-0.394339	-2.993661	-0.613537
H	0.952424	-2.836403	0.553836
H	2.028861	2.719935	0.665898
H	2.143205	2.441454	-1.085229
H	-1.960022	2.413857	-1.968897
H	-0.830979	3.792225	-1.922511
H	-0.364537	2.275957	-2.737172
H	-2.776312	-3.169541	-0.338443
H	-4.356362	-2.378622	-0.571996
H	-3.086534	-2.234370	-1.817409
H	-3.660166	0.675069	-1.672245
H	-4.845619	0.255205	-0.414210
H	-3.651824	1.537327	-0.111797
H	-0.973770	4.130526	0.819333
H	-0.633654	2.859694	2.021951
H	-2.129278	2.798941	1.067006
H	-2.716132	-1.762843	2.346263
H	-3.009919	-0.013643	2.441255
H	-4.310599	-1.105271	1.891829
H	1.415183	3.948686	-0.468744

CX-D90

B3lyp/lanl2dz optimized geometry
Energy = -723.759027 a.u.
Enthalpy Correction (inc. ZPVE) = 0.428094
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.822070

Atom	x-coord	y-coord	z-coord
N	2.719025	-0.555889	1.095735
C	1.886655	-0.505180	0.000365
C	2.267529	-0.558944	2.495243
N	2.732867	-0.569872	-1.084167
C	2.298419	-0.597939	-2.489168
C	4.065270	-0.647557	0.700006
C	4.074041	-0.657816	-0.669961
H	1.207896	-0.547586	-2.514614
H	2.718641	0.251705	-3.038304
H	2.621493	-1.528926	-2.966467
H	4.878224	-0.702073	1.405700
H	4.895875	-0.722910	-1.364377
H	1.175803	-0.539805	2.506392
H	2.611288	-1.467080	3.001168
H	2.656036	0.316546	3.027205
Pd	-0.158190	-0.447312	-0.015899
P	-0.189605	2.032482	-0.010193

P	-2.620483	-0.742940	-0.005079
C	-0.021755	-2.545869	-0.003987
C	-3.354422	-0.691007	1.732363
C	-1.315341	2.912522	1.230069
C	1.466320	2.859232	0.371663
C	-0.651251	2.868704	-1.642183
C	-3.280227	-2.375470	-0.677436
C	-3.695010	0.490206	-0.950408
H	-0.589469	-2.918463	0.858848
H	-0.467531	-2.907099	-0.938543
H	1.010955	-2.896678	0.067076
H	1.785098	2.601712	1.386565
H	2.228009	2.512093	-0.332662
H	-1.653862	2.563724	-1.954654
H	-0.625590	3.959163	-1.535628
H	0.059957	2.571694	-2.419655
H	-2.828794	-3.216082	-0.145304
H	-4.368189	-2.415314	-0.554499
H	-3.036291	-2.464176	-1.740644
H	-3.412206	0.488819	-2.007778
H	-4.750613	0.208632	-0.867006
H	-3.570706	1.500718	-0.550869
H	-1.181671	3.998171	1.163850
H	-1.067615	2.586255	2.245309
H	-2.365167	2.675450	1.033510
H	-2.909187	-1.485550	2.339133
H	-3.134627	0.271180	2.204693
H	-4.440215	-0.834424	1.697354
H	1.375906	3.948577	0.294275

6. Twist-Angle Transition Structures

TS-D15
B3lyp/lanl2dz optimized geometry
Energy = -723.691682 a.u.
Enthalpy Correction (inc. ZPVE) = 0.425510
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.751851

Atom	x-coord	y-coord	z-coord
C	3.975903	-1.300545	-0.570959
N	2.625386	-1.545154	-0.298188
C	1.975892	-0.371572	0.094370
N	2.971708	0.597305	0.020046

C	4.178904	0.046845	-0.432442
Pd	-0.051403	-0.147390	-0.010898
C	1.118593	-0.785551	1.864335
C	2.817526	2.008887	0.385739
C	2.007905	-2.870813	-0.451148
P	-0.862902	2.189456	-0.187022
C	-2.472159	2.428199	-1.166279
P	-2.162426	-1.448709	-0.034316
C	-2.030526	-3.264132	0.498384
C	-1.442009	2.670426	1.556215
C	0.011280	3.801995	-0.702175
C	-2.965481	-1.632041	-1.738284
C	-3.635708	-0.898924	1.024099
H	0.192814	-0.427178	2.329905
H	1.216146	-1.867086	1.954396
H	1.965146	-0.282056	2.337207
H	2.618406	2.617388	-0.500854
H	1.984595	2.112363	1.082622
H	3.732490	2.363570	0.869950
H	0.989228	-2.837283	-0.062428
H	1.963821	-3.147462	-1.510025
H	2.590708	-3.621469	0.093395
H	5.070048	0.637441	-0.569414
H	4.645968	-2.072812	-0.912424
H	-0.706002	4.630775	-0.698079
H	0.820802	4.043108	-0.007486
H	0.424197	3.695563	-1.710645
H	-3.201556	1.664085	-0.882712
H	-2.901955	3.418116	-0.973655
H	-2.264475	2.332341	-2.237220
H	-3.956641	0.106992	0.735862
H	-4.477841	-1.588501	0.895606
H	-3.348062	-0.884802	2.080769
H	-1.659253	-3.325230	1.526963
H	-3.009578	-3.754366	0.445836
H	-1.336827	-3.796555	-0.161107
H	-1.928601	3.652553	1.541287
H	-2.153402	1.926447	1.927938
H	-0.588535	2.707832	2.241517
H	-3.866261	-2.253446	-1.678018
H	-3.234537	-0.646584	-2.130472
H	-2.256770	-2.096739	-2.431483

TS-D30

B3lyp/lanl2dz optimized geometry
Energy = -723.700565 a.u.
Enthalpy Correction (inc. ZPVE) = 0.425374
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.760667

Atom	x-coord	y-coord	z-coord
C	3.850241	-1.445872	-0.707538
N	2.477105	-1.668115	-0.530601
C	1.879512	-0.588322	0.126786

N	2.929286	0.316279	0.300706
C	4.117959	-0.179502	-0.264495
Pd	-0.122388	-0.225229	0.017991
C	0.977403	-1.357888	1.715072
C	2.887104	1.501808	1.160600
C	1.782763	-2.857780	-1.043059
P	-0.485590	2.209900	-0.279720
C	-2.075010	2.713061	-1.182612
P	-2.433443	-1.124414	0.047795
C	-2.555300	-2.940955	0.570123
C	-0.754794	3.081050	1.383425
C	0.737736	3.369337	-1.149394
C	-3.370803	-1.148217	-1.595116
C	-3.705796	-0.338172	1.209229
H	0.124442	-0.966725	2.282251
H	0.893126	-2.432955	1.553359
H	1.888733	-1.133567	2.275863
H	3.420484	2.331846	0.687298
H	1.849029	1.785390	1.329181
H	3.356484	1.290571	2.129848
H	0.768104	-2.884989	-0.639624
H	1.715902	-2.821034	-2.135991
H	2.322475	-3.763441	-0.746230
H	5.044882	0.369989	-0.234711
H	4.484738	-2.149120	-1.222675
H	0.400339	4.409658	-1.075036
H	1.734821	3.284663	-0.711201
H	0.800073	3.089991	-2.206294
H	-2.942919	2.265507	-0.688586
H	-2.191792	3.802985	-1.183229
H	-2.036162	2.358570	-2.217612
H	-3.854652	0.714743	0.949184
H	-4.667229	-0.859443	1.138176
H	-3.346993	-0.394853	2.242304
H	-2.110283	-3.073242	1.561884
H	-3.601185	-3.266599	0.603919
H	-2.013282	-3.569248	-0.144841
H	-1.027066	4.130690	1.223332
H	-1.562386	2.582917	1.929358
H	0.150549	3.041776	1.996875
H	-4.351864	-1.621804	-1.474173
H	-3.509556	-0.126050	-1.960221
H	-2.794337	-1.706409	-2.339959

TS-D45

B3lyp/lanl2dz optimized geometry
Energy = -723.709945 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426065
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.770289

Atom	x-coord	y-coord	z-coord
C	-3.851150	-1.272683	0.784757
N	-2.478927	-1.561404	0.714417

C	-1.832323	-0.678968	-0.156480
N	-2.848920	0.185585	-0.574898
C	-4.071177	-0.146083	0.040845
Pd	0.159797	-0.289609	-0.063335
C	-0.926684	-1.751428	-1.502961
C	-2.724408	1.136770	-1.682401
C	-1.830348	-2.610682	1.512014
P	0.323475	2.153107	0.332578
C	1.673864	2.757574	1.514741
P	2.546541	-0.962663	-0.092557
C	2.887869	-2.685117	-0.798029
C	0.762593	3.121897	-1.234740
C	-1.164726	3.111841	1.000657
C	3.393309	-1.070942	1.595484
C	3.780376	0.083467	-1.075322
H	-0.151551	-1.401991	-2.195139
H	-0.701936	-2.748165	-1.120332
H	-1.873759	-1.777835	-2.049846
H	-3.342488	2.019644	-1.492446
H	-1.680648	1.439262	-1.783098
H	-3.049320	0.680244	-2.626474
H	-0.800094	-2.739066	1.172797
H	-1.808432	-2.330465	2.571252
H	-2.371848	-3.556434	1.401969
H	-4.982301	0.396133	-0.153571
H	-4.521976	-1.823162	1.424651
H	-0.958331	4.188207	1.009018
H	-2.049584	2.920263	0.389004
H	-1.373939	2.779659	2.022624
H	2.656322	2.434928	1.155468
H	1.665285	3.851471	1.586355
H	1.507403	2.332413	2.509521
H	3.803004	1.105247	-0.682491
H	4.787936	-0.342500	-1.008587
H	3.479452	0.119465	-2.127520
H	2.524971	-2.744214	-1.829537
H	3.961322	-2.904966	-0.786447
H	2.365336	-3.439438	-0.200354
H	0.921759	4.179880	-0.995918
H	1.677241	2.713358	-1.675516
H	-0.040888	3.044291	-1.973595
H	4.428110	-1.416631	1.489940
H	3.392118	-0.087425	2.075796
H	2.847686	-1.769974	2.237561

TS-D60
B3lyp/lanl2dz optimized geometry
Energy = -723.717234 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426138
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.777192

Atom	x-coord	y-coord	z-coord
C	-3.846935	-1.089310	0.811643
N	-2.476794	-1.394558	0.879265
C	-1.779965	-0.765338	-0.157570
N	-2.763961	-0.034668	-0.832339
C	-4.021131	-0.212682	-0.223986
Pd	0.196480	-0.315548	-0.074812
C	-0.835926	-2.080285	-1.178058
C	-2.547658	0.666808	-2.100686
C	-1.875270	-2.210832	1.941063
P	0.183485	2.131945	0.325204
C	1.339145	2.820523	1.654779
P	2.618480	-0.848227	-0.098664
C	3.088751	-2.408217	-1.061059
C	0.695625	3.145088	-1.188407
C	-1.453659	2.941902	0.812813
C	3.391590	-1.195078	1.592714
C	3.838246	0.403790	-0.823545
H	-0.106859	-1.847072	-1.962831
H	-0.513493	-2.934210	-0.578615
H	-1.781496	-2.328441	-1.669213
H	-3.183278	1.556631	-2.150217
H	-1.499766	0.968650	-2.171133
H	-2.785352	0.019968	-2.955167
H	-0.847115	-2.461151	1.670339
H	-1.855180	-1.660365	2.888874
H	-2.447867	-3.134736	2.075616
H	-4.916379	0.257408	-0.597434
H	-4.555784	-1.461033	1.533824
H	-1.346728	4.031661	0.858525
H	-2.231601	2.687089	0.088042
H	-1.762498	2.570720	1.795256
H	2.375144	2.554314	1.422688
H	1.257840	3.912106	1.712441
H	1.077202	2.390333	2.626617
H	3.795198	1.340215	-0.257644
H	4.861637	0.013896	-0.782464
H	3.579452	0.610757	-1.867151
H	2.820134	-2.289366	-2.116081
H	4.165528	-2.598761	-0.989369
H	2.548410	-3.271626	-0.658950
H	0.736460	4.211912	-0.939543
H	1.681294	2.820323	-1.534935
H	-0.023451	2.998361	-2.000478
H	4.453650	-1.445435	1.489670
H	3.292465	-0.313943	2.234747
H	2.873323	-2.032408	2.071143

TS-D75
B3lyp/lanl2dz optimized geometry
Energy = -723.721417 a.u.

Enthalpy Correction (inc. ZPVE) = 0.426022
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.781286

Atom	x-coord	y-coord	z-coord
C	-3.895510	-0.776671	0.791346
N	-2.541337	-1.072393	1.028927
C	-1.770405	-0.794409	-0.104754
N	-2.690667	-0.275833	-1.023612
C	-3.987245	-0.268045	-0.475447
Pd	0.207674	-0.344452	-0.058505
C	-0.829466	-2.324716	-0.688044
C	-2.366920	0.075775	-2.409757
C	-2.028063	-1.608660	2.295660
P	0.159680	2.118796	0.225227
C	1.294362	2.890682	1.525374
P	2.641120	-0.822539	-0.071604
C	3.142221	-2.506190	-0.775329
C	0.627884	3.087868	-1.329592
C	-1.511209	2.877099	0.675587
C	3.476683	-0.855983	1.624810
C	3.782846	0.334305	-1.039512
H	-0.165076	-2.303458	-1.559195
H	-0.416916	-2.947287	0.110198
H	-1.781640	-2.758470	-1.009195
H	-3.033497	0.872339	-2.754519
H	-1.333538	0.429175	-2.462570
H	-2.480608	-0.788731	-3.076543
H	-0.940028	-1.685012	2.239366
H	-2.281691	-0.937285	3.123794
H	-2.451665	-2.599278	2.498527
H	-4.845039	0.085632	-1.024072
H	-4.656007	-0.912059	1.543241
H	-1.454721	3.971614	0.671901
H	-2.271071	2.552113	-0.041487
H	-1.808910	2.537639	1.672777
H	2.337583	2.642356	1.304952
H	1.184231	3.981162	1.536497
H	1.042469	2.496203	2.514887
H	3.732626	1.344935	-0.620611
H	4.820269	-0.015562	-0.992256
H	3.467503	0.372651	-2.087280
H	2.869859	-2.561418	-1.834732
H	4.222771	-2.661815	-0.679046
H	2.619747	-3.305309	-0.238930
H	0.609936	4.165849	-1.130959
H	1.630951	2.801231	-1.659562
H	-0.079768	2.863317	-2.134032
H	4.550617	-1.050952	1.525959
H	3.331471	0.104493	2.129260
H	3.028110	-1.641862	2.241245

TS-D90
B3lyp/lanl2dz optimized geometry
Energy = -723.722773 a.u.
Enthalpy Correction (inc. ZPVE) = 0.426123
NIMAG = 1

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.782767

Atom	x-coord	y-coord	z-coord
C	-3.944265	-0.471390	0.695607
N	-2.612315	-0.661888	1.106996
C	-1.770142	-0.801778	-0.001550
N	-2.622998	-0.643498	-1.100173
C	-3.951242	-0.460931	-0.672630
Pd	0.209428	-0.351040	-0.007975
C	-0.826160	-2.428910	-0.016139
C	-2.210678	-0.757949	-2.503892
C	-2.184146	-0.784985	2.505162
P	0.161989	2.128456	0.007752
C	1.307439	3.018035	1.219775
P	2.644277	-0.822113	-0.006311
C	3.136276	-2.558760	-0.576233
C	0.599257	2.956842	-1.633753
C	-1.512089	2.908417	0.404833
C	3.489321	-0.725184	1.682880
C	3.784959	0.250126	-1.068391
H	-0.257270	-2.711551	-0.907557
H	-0.305019	-2.724459	0.899697
H	-1.783517	-2.958804	-0.046685
H	-2.735661	-0.011006	-3.108263
H	-1.135957	-0.575040	-2.579353
H	-2.435349	-1.754980	-2.903323
H	-1.115132	-0.568689	2.575346
H	-2.727770	-0.064251	3.124514
H	-2.373913	-1.794252	2.891639
H	-4.766763	-0.321910	-1.363671
H	-4.752636	-0.342020	1.396809
H	-1.464924	3.999358	0.310494
H	-2.269305	2.518496	-0.282303
H	-1.805486	2.651255	1.427524
H	2.349798	2.763909	1.001994
H	1.183542	4.104257	1.141614
H	1.078263	2.705771	2.243549
H	3.743448	1.290452	-0.728741
H	4.820801	-0.101118	-1.000663
H	3.463171	0.209258	-2.114109
H	2.857428	-2.697134	-1.626214
H	4.216767	-2.710838	-0.473322
H	2.614532	-3.310323	0.025581
H	0.570194	4.048153	-1.534698
H	1.601583	2.652138	-1.949197
H	-0.116037	2.650087	-2.403457
H	4.562033	-0.931027	1.593949

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H     3.350044    0.272423    2.111300
H     3.041442   -1.458944    2.361034
```

7. Twist-Angle Products

PR-D

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B3lyp/lanl2dz optimized geometry
Energy = -723.764941 a.u.
Enthalpy Correction (inc. ZPVE) = 0.429432
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1393.825122

Atom  x-coord     y-coord     z-coord

C     4.559937   -1.081970    0.543259
N     3.790294   -1.307637   -0.606441
C     2.481914   -1.477684   -0.248997
N     2.418819   -1.361286    1.108788
C     3.701445   -1.118800    1.615079
Pd   -1.138714    0.455409   -0.025723
C     1.327133   -1.728551   -1.152685
C     1.182612   -1.478796    1.915712
C     4.318628   -1.349246   -1.985959
P     0.185071    2.552537   -0.019036
C    -0.515871    3.856217   -1.195535
P    -2.967881   -1.218509   -0.076188
C    -2.895048   -2.769415    1.009786
C     0.219113    3.503324    1.616546
C     2.021165    2.588792   -0.497283
C    -3.405272   -1.965612   -1.758576
C    -4.627554   -0.482728    0.450531
H     0.509412   -0.998388   -0.947244
H     1.615326   -1.639452   -2.202811
H     0.912354   -2.732364   -0.992634
H     1.383051   -1.097644    2.919487
H     0.379103   -0.878398    1.454542
H     0.874896   -2.527681    1.982638
H     5.405393   -1.253586   -1.946946
H     4.067740   -2.301206   -2.461939
H     3.912803   -0.523240   -2.577375
H     3.893613   -0.998093    2.668076
H     5.624252   -0.920512    0.505195
H     2.413188    3.612138   -0.458970
H     2.597832    1.962865    0.193335
H     2.138889    2.202510   -1.515766
```

H	-1.563241	4.044168	-0.940099
H	0.047725	4.794447	-1.126185
H	-0.475935	3.482442	-2.223480
H	-4.871981	0.361533	-0.201480
H	-5.426255	-1.231689	0.389307
H	-4.553802	-0.113934	1.478291
H	-2.774554	-2.475678	2.057710
H	-3.813704	-3.359494	0.908566
H	-2.041790	-3.391258	0.717109
H	0.727764	4.467908	1.500164
H	-0.807967	3.675889	1.952606
H	0.734768	2.912266	2.380593
H	-4.290109	-2.609071	-1.683709
H	-3.605831	-1.158588	-2.470200
H	-2.562953	-2.555847	-2.134850

8. Twist-Angle Separated Products

Pdbis(TMP)
B3lyp/lanl2dz optimized geometry
Energy = -379.246117 a.u.
Enthalpy Correction (inc. ZPVE) = 0.249051
NIMAG = 0

B3lyp/lanl2dzaug:6-311+G(2d,p) single point
Energy = -1049.160267

Atom	x-coord	y-coord	z-coord
C	-3.348744	1.630737	-0.420653
H	-4.440506	1.518720	-0.401051
H	-3.048051	2.394509	0.304007
P	-2.480045	-0.000544	-0.001396
C	-3.326971	-1.177017	-1.222128
H	-3.017379	-2.204297	-1.003478
H	-4.420171	-1.103125	-1.155617
H	-3.006028	-0.931418	-2.239726
C	-3.364813	-0.468119	1.608023
H	-4.455430	-0.442636	1.485677
H	-3.055370	-1.474443	1.908845
H	-3.070102	0.231642	2.396964
H	-3.034049	1.960029	-1.416373
Pd	-0.000114	0.006385	0.015679
P	2.479824	-0.000704	-0.000385
C	3.343947	1.529223	-0.710297
H	3.047181	2.410491	-0.132186
H	4.435905	1.422099	-0.678381
H	3.022094	1.674520	-1.746710
C	3.327064	-1.376047	-0.991977
H	3.020947	-2.348073	-0.591529
H	3.003082	-1.317951	-2.036257
H	4.420247	-1.288759	-0.943004
C	3.370344	-0.167688	1.663985
H	3.076198	0.662797	2.314170
H	3.064587	-1.103466	2.143280

```
H     4.460424   -0.162179    1.535120
```

2-Methyl-Imidazolium **NN_2Me$^+$**
B3lyp/LANL2DZ optimized geometry
Energy = -344.496943 a.u.
Enthalpy Correction (inc. ZPVE) = 0.179209
NIMAG =

B3lyp/6-311+G(2d,p) single point
Energy = -344.649607

Atom	x-coord	y-coord	z-coord
C	2.505902	0.207988	0.008655
N	1.098118	-0.250047	-0.002010
C	0.000000	0.559101	0.002976
N	-1.098161	-0.249933	-0.001937
C	-2.505926	0.208186	0.008616
C	0.686893	-1.589047	-0.004264
C	-0.687057	-1.588977	-0.004227
H	-2.666113	0.960020	-0.768401
H	-2.764998	0.624458	0.986963
H	-3.153497	-0.646469	-0.195478
H	2.665623	0.961403	-0.766919
H	3.153345	-0.646250	-0.197591
H	2.765542	0.622307	0.987686
H	1.384976	-2.409570	-0.006886
H	-1.385221	-2.409430	-0.006823
C	0.000180	2.052857	-0.007486
H	0.882684	2.448964	0.503037
H	0.001920	2.444640	-1.033683
H	-0.883916	2.449135	0.500100

9. Twist-Angle CDA Model Complexes

CX-MOD-D0
B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1118.298920 a.u.

Atom	x-coord	y-coord	z-coord
N	2.129531	1.001860	-0.000037
C	1.324691	-0.101727	-0.000004
C	1.703615	2.398280	-0.000122
N	2.201944	-1.149554	-0.000022
C	1.882325	-2.580483	0.000089
C	3.467544	0.648966	-0.000048
C	3.511561	-0.705115	-0.000058
H	1.313966	-2.843685	0.893650
H	1.313960	-2.843817	-0.893434
H	2.821496	-3.135849	0.000110
H	4.257731	1.383208	-0.000101
H	4.350499	-1.382894	-0.000084
H	1.124100	2.620510	0.897820
H	2.592886	3.029997	-0.000214

H	1.123988	2.620348	-0.898026
Pd	-0.772757	-0.246902	0.000059
P	-1.623681	2.087208	0.000061
P	-2.928839	-1.211670	-0.000148
H	-0.431729	-1.762274	0.000376
H	-1.347925	2.970454	1.066786
H	-1.347706	2.970915	-1.066251
H	-3.028776	2.230710	-0.000058
H	-4.099597	-0.421959	-0.000646
H	-3.233808	-2.068235	1.075290
H	-3.233191	-2.068667	-1.075381

CX-MOD-D15

B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1118.301069 a.u.

Atom	x-coord	y-coord	z-coord
N	-2.138738	0.941858	-0.201996
C	-1.307849	-0.138224	-0.146715
C	-1.765032	2.308399	-0.558084
N	-2.136846	-1.184408	0.136546
C	-1.748585	-2.584624	0.329732
C	-3.454585	0.573973	0.022039
C	-3.450999	-0.763755	0.240435
H	-1.319287	-2.988787	-0.589360
H	-1.025211	-2.669607	1.141671
H	-2.643768	-3.153204	0.585930
H	-4.264643	1.286057	-0.005368
H	-4.259712	-1.446102	0.450027
H	-0.898188	2.286090	-1.217638
H	-2.593500	2.772573	-1.096729
H	-1.551994	2.900269	0.336668
Pd	0.779159	-0.234219	-0.088128
P	1.464359	2.079013	0.482663
P	2.979618	-1.095207	-0.156032
H	0.484554	-1.680296	-0.592458
H	1.592385	2.987978	-0.590650
H	0.759330	2.917718	1.372831
H	2.751032	2.256253	1.037405
H	4.106158	-0.301349	0.151898
H	3.410821	-1.634838	-1.383067
H	3.242441	-2.192549	0.686969

CX-MOD-D30

B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1118.304594 a.u.

Atom	x-coord	y-coord	z-coord
N	-2.130981	0.884252	-0.338792
C	-1.286234	-0.168905	-0.164350
C	-1.770768	2.202140	-0.857376
N	-2.090786	-1.192077	0.233283
C	-1.655790	-2.551814	0.563238
C	-3.441596	0.518503	-0.074879
C	-3.413820	-0.786899	0.290875

H	-1.274353	-3.052728	-0.329397
H	-0.877217	-2.523585	1.326577
H	-2.515354	-3.103522	0.946506
H	-4.264594	1.208254	-0.180455
H	-4.209627	-1.456665	0.577129
H	-0.793329	2.141488	-1.334917
H	-2.503213	2.506476	-1.608531
H	-1.757254	2.944684	-0.053925
Pd	0.788796	-0.224178	-0.119805
P	1.302798	2.022301	0.775899
P	3.028574	-0.967492	-0.293788
H	0.523621	-1.611268	-0.795267
H	1.618070	3.025300	-0.167318
H	0.385145	2.759348	1.555078
H	2.432114	2.177655	1.609331
H	4.122433	-0.177668	0.122593
H	3.477183	-1.312333	-1.583241
H	3.342812	-2.158777	0.388736

CX-MOD-D45

B3lyp/lanl2dz:6-31G(d) optimized geometry

Energy = -1118.307582 a.u.

Atom	x-coord	y-coord	z-coord
N	-2.095387	0.850433	-0.471446
C	-1.267785	-0.188098	-0.179479
C	-1.700547	2.105718	-1.107510
N	-2.085938	-1.168293	0.285077
C	-1.662369	-2.469275	0.804132
C	-3.415799	0.517733	-0.206186
C	-3.407645	-0.749176	0.277083
H	-0.754231	-2.781279	0.289113
H	-1.470348	-2.408892	1.879231
H	-2.453753	-3.197726	0.617268
H	-4.231157	1.197530	-0.400101
H	-4.214288	-1.385872	0.606006
H	-0.648887	2.041977	-1.386834
H	-2.292293	2.261896	-2.013023
H	-1.859581	2.946619	-0.425889
Pd	0.798584	-0.221802	-0.145243
P	1.177022	1.890229	1.074882
P	3.065476	-0.844995	-0.428693
H	0.559318	-1.514303	-1.002569
H	1.696601	2.978389	0.339141
H	0.113989	2.566034	1.711592
H	2.098519	1.917990	2.144349
H	4.134001	-0.082194	0.090656
H	3.512371	-0.982947	-1.756882
H	3.431551	-2.109238	0.072627

CX-MOD-D60

B3lyp/lanl2dz:6-31G(d) optimized geometry

Energy = -1118.310152 a.u.

Atom	x-coord	y-coord	z-coord

N	-2.076793	0.832633	-0.574737
C	-1.261321	-0.170732	-0.160141
C	-1.649834	2.044757	-1.270859
N	-2.090163	-1.116223	0.348459
C	-1.674233	-2.380593	0.954655
C	-3.406210	0.513214	-0.334603
C	-3.413283	-0.710146	0.250833
H	-0.626417	-2.554479	0.710620
H	-1.795694	-2.338999	2.040873
H	-2.281283	-3.194292	0.550684
H	-4.215436	1.172646	-0.608332
H	-4.230037	-1.323045	0.599780
H	-0.571179	1.997759	-1.423167
H	-2.140209	2.104955	-2.245924
H	-1.905915	2.930696	-0.682501
Pd	0.800728	-0.208456	-0.159575
P	1.144643	1.733422	1.321816
P	3.066020	-0.768286	-0.563431
H	0.536252	-1.414996	-1.130560
H	1.934798	2.812209	0.866695
H	0.038135	2.475779	1.786917
H	1.784224	1.529387	2.564066
H	4.140641	-0.058189	0.014664
H	3.479210	-0.743242	-1.909510
H	3.457431	-2.078136	-0.225001

CX-MOD-D75
B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1118.311440 a.u.

Atom	x-coord	y-coord	z-coord
N	-2.070559	0.834220	-0.636553
C	-1.254209	-0.136301	-0.155063
C	-1.634899	2.032939	-1.350779
N	-2.081391	-1.077295	0.362297
C	-1.656322	-2.321709	1.001758
C	-3.401621	0.501772	-0.423495
C	-3.407722	-0.698934	0.207726
H	-0.587613	-2.451018	0.829195
H	-1.853487	-2.283732	2.076916
H	-2.197511	-3.162798	0.561531
H	-4.212396	1.139022	-0.741577
H	-4.225113	-1.311671	0.555555
H	-0.545948	2.026681	-1.406940
H	-2.043311	2.031401	-2.364811
H	-1.973668	2.929676	-0.824372
Pd	0.808153	-0.174506	-0.186262
P	1.107622	1.472841	1.623000
P	3.064463	-0.646069	-0.710440
H	0.518553	-1.216202	-1.327602
H	0.325763	2.648061	1.605007
H	0.801238	1.051012	2.934857
H	2.359131	2.069835	1.891127
H	4.137130	-0.025124	-0.034492
H	3.459509	-0.395612	-2.038829
H	3.473680	-1.988900	-0.597023

CX-MOD-D90
B3lyp/lanl2dz:6-31G(d) optimized geometry
Energy = -1118.311744 a.u.

Atom	x-coord	y-coord	z-coord
N	2.076914	-1.054284	-0.274105
C	1.254593	0.019678	-0.185409
C	1.644214	-2.441352	-0.435339
N	2.074860	1.094186	-0.085251
C	1.638742	2.486306	0.010475
C	3.405837	-0.655778	-0.224279
C	3.404474	0.695587	-0.104950
H	0.559177	2.521010	-0.139846
H	1.888024	2.896144	0.993448
H	2.128011	3.079819	-0.765844
H	4.220831	-1.360892	-0.280780
H	4.218077	1.401165	-0.035570
H	0.558758	-2.454467	-0.539590
H	2.095558	-2.867595	-1.334945
H	1.938486	-3.034035	0.435461
Pd	-0.807264	0.026204	-0.250249
P	-1.115372	-0.233881	2.181632
P	-3.056664	0.104073	-0.971064
H	-0.501637	0.188990	-1.784273
H	-0.593402	-1.395181	2.791333
H	-0.512095	0.722579	3.026401
H	-2.394512	-0.251610	2.780085
H	-4.136512	0.020644	-0.065652
H	-3.455754	-0.884816	-1.891003
H	-3.447905	1.254034	-1.683766

10. LANL2DZAUG:6-311+G(2d,p) Basis Set Implementation

Gaussian98 Basis Set and Pseudopotential genecp cards:

```
! basis set for high-level single points
-C -H -N -P 0
6-311+G(2d,p)
****
-Pd 0
S 3 1.00
           0.278700D+01 -.161024D+01
           0.196500D+01 0.184898D+01
           0.624300D+00 0.603749D+00
S 3 1.00
           0.278700D+01 0.135408D+01
           0.196500D+01 -.167809D+01
           0.624300D+00 -.855938D+00
S 1 1.00
           0.208100D+00 0.100000D+01
S 1 1.00
           0.832000D-01 0.100000D+01
```

```
S 1 1.00
           0.333000D-01 0.100000D+01
P 3 1.00
           0.599900D+01 -.103491D+00
           0.144300D+01 0.745695D+00
           0.526400D+00 0.365649D+00
P 1 1.00
           0.175500D+00 0.100000D+01
P 1 1.00
           0.585000D-01 0.100000D+01
P 1 1.00
           0.195000D-01 0.100000D+01
D 2 1.00
           0.609100D+01 0.376146D-01
           0.171900D+01 0.520048D+00
D 1 1.00
           0.605600D+00 0.100000D+01
D 1 1.00
           0.188300D+00 0.100000D+01
D 1 1.00
           0.628000D-01 0.100000D+01
F 2 1.00
           0.361217D+01 0.173786D+00
           0.129541D+01 0.597338D+00
F 1 1.00
           0.554710D+00 0.100000D+01
F 1 1.00
           0.237530D+00 0.100000D+01
****
```