Table S1. The Coordinates of Atoms in **1** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -154.37333
MP4/BS2//MP2/BS1 = -155.43489

atom	x	y	z
C	0.000000	0.000000	0.000000
C	1.323944	0.000000	0.000000
H	1.894257	-0.925275	0.000000
H	1.894257	0.925275	0.000000
C	-1.263378	0.787698	0.000000
H	-1.568601	1.281083	-0.916682
H	-1.568601	1.281083	0.916682
C	-1.263378	-0.787698	0.000000
H	-1.568601	-1.281083	-0.916682
H	-1.568601	-1.281083	0.916682

Table S2. The Coordinates of Atoms in **1** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -155.10351
B3LYP/BS2//B3LYP/BS1 = -155.96220

atom	x	y	z
C	0.000000	0.000000	0.000000
C	1.315557	0.000000	0.000000
H	1.884434	-0.925304	0.000000
H	1.884434	0.925304	0.000000
C	-1.258110	0.780549	0.000000
H	-1.559505	1.278365	-0.916408
H	-1.559505	1.278365	0.916408
C	-1.258110	-0.780549	0.000000
H	-1.559505	-1.278365	-0.916408
H	-1.559505	-1.278365	0.916408

Table S3. The Coordinates of Atoms in **2** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -807.61245
MP4/BS2//MP2/BS1 = -811.43724

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	2.368247	0.000000	0.003593
H	3.083561	0.000000	-1.235190
H	3.079956	-1.074018	0.625036
H	3.079956	1.074018	0.625036
P	-2.368247	0.000000	0.003593
H	-3.083561	0.000000	-1.235190
H	-3.079956	1.074018	0.625036
H	-3.079956	-1.074018	0.625036

Table S4. The Coordinates of Atoms in **2** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -809.59228
B3LYP/BS2//B3LYP/BS1 = -813.08750

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	2.349295	0.000000	0.000000
H	3.075553	0.000000	-1.236875
H	3.075553	-1.071165	0.618437
H	3.075553	1.071165	0.618437
P	-2.349295	0.000000	0.000000
H	-3.075553	0.000000	-1.236875
H	-3.075553	1.071165	0.618437
H	-3.075553	-1.071165	0.618437

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Table S5. The Coordinates of Atoms in **3(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -961.97591
MP4/BS2//MP2/BS1 = -966.85762

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	2.044499	0.000000	-1.274508
H	2.300179	-1.058216	-2.211983
H	3.363617	-0.014944	-0.688729
H	2.314074	1.074581	-2.189230
P	-2.044499	0.000000	-1.274508
H	-2.300179	-1.058216	-2.211983
H	-3.363617	-0.014944	-0.688729
H	-2.314074	1.074581	-2.189230
C	0.000000	-0.007793	3.427677
C	-0.904839	-0.003669	2.253549
H	-1.427464	0.922919	2.029242
H	-1.427626	-0.928740	2.023333
C	0.904839	-0.003669	2.253549
H	1.427464	0.922919	2.029242
H	1.427626	-0.928740	2.023333
C	0.000000	-0.013020	4.755433
H	0.926377	-0.014739	5.325394
H	-0.926377	-0.014739	5.325394

Table S6. The Coordinates of Atoms in **3(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -964.67378
B3LYP/BS2//B3LYP/BS1 = -969.02121

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	2.006033	0.000000	-1.369302
H	2.183090	-0.979727	-2.410952
H	3.354931	-0.121463	-0.860904
H	2.295354	1.133984	-2.209688
P	-2.008608	0.000000	-1.371060
H	-2.263169	-1.121727	-2.238361
H	-3.363179	0.074671	-0.868660
H	-2.203990	0.998328	-2.391445
C	0.002428	-0.011814	3.399977
C	-0.903436	-0.001707	2.238419

H	-1.429899	0.926739	2.033125
H	-1.444280	-0.920852	2.028786
C	0.906557	-0.016847	2.237171
H	1.447804	0.903035	2.031741
H	1.432073	-0.944592	2.026454
C	0.004119	-0.014087	4.719395
H	0.931150	-0.022769	5.286061
H	-0.921375	-0.007396	5.288592

Table S7. The Coordinates of Atoms in **4** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -962.02350
MP4/BS2//MP2/BS1 = -966.88494

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	-0.583465	2.561730
C	0.000000	-1.556800	3.489302
H	-0.927281	-1.975435	3.874106
H	0.927281	-1.975435	3.874106
C	1.165276	0.000000	1.799449
C	-1.165276	0.000000	1.799449
H	1.357786	1.059171	2.001434
H	2.067318	-0.613649	1.724779
H	-1.357786	1.059171	2.001434
H	-2.067318	-0.613649	1.724779
P	1.929770	-0.036714	-1.500781
H	2.902705	-1.055663	-1.253350
H	2.814698	1.085495	-1.428334
H	1.902596	-0.153155	-2.931320
P	-1.929770	-0.036714	-1.500781
H	-2.902705	-1.055663	-1.253350
H	-2.814698	1.085495	-1.428334
H	-1.902596	-0.153155	-2.931320

Table S8. The Coordinates of Atoms in **4** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -964.71935
B3LYP/BS2//B3LYP/BS1 = -969.05503

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	-0.563547	2.534295
C	0.000000	-1.540329	3.448206
H	-0.926669	-1.958416	3.831061
H	0.926669	-1.958416	3.831061
C	1.165355	0.000000	1.766502
C	-1.165355	0.000000	1.766502
H	1.377431	1.052686	1.985633
H	2.067892	-0.615027	1.731771
H	-1.377431	1.052686	1.985633
H	-2.067892	-0.615027	1.731771
P	1.921960	-0.032072	-1.530163
H	2.809596	-1.149201	-1.408390
H	2.903299	0.991527	-1.331718
H	1.908032	0.020533	-2.967433
P	-1.921960	-0.032072	-1.530163
H	-2.809596	-1.149201	-1.408390
H	-2.903299	0.991527	-1.331718
H	-1.908032	0.020533	-2.967433

Table S9. The Coordinates of Atoms in **5(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -961.99579
MP4/BS2//MP2/BS1 = -966.86019

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.350233
P	2.296795	0.000000	-0.722898
H	1.242755	0.099939	3.054721
H	-0.697493	1.019950	3.078146
H	-0.528777	-1.111944	3.086618
H	2.516361	0.026713	-2.133966
H	3.180278	-1.084521	-0.414105
H	3.194731	1.059299	-0.370698
C	-2.185697	-0.001807	-0.437673
H	-2.634778	-0.931972	-0.095007
H	-2.635425	0.927819	-0.094460

C	-1.377116	-0.001235	-1.645200
C	-0.800118	-1.285285	-1.975144
H	-1.351135	-2.182666	-1.709920
H	-0.116276	-1.355455	-2.818168
C	-0.798174	1.284435	-1.969041
H	-1.351466	2.180822	-1.705133
H	-0.111283	1.356394	-2.809513

Table S10. The Coordinates of Atoms in **5(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -964.68129
B3LYP/BS2//B3LYP/BS1 = -969.02158

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	2.367945
P	2.332283	0.000000	-0.639881
H	1.215515	-0.212357	3.097251
H	-0.437988	1.155593	3.101221
H	-0.801646	-0.952727	3.081450
H	2.597433	0.060829	-2.041780
H	3.198966	-1.101948	-0.335267
H	3.235371	1.039245	-0.236521
C	-2.133356	0.001800	-0.323505
H	-2.586864	-0.921811	0.027304
H	-2.588004	0.925333	0.025933
C	-1.454324	0.001905	-1.612614
C	-0.941223	-1.270626	-2.012085
H	-1.434055	-2.171811	-1.668411
H	-0.303946	-1.346765	-2.886472
C	-0.940174	1.274887	-2.009632
H	-1.434093	2.175914	-1.667057
H	-0.298244	1.351641	-2.880548

Table S11. The Coordinates of Atoms in **6(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -961.96483
MP4/BS2//MP2/BS1 = -966.84793

atom	x	y	z
Pd	0.000000	0.000000	0.000000

C	0.000000	0.000000	3.492424
C	0.881110	0.000000	2.299609
C	-0.806513	-0.254791	2.189981
C	2.205981	-0.018954	2.106450
H	2.685515	-0.081605	1.139002
H	2.864608	0.034637	2.977813
H	0.072398	-0.846908	4.171968
H	-0.180562	0.952175	3.987001
H	-1.171804	-1.268496	2.063604
H	-1.479450	0.551853	1.900651
P	1.628462	0.972547	-1.454322
H	2.060893	0.246083	-2.616409
H	2.951365	1.382558	-1.050384
H	1.305866	2.186213	-2.150365
P	-1.939692	-0.959700	-1.114064
H	-2.984634	-1.651094	-0.397650
H	-2.823844	-0.081626	-1.829456
H	-1.824036	-1.932197	-2.164730

Table S12. The Coordinates of Atoms in **6(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -964.65920
B3LYP/BS2//B3LYP/BS1 = -969.00578

atom	x	y	z
Pd	-0.113324	0.007295	-0.202613
C	-0.131249	0.020011	3.249237
C	0.758907	-0.008624	2.073223
C	-0.966380	-0.019474	1.959406
C	2.079387	-0.037571	1.926457
H	2.587335	-0.068418	0.973605
H	2.710415	-0.031531	2.819213
H	-0.166727	-0.873553	3.870364
H	-0.178538	0.948350	3.816428
H	-1.487630	-0.954781	1.778296
H	-1.514034	0.893602	1.742983
P	1.790801	0.065958	-1.719173
H	1.652294	0.143150	-3.150411
H	2.746252	-1.013456	-1.744069
H	2.781872	1.109976	-1.633474
P	-2.185189	-0.060217	-1.517601
H	-3.512283	-0.117137	-0.944320
H	-2.501673	1.001841	-2.438862
H	-2.421759	-1.120360	-2.464584

Table S13. The Coordinates of Atoms in **7** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -962.01523
MP4/BS2//MP2/BS1 = -966.87720

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.062001
C	1.936803	0.000000	0.874795
C	1.452706	0.346581	2.318937
C	-0.962928	-0.297845	2.946043
H	-1.974195	-0.580474	2.665359
H	-0.764378	-0.279128	4.022173
H	2.320265	-1.018164	0.770155
H	2.564333	0.747345	0.382154
H	1.572013	1.421331	2.507916
H	1.943599	-0.215504	3.128361
P	-2.432028	0.102840	-0.331777
H	-3.019781	1.407178	-0.385313
H	-3.245921	-0.425833	0.717375
H	-3.155396	-0.464576	-1.433915
P	0.791653	0.005297	-2.316755
H	1.387860	1.216886	-2.792949
H	1.891586	-0.862875	-2.603594
H	0.022121	-0.285619	-3.492444

Table S14. The Coordinates of Atoms in **7** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -964.71049
B3LYP/BS2//B3LYP/BS1 = -969.04434

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.043032
C	1.943017	0.000000	0.789069
C	1.484535	0.176857	2.269000
C	-0.975157	-0.149696	2.938242
H	-2.018136	-0.290496	2.665847
H	-0.769608	-0.142838	4.011996
H	2.411252	-0.967914	0.590517
H	2.535692	0.827103	0.389828
H	1.711892	1.187264	2.634754
H	1.923086	-0.551925	2.965850

P	-2.461270	0.030345	-0.296956
H	-3.144435	1.197047	0.173367
H	-3.210556	-0.927501	0.457357
H	-3.190253	-0.112193	-1.527283
P	0.741017	-0.012405	-2.363840
H	1.769989	0.926167	-2.696130
H	1.437955	-1.187238	-2.796177
H	-0.040340	0.164523	-3.558243

Table S15. The Coordinates of Atoms in **8** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -962.02276
MP4/BS2//MP2/BS1 = -966.90323

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.702709	0.000000	2.106273
C	-0.702709	0.000000	2.017862
H	1.236108	0.926666	2.314702
H	1.236108	-0.926666	2.314702
C	-1.848618	0.781472	2.605230
H	-2.550242	1.280541	1.945264
H	-1.690232	1.273198	3.561159
C	-1.848618	-0.781472	2.605230
H	-2.550242	-1.280541	1.945264
H	-1.690232	-1.273198	3.561159
P	1.937015	0.000000	-1.462423
H	1.898649	0.000000	-2.898279
H	2.880575	-1.070263	-1.327952
H	2.880575	1.070263	-1.327952
P	-2.055367	0.000000	-1.299236
H	-2.161015	0.000000	-2.731084
H	-2.980726	1.070843	-1.067907
H	-2.980726	-1.070843	-1.067907

Table S16. The Coordinates of Atoms in **8** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -964.71487
B3LYP/BS2//B3LYP/BS1 = -969.06410

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.696459	0.000000	2.088063
C	-0.696459	0.000000	2.033137
H	1.236540	0.923765	2.285374
H	1.236540	-0.923765	2.285374
C	-1.846262	0.776984	2.597808
H	-2.533035	1.275843	1.922811
H	-1.705027	1.269776	3.555656
C	-1.846262	-0.776984	2.597808
H	-2.533035	-1.275843	1.922811
H	-1.705027	-1.269776	3.555656
P	1.971952	0.000000	-1.446332
H	1.975303	0.000000	-2.887628
H	2.924236	-1.066131	-1.303721
H	2.924236	1.066131	-1.303721
P	-1.979587	0.000000	-1.425450
H	-1.992863	0.000000	-2.865188
H	-2.932211	1.065972	-1.275061
H	-2.932211	-1.065972	-1.275061

Table S17. The Coordinates of Atoms in **9** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.03455
MP4/BS2//MP2/BS1 = -702.61353

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	-2.100549	0.000000	-1.243827
H	-2.242752	0.026247	-2.670545
H	-2.966237	-1.109570	-0.985691
H	-3.028832	1.042265	-0.935329
C	0.000000	0.000000	2.666933
C	-1.075191	0.576558	1.783365
H	-1.089080	1.670621	1.733209
H	-2.066994	0.118363	1.842708
C	1.206343	0.199316	1.790103
H	1.568458	1.231121	1.730623

H	1.995119	-0.553419	1.837893
C	-0.124425	-0.723393	3.792421
H	0.737033	-1.187205	4.267459
H	-1.093321	-0.887799	4.258574
C	2.000560	-0.552949	-0.967443
H	2.612646	0.334823	-0.838270
H	2.319612	-1.449058	-0.443836
C	1.050749	-0.623986	-1.976947
H	0.897988	0.210471	-2.656161
H	0.615649	-1.578080	-2.262904

Table S18. The Coordinates of Atoms in **9** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.48453
B3LYP/BS2//B3LYP/BS1 = -704.49676

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	-2.082128	0.000000	-1.311373
H	-2.234557	-0.089009	-2.737511
H	-3.026329	-1.018255	-0.964692
H	-2.945262	1.121886	-1.106119
C	0.000000	0.000000	2.620305
C	-1.079512	0.563253	1.740619
H	-1.113517	1.658255	1.720444
H	-2.069489	0.109626	1.834298
C	1.206607	0.199659	1.752583
H	1.572860	1.231843	1.722754
H	2.008393	-0.533794	1.846635
C	-0.125628	-0.745398	3.723247
H	0.735818	-1.210971	4.193351
H	-1.094804	-0.921519	4.181036
C	2.048388	-0.589425	-0.995878
H	2.656036	0.292850	-0.827934
H	2.331424	-1.484916	-0.454131
C	1.124309	-0.634408	-2.002222
H	0.971197	0.214195	-2.661394
H	0.654148	-1.569837	-2.288644

Table S19. The Coordinates of Atoms in **10** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.03249
MP4/BS2//MP2/BS1 = -702.61297

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	-1.946613	0.000000	-1.522959
H	-1.931249	-0.374505	-2.909743
H	-3.070488	-0.794795	-1.132492
H	-2.642970	1.240191	-1.676463
C	0.000000	0.000000	2.631505
C	-1.062109	0.632558	1.762097
H	-1.031601	1.726919	1.729261
H	-2.070279	0.213274	1.820701
C	1.212146	0.150582	1.746053
H	1.634435	1.160213	1.706531
H	1.953068	-0.653685	1.757810
C	-0.144075	-0.726283	3.753105
H	0.700668	-1.231204	4.216258
H	-1.114470	-0.850630	4.228340
C	1.381949	-1.334148	-1.339999
H	1.821208	-2.007482	-0.609280
H	0.729883	-1.779313	-2.085907
C	1.821372	-0.031136	-1.460521
H	2.622723	0.349599	-0.835156
H	1.515126	0.590365	-2.298009

Table S20. The Coordinates of Atoms in **10** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.48396
B3LYP/BS2//B3LYP/BS1 = -704.49535

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	-1.984887	0.000000	-1.499791
H	-2.029839	-0.184319	-2.926734
H	-3.012122	-0.943505	-1.174109
H	-2.804842	1.171758	-1.450626
C	0.000000	0.000000	2.600000
C	-1.059594	0.623618	1.731329
H	-1.036454	1.718992	1.717980
H	-2.071305	0.222771	1.828989
C	1.211436	0.137908	1.719933

H	1.645581	1.144075	1.708000
H	1.963632	-0.652220	1.785735
C	-0.153264	-0.744519	3.700260
H	0.687384	-1.256430	4.159941
H	-1.125900	-0.872539	4.166778
C	1.379730	-1.295265	-1.458217
H	1.788081	-2.024169	-0.765993
H	0.698698	-1.670237	-2.215063
C	1.845428	-0.014689	-1.494964
H	2.644613	0.312130	-0.839729
H	1.544378	0.674375	-2.278240

Table S21. The Coordinates of Atoms in **11(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.00623
MP4/BS2//MP2/BS1 = -702.58691

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.154628
C	1.398330	0.000000	1.763376
H	1.961696	-0.930734	1.781912
H	1.962186	0.930351	1.784093
C	-0.649241	-1.278519	1.983242
H	-0.069087	-2.181797	2.146035
H	-1.726461	-1.346675	2.114822
C	-0.649122	1.278815	1.983091
H	-0.069009	2.182068	2.146054
H	-1.726539	1.346878	2.113298
C	-1.791418	-0.699073	-1.204439
H	-2.426730	-1.242483	-0.513055
H	-1.404316	-1.262140	-2.048958
C	-1.783045	0.706098	-1.213117
H	-2.410894	1.265784	-0.527902
H	-1.390903	1.254700	-2.064788
P	1.577627	-0.010889	-1.764260
H	1.017084	-0.089829	-3.080574
H	2.468403	1.087353	-2.008568
H	2.556622	-1.048573	-1.915797

Table S22. The Coordinates of Atoms in **11(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.44812
B3LYP/BS2//B3LYP/BS1 = -704.46316

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	1.625358	0.000000	-1.739392
H	1.158046	-0.003237	-3.094892
H	2.570052	1.072416	-1.876843
H	2.574651	-1.068771	-1.873123
C	-1.859005	-0.689219	-1.218930
H	-2.425273	-1.251253	-0.486234
H	-1.460690	-1.250835	-2.057639
C	-1.859775	0.689269	-1.217812
H	-2.426632	1.249480	-0.484178
H	-1.462062	1.252705	-2.055586
C	0.000000	0.000000	2.181419
C	1.367837	0.000131	1.683040
H	1.939107	-0.923608	1.724333
H	1.938956	0.923957	1.724442
C	-0.646835	-1.269403	2.114652
H	-0.054118	-2.172560	2.192400
H	-1.712584	-1.346025	2.300351
C	-0.647007	1.269297	2.114292
H	-0.054371	2.172533	2.191722
H	-1.712739	1.345860	2.300102

Table S23. The Coordinates of Atoms in **12** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.04287
MP4/BS2//MP2/BS1 = -702.63901

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	1.747330	0.000000	-1.701864
H	1.476098	0.000000	-3.108882
H	2.695089	-1.073453	-1.704026
H	2.695089	1.073453	-1.704026
C	0.000000	0.000000	2.162825
C	1.348258	0.000000	1.785936
H	1.918882	-0.928112	1.799888
H	1.918882	0.928112	1.799888

C	-0.915336	-0.782183	3.061533
H	-1.782715	-1.276645	2.639336
H	-0.475869	-1.275465	3.924091
C	-0.915336	0.782183	3.061533
H	-1.782715	1.276645	2.639336
H	-0.475869	1.275465	3.924091
C	-2.227999	0.000000	-0.095459
H	-2.563041	-0.925294	0.367149
H	-2.563041	0.925294	0.367149
C	-1.742739	0.000000	-1.415295
H	-1.708814	-0.925031	-1.986422
H	-1.708814	0.925031	-1.986422

Table S24. The Coordinates of Atoms in **12** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.48884
B3LYP/BS2//B3LYP/BS1 = -704.51262

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	1.803853	0.000000	-1.673078
H	1.590325	0.000000	-3.094024
H	2.762131	-1.068874	-1.660427
H	2.762131	1.068874	-1.660427
C	0.000000	0.000000	2.201400
C	1.322640	0.000000	1.801754
H	1.893854	-0.925857	1.796246
H	1.893854	0.925857	1.796246
C	-0.934458	-0.777923	3.069019
H	-1.790077	-1.269352	2.620164
H	-0.519821	-1.275828	3.940797
C	-0.934458	0.777923	3.069019
H	-1.790077	1.269352	2.620164
H	-0.519821	1.275828	3.940797
C	-2.234181	0.000000	-0.132390
H	-2.569732	-0.922162	0.333285
H	-2.569732	0.922162	0.333285
C	-1.738941	0.000000	-1.429568
H	-1.682822	-0.922582	-2.000495
H	-1.682822	0.922582	-2.000495

Table S25. The Coordinates of Atoms in **13** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.04195
MP4/BS2//MP2/BS1 = -702.63795

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.226894
C	1.309364	0.000000	1.733075
H	-0.461152	0.927656	2.562201
H	-0.461152	-0.927656	2.562201
C	2.578366	0.782756	1.927622
H	3.037743	1.281392	1.080569
H	2.727957	1.275344	2.884132
C	2.578366	-0.782756	1.927622
H	3.037743	-1.281392	1.080569
H	2.727957	-1.275344	2.884132
C	-2.230305	0.000000	-0.141133
H	-2.570927	0.924209	0.318768
H	-2.570927	-0.924209	0.318768
C	-1.723290	0.000000	-1.451529
H	-1.678222	-0.924874	-2.022127
H	-1.678222	0.924874	-2.022127
P	1.799372	0.000000	-1.641462
H	1.598723	0.000000	-3.059376
H	2.747242	-1.073837	-1.594185
H	2.747242	1.073837	-1.594185

Table S26. The Coordinates of Atoms in **13** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.48822
B3LYP/BS2//B3LYP/BS1 = -704.51201

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.229969
C	1.303043	0.000000	1.768967
H	-0.471648	0.924645	2.553472
H	-0.471648	-0.924645	2.553472
C	2.569447	0.778373	1.930026
H	3.003913	1.276513	1.070167
H	2.743737	1.272495	2.881379
C	2.569447	-0.778373	1.930026

H	3.003913	-1.276513	1.070167
H	2.743737	-1.272495	2.881379
C	-2.255941	0.000000	-0.107937
H	-2.578759	0.921688	0.366383
H	-2.578759	-0.921688	0.366383
C	-1.774157	0.000000	-1.407730
H	-1.717651	-0.923172	-1.977451
H	-1.717651	0.923172	-1.977451
P	1.755684	0.000000	-1.703738
H	1.505713	0.000000	-3.117533
H	2.715550	-1.068777	-1.715243
H	2.715550	1.068777	-1.715243

Table S27. The Coordinates of Atoms in **14(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -698.98769
MP4/BS2//MP2/BS1 = -702.57190

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	-1.525871	0.000000	-1.711109
H	-1.261758	-0.638581	-2.963602
H	-2.805724	-0.575883	-1.449126
H	-1.962747	1.262468	-2.21494
C	0.000000	0.000000	2.314324
C	-1.07894	0.835719	1.716452
H	-0.909548	1.914913	1.737052
H	-2.104041	0.534879	1.943500
C	1.381697	0.474174	1.869547
H	1.417301	1.543049	1.645416
H	2.171557	0.187515	2.565197
C	-0.174354	-1.214943	2.918823
H	0.673680	-1.831724	3.208925
H	-1.164637	-1.572592	3.187354
C	2.353393	-0.487364	0.456768
H	3.156664	0.250429	0.426054
H	2.575578	-1.347651	1.089181
C	1.775686	-0.853761	-0.849506
H	2.066001	-0.259608	-1.714651
H	1.600060	-1.910900	-1.038672

Table S28. The Coordinates of Atoms in **14(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.44666
B3LYP/BS2//B3LYP/BS1 = -704.46103

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	-1.631919	0.000000	-1.631866
H	-1.378353	-0.396184	-2.985150
H	-2.780545	-0.815290	-1.393929
H	-2.305278	1.230027	-1.906346
C	0.000000	0.000000	2.428444
C	-1.064048	0.763642	1.711413
H	-0.925566	1.849404	1.712053
H	-2.088698	0.463715	1.935545
C	1.377550	0.360229	1.891310
H	1.488507	1.428436	1.690847
H	2.167643	0.018029	2.557802
C	-0.190428	-1.039234	3.271810
H	0.641029	-1.625496	3.651670
H	-1.184206	-1.312287	3.610416
C	2.316370	-0.602041	0.440261
H	3.155892	0.090477	0.488351
H	2.474582	-1.510651	1.018036
C	1.748067	-0.821153	-0.899233
H	2.120223	-0.184670	-1.700822
H	1.570789	-1.855897	-1.186889

Table S29. The Coordinates of Atoms in **15(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -698.98978
MP4/BS2//MP2/BS1 = -702.56576

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.134300
P	1.252586	0.000000	-1.963247
H	0.716960	0.641294	-3.129773
H	2.574693	0.550531	-2.055226
H	1.553596	-1.260244	-2.573003
C	1.384516	-0.219281	1.797787
H	1.793452	-1.226882	1.846204
H	2.090001	0.607771	1.851554

C	-0.455015	1.393928	2.175803
H	-1.327259	1.636966	2.774677
H	0.309006	2.167028	2.115483
C	-0.909549	-1.095654	1.914175
H	-1.972504	-0.931012	2.077771
H	-0.547689	-2.114049	2.028470
C	-1.949459	1.599529	0.296831
H	-2.648785	1.514322	1.121081
H	-1.615027	2.606627	0.066892
C	-2.026832	0.625034	-0.733522
H	-2.709560	-0.211935	-0.626476
H	-1.756168	0.904318	-1.748992

Table S30. The Coordinates of Atoms in **15(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.44080
B3LYP/BS2//B3LYP/BS1 = -704.45215

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.373154
P	1.646154	0.000000	-1.772286
H	1.563555	-1.087914	-2.700247
H	1.722710	1.054126	-2.742585
H	3.053889	-0.097116	-1.513366
C	1.101807	-0.711777	1.789871
H	1.006226	-1.788942	1.661540
H	2.115262	-0.333827	1.907592
C	0.097883	1.248128	2.992018
H	-0.742341	1.597353	3.580105
H	1.073916	1.625438	3.284884
C	-1.241211	-0.435890	1.694227
H	-2.128326	0.174140	1.837820
H	-1.429728	-1.510106	1.648657
C	-0.576685	2.693178	1.292445
H	-1.286660	3.040218	2.032786
H	0.393573	3.177392	1.318332
C	-1.042032	2.140262	0.097899
H	-2.107286	1.970491	-0.027486
H	-0.488229	2.334672	-0.820761

Table S31. The Coordinates of Atoms in **16(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -698.95635
MP4/BS2//MP2/BS1 = -702.54059

atom	x	y	z
Pd	0.457393	-0.202142	-0.238207
C	0.528788	-0.345244	1.965852
P	1.01832	-0.205845	-2.557578
H	1.612785	0.927256	-3.195891
H	1.993739	-1.174180	-2.956818
H	0.049261	-0.494248	-3.573179
C	-0.086132	0.860593	1.605876
H	-0.075093	-1.187097	2.295522
H	1.577489	-0.338469	2.260426
C	0.318456	2.234624	1.711579
H	0.091693	2.924785	0.906267
H	0.852655	2.615147	2.580266
C	-1.517163	1.220600	1.639949
H	-1.913210	1.808061	0.816877
H	-2.018322	1.302197	2.602504
C	-2.506352	-0.743969	0.822426
H	-3.310063	-0.119456	0.443175
H	-2.602454	-1.072107	1.853174
C	-1.672931	-1.421216	-0.054981
H	-1.129218	-2.306522	0.272723
H	-1.832148	-1.331470	-1.128054

Table S32. The Coordinates of Atoms in **16(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.40931
B3LYP/BS2//B3LYP/BS1 = -704.42736

atom	x	y	z
Pd	0.519540	-0.233805	-0.242620
C	0.521775	-0.246140	1.962923
P	1.009643	-0.239461	-2.580688
H	1.866384	0.744481	-3.176623
H	1.683347	-1.387792	-3.117148
H	-0.021035	-0.179058	-3.578767
C	-0.139307	0.925516	1.608373
H	-0.044559	-1.110575	2.293455
H	1.563984	-0.196875	2.270587

C	0.190531	2.299448	1.757525
H	-0.100836	3.015949	1.000785
H	0.804783	2.654195	2.580793
C	-1.580864	1.193743	1.647798
H	-2.019781	1.803217	0.869259
H	-2.091309	1.161772	2.604441
C	-2.547836	-0.711352	0.835819
H	-3.350055	-0.086556	0.456515
H	-2.668325	-1.071052	1.852181
C	-1.719852	-1.376596	-0.037691
H	-1.176341	-2.263319	0.276015
H	-1.836415	-1.245154	-1.109158

Table S33. The Coordinates of Atoms in **17** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.05269
MP4/BS2//MP2/BS1 = -702.63932

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	2.387719	0.000000	-0.633503
H	2.953349	-1.043328	-1.434771
H	2.996848	1.102117	-1.316360
H	3.316405	-0.077131	0.452194
C	0.000000	0.000000	2.120848
H	-0.601893	-0.841528	2.472518
H	1.066164	-0.144952	2.332870
C	-0.516437	1.336572	2.531267
C	0.292998	2.331710	2.958531
H	-0.100155	3.302987	3.249224
H	1.371112	2.200307	3.031594
C	-2.027618	1.508032	2.446203
H	-2.508849	0.741049	3.071692
H	-2.314994	2.494288	2.834944
C	-2.525971	1.342110	0.982487
H	-3.626315	1.413887	0.975880
H	-2.136326	2.178442	0.386697
C	-2.057630	0.008703	0.376016
H	-2.390652	-0.857811	0.958374
H	-2.374246	-0.101231	-0.677654

Table S34. The Coordinates of Atoms in **17** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.51411
B3LYP/BS2//B3LYP/BS1 = -704.52831

atom	x	y	z
Pd	0.000000	0.000000	0.000000
P	2.448223	0.000000	-0.481105
H	3.044120	-0.899380	-1.426883
H	3.129622	1.183647	-0.920613
H	3.321393	-0.301147	0.614227
C	0.000000	0.000000	2.094887
H	-0.502236	-0.927449	2.383586
H	1.058779	-0.023996	2.369985
C	-0.697727	1.218957	2.572573
C	-0.043287	2.267820	3.100073
H	-0.569346	3.153087	3.443580
H	1.037514	2.268086	3.211220
C	-2.209125	1.218751	2.426825
H	-2.616428	0.323672	2.920213
H	-2.633898	2.099615	2.921723
C	-2.631459	1.193553	0.934809
H	-3.732570	1.188388	0.883804
H	-2.287722	2.120820	0.458568
C	-2.055669	-0.022224	0.198817
H	-2.387172	-0.960894	0.659646
H	-2.354441	-0.021764	-0.865364

Table S35. The Coordinates of Atoms in **18** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.05357
MP4/BS2//MP2/BS1 = -702.63995

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.086437
C	1.442029	0.000000	2.463121
H	-0.584295	0.807871	2.535599
H	-0.488006	-0.980069	2.231784
C	2.136373	-1.113466	2.791042
H	3.198742	-1.077385	3.021578
H	1.657441	-2.089315	2.843774
C	2.104943	1.372414	2.411275

H	1.564631	2.054835	3.084298
H	3.145441	1.304169	2.755966
C	2.061177	1.956391	0.970926
H	2.478596	2.977755	0.992463
H	2.707616	1.347051	0.326131
C	0.637108	1.993411	0.396076
H	-0.076348	2.499719	1.052356
H	0.597262	2.412613	-0.616629
P	-0.027790	-0.171261	-2.452747
H	0.207006	1.048856	-3.161419
H	0.881080	-0.992901	-3.194889
H	-1.223656	-0.558127	-3.138695

Table S36. The Coordinates of Atoms in **18** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.51466
B3LYP/BS2//B3LYP/BS1 = -704.52877

atom	x	y	z
Pd	0.584680	-0.376797	-0.245805
C	-1.304331	-0.962726	-0.868639
C	-2.292853	-0.488993	0.132711
H	-1.498816	-0.583905	-1.877204
H	-1.200033	-2.059542	-0.882010
C	-2.859461	-1.280098	1.059744
H	-3.553979	-0.887665	1.796392
H	-2.651236	-2.345475	1.101981
C	-2.596069	0.999611	0.068678
H	-2.937832	1.252382	-0.946067
H	-3.399434	1.253681	0.769375
C	-1.337961	1.846747	0.386959
H	-1.605729	2.913502	0.298151
H	-1.047031	1.671935	1.430242
C	-0.162224	1.550538	-0.546562
H	-0.441343	1.640957	-1.601065
H	0.697659	2.196811	-0.334905
P	2.891299	0.099375	0.530125
H	3.202369	0.276633	1.919190
H	3.980875	-0.782213	0.222991
H	3.507161	1.304482	0.060754

Table S37. The Coordinates of Atoms in **19** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.02579
MP4/BS2//MP2/BS1 = -702.60573

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.077024
C	1.932067	0.000000	0.946504
C	1.425394	0.413877	2.359821
C	-0.946091	-0.393375	2.940890
H	-1.930463	-0.747638	2.647880
H	-0.752192	-0.384708	4.017534
H	2.301246	-1.026041	0.887969
H	2.561129	0.719746	0.420341
H	1.504773	1.501444	2.482461
H	1.914393	-0.082152	3.212137
P	-2.420483	0.270370	-0.198489
H	-2.869089	1.595932	-0.498144
H	-3.223083	0.046493	0.961508
H	-3.241707	-0.42337	-1.147528
C	1.241874	-0.211372	-1.918617
H	1.924407	0.632524	-1.898730
H	1.682752	-1.199753	-1.824679
C	-0.066722	-0.053278	-2.348108
H	-0.428787	0.917737	-2.676557
H	-0.674402	-0.917458	-2.602611

Table S38. The Coordinates of Atoms in **19** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.47532
B3LYP/BS2//B3LYP/BS1 = -704.48654

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.053075
C·	1.939932	0.000000	0.841974
C	1.459403	0.302001	2.288354
C	-0.944063	-0.297803	2.943568
H	-1.966170	-0.554382	2.680030
H	-0.720913	-0.307944	4.013482
H	2.369281	-0.997821	0.725972
H	2.564680	0.770177	0.385086

H	1.601576	1.365039	2.524429
H	1.936940	-0.298316	3.076803
P	-2.444897	0.233330	-0.243627
H	-2.940545	1.510369	-0.663681
H	-3.228427	0.111591	0.944386
H	-3.274483	-0.566262	-1.100715
C	1.210022	-0.251489	-2.029106
H	1.937641	0.548121	-1.957250
H	1.588246	-1.263754	-1.934858
C	-0.071230	-0.008287	-2.426936
H	-0.397659	0.995029	-2.682127
H	-0.745561	-0.823737	-2.667045

Table S39. The Coordinates of Atoms in **20** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.02491
MP4/BS2//MP2/BS1 = -702.60519

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.095889
C	1.924008	0.000000	0.924646
C	1.440555	0.390192	2.350344
C	-0.934682	-0.324114	2.999323
H	-1.944341	-0.634737	2.749934
H	-0.704276	-0.289723	4.068690
H	2.289283	-1.026907	0.844215
H	2.552772	0.725361	0.402164
H	1.533254	1.474236	2.493990
H	1.943778	-0.126418	3.182030
P	0.970524	0.008466	-2.23872
H	2.396455	0.014601	-2.349867
H	0.710192	-1.071391	-3.142668
H	0.701690	1.079674	-3.151242
C	-2.297559	-0.036283	0.158630
H	-2.500832	-1.001793	0.611605
H	-2.512604	0.843103	0.756287
C	-2.035957	0.065450	-1.196383
H	-2.047818	-0.817503	-1.830321
H	-2.052084	1.031942	-1.693666

Table S40. The Coordinates of Atoms in **20** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.47452
B3LYP/BS2//B3LYP/BS1 = -704.48592

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.074094
C	1.926822	0.000000	0.820474
C	1.477154	0.243708	2.285824
C	-0.929333	-0.215452	3.002979
H	-1.974163	-0.409122	2.781505
H	-0.669722	-0.208558	4.065060
H	2.361196	-0.989707	0.654865
H	2.536288	0.792224	0.378051
H	1.661203	1.285591	2.580214
H	1.950200	-0.416604	3.027165
P	0.879469	0.026027	-2.306520
H	2.303692	0.023721	-2.440291
H	0.608715	-1.025459	-3.244217
H	0.617402	1.121014	-3.195989
C	-2.369622	-0.073143	0.167175
H	-2.515439	-1.045605	0.624246
H	-2.552966	0.792890	0.791884
C	-2.145292	0.050135	-1.170016
H	-2.119752	-0.822243	-1.815318
H	-2.151232	1.022577	-1.652401

Table S41. The Coordinates of Atoms in **21** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.02481
MP4/BS2//MP2/BS1 = -702.60630

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.051894
C	1.943773	0.000000	0.876689
C	1.465422	0.220140	2.350220
C	-1.039026	-0.179266	2.878595
H	-2.057011	-0.347559	2.533797
H	-0.908737	-0.170352	3.964748
H	2.366500	-0.989911	0.686545
H	2.530139	0.810340	0.437342

H	1.661559	1.251011	2.673109
H	1.905472	-0.473094	3.081557
P	0.710380	-0.016555	-2.367972
H	1.691533	0.948299	-2.759639
H	1.409199	-1.179449	-2.824781
H	-0.150486	0.129975	-3.508205
C	-2.219567	0.734477	-0.274545
H	-2.410909	1.194144	0.689594
H	-2.174689	1.396145	-1.135716
C	-2.241313	-0.634229	-0.424982
H	-2.448766	-1.287093	0.417513
H	-2.220316	-1.094870	-1.408780

Table S42. The Coordinates of Atoms in **21** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.47638
B3LYP/BS2//B3LYP/BS1 = -704.48681

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.036425
C	1.947260	0.000000	0.791634
C	1.488861	0.038456	2.283699
C	-1.014798	-0.029031	2.898077
H	-2.057735	-0.056406	2.590020
H	-0.846319	-0.028209	3.978017
H	2.459681	-0.922737	0.507678
H	2.497126	0.886349	0.465443
H	1.802877	0.960456	2.791609
H	1.851471	-0.819764	2.866041
P	0.721943	0.006676	-2.397461
H	1.474789	1.148116	-2.824752
H	1.702614	-0.978459	-2.740121
H	-0.071486	-0.124152	-3.591131
C	-2.280171	0.671296	-0.332221
H	-2.451503	1.222543	0.585619
H	-2.243969	1.248255	-1.251068
C	-2.272888	-0.689562	-0.346574
H	-2.438862	-1.262036	0.559253
H	-2.230802	-1.246589	-1.277320

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Table S43. The Coordinates of Atoms in **22(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -698.97082
MP4/BS2//MP2/BS1 = -702.55669

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.078019
C	0.764853	0.000000	3.180335
H	1.849703	0.087490	3.143244
H	0.339300	-0.098215	4.185762
C	-1.540897	-0.152466	2.106696
H	-1.943980	-0.607151	3.033219
H	-2.013264	0.832134	1.987688
C	-1.919434	-1.052317	0.869805
H	-2.987804	-1.282123	0.892865
H	-1.356185	-1.991491	0.891081
C	-2.127613	-0.544085	-0.957565
H	-2.552871	-1.517862	-1.205568
H	-2.894794	0.219907	-0.829441
C	-1.004472	-0.144985	-1.863488
H	-0.619412	-0.921506	-2.523122
H	-1.088868	0.839558	-2.322557
P	2.031828	0.948268	-0.445102
H	2.649105	0.953322	-1.734072
H	3.134644	0.482235	0.329128
H	2.122992	2.341358	-0.154899

Table S44. The Coordinates of Atoms in **22(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.43087
B3LYP/BS2//B3LYP/BS1 = -704.44511

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.351130
C	1.919518	0.000000	0.765591
C	1.452330	0.551367	2.117221
C	3.165909	-0.369551	0.478745
H	3.446898	-0.777629	-0.490661
H	3.979461	-0.291998	1.206703
H	-0.386560	0.393736	3.292354
H	0.007500	-1.092002	2.405542

H	2.097035	0.282017	2.975095
H	1.413528	1.648218	2.069076
C	-1.744847	0.496207	1.574772
H	-2.230617	-0.181165	2.275309
H	-1.761048	1.530210	1.913469
C	-2.106618	0.290553	0.159022
H	-2.690803	-0.599932	-0.066494
H	-2.408635	1.179472	-0.392573
P	0.467795	-0.155534	-2.257297
H	-0.428368	-0.732478	-3.212558
H	1.659501	-0.845190	-2.636990
H	0.716371	1.080314	-2.928175

Table S45. The Coordinates of Atoms in **23(TS)** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -698.97793
MP4/BS2//MP2/BS1 = -702.56089

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.143488
C	1.986828	0.000000	0.846585
C	1.400169	0.60909	2.190308
C	-0.34468	-1.139228	2.780837
H	-1.301236	-1.633128	2.622010
H	0.323319	-1.590328	3.516168
H	2.328687	-1.026869	1.015980
H	2.755459	0.615083	0.367910
H	1.343763	1.700361	2.098630
H	1.946408	0.361936	3.118435
P	0.414603	-0.188516	-2.266373
H	1.638112	0.332203	-2.786697
H	0.531692	-1.525591	-2.755874
H	-0.465896	0.318019	-3.275757
C	-1.582437	0.940123	1.507098
H	-2.184221	0.512403	2.303926
H	-1.263426	1.960647	1.720833
C	-2.070974	0.674370	0.143162
H	-2.850723	-0.074286	0.022071
H	-2.101708	1.510557	-0.552871

Table S46. The Coordinates of Atoms in **23(TS)** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.43415
B3LYP/BS2//B3LYP/BS1 = -704.44591

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.171053
C	1.969821	0.000000	0.815078
C	1.401818	0.601929	2.157680
C	-0.341139	-1.021565	2.964096
H	-1.300542	-1.527991	2.904503
H	0.346831	-1.375887	3.732233
H	2.363918	-1.007662	0.977859
H	2.706913	0.640820	0.321016
H	1.354764	1.694345	2.075304
H	1.969257	0.349213	3.070196
P	0.476755	-0.249108	-2.267154
H	1.693859	0.307655	-2.769934
H	0.676337	-1.595168	-2.704653
H	-0.386303	0.174983	-3.331562
C	-1.655050	0.874573	1.490642
H	-2.240909	0.375061	2.252850
H	-1.387885	1.894813	1.760802
C	-2.076487	0.638374	0.111578
H	-2.829670	-0.128861	-0.051742
H	-2.141602	1.500292	-0.549055

Table S47. The Coordinates of Atoms in **24** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.05149
MP4/BS2//MP2/BS1 = -702.63795

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.024694
C	1.192850	0.000000	2.655536
H	2.128326	-0.220752	2.147823
H	1.273720	0.234039	3.721620
C	-1.331355	0.163630	2.732803
H	-1.171677	0.455219	3.784189
H	-1.936501	0.941402	2.247664
C	-2.102499	-1.183743	2.688317

H	-1.537392	-1.924803	3.269499
H	-3.092186	-1.069162	3.150396
C	-2.252867	-1.700753	1.236547
H	-2.764176	-2.678021	1.267036
H	-2.890389	-1.014094	0.665183
C	-0.899687	-1.868176	0.529069
H	-0.196000	-2.474104	1.106297
H	-1.004561	-2.257854	-0.491616
P	0.073524	0.236304	-2.448789
H	-1.116920	-0.018686	-3.199616
H	0.414049	1.482260	-3.067857
H	0.955451	-0.591647	-3.212540

Table S48. The Coordinates of Atoms in **24** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.51057
B3LYP/BS2//B3LYP/BS1 = -704.52447

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.010472
C	1.199678	0.000000	2.609285
H	2.128743	-0.173980	2.071658
H	1.302792	0.180840	3.682657
C	-1.306658	0.136203	2.753699
H	-1.119912	0.259093	3.831698
H	-1.849993	1.024941	2.402410
C	-2.204807	-1.106657	2.530803
H	-1.675751	-1.996775	2.895625
H	-3.126083	-0.998744	3.117887
C	-2.562775	-1.303809	1.043926
H	-3.253636	-2.161083	0.967085
H	-3.105327	-0.422780	0.677256
C	-1.349291	-1.584794	0.155320
H	-0.776291	-2.445019	0.517230
H	-1.647330	-1.750511	-0.887242
P	0.189108	0.209426	-2.477750
H	-0.803185	0.929533	-3.220207
H	1.334927	0.798662	-3.106653
H	0.157811	-0.987127	-3.265390

Table S49. The Coordinates of Atoms in **25** Optimized at the MP2/BS1 Level.

Total Energy (in a.u.) MP2/BS1 = -699.04611
MP4/BS2//MP2/BS1 = -702.63400

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.083002
C	1.400717	0.000000	2.727029
H	-0.638249	0.789321	2.494801
H	-0.494955	-0.984121	2.189909
H	1.334851	-0.204626	3.808675
H	2.012035	-0.794169	2.274127
C	2.088058	1.343937	2.532561
C	2.477203	2.115756	3.563028
H	2.343376	1.799540	4.595021
H	2.946160	3.085068	3.409068
C	2.237958	1.783049	1.084662
H	2.737976	2.766863	1.068407
H	2.879809	1.074160	0.543008
C	0.874578	1.893290	0.377597
H	0.163395	2.502188	0.942923
H	0.969240	2.257221	-0.653183
P	-0.092205	-0.176965	-2.465896
H	0.298671	0.997601	-3.182911
H	0.709269	-1.113184	-3.195424
H	-1.323303	-0.414982	-3.157939

Table S50. The Coordinates of Atoms in **25** Optimized at the B3LYP/BS1 Level.

Total Energy (in a.u.) B3LYP/BS1 = -701.50758
B3LYP/BS2//B3LYP/BS1 = -704.52271

atom	x	y	z
Pd	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.059654
C	1.385017	0.000000	2.730995
H	-0.615274	0.823932	2.438666
H	-0.521432	-0.957922	2.244336
H	1.284542	-0.135212	3.818678
H	1.976368	-0.844106	2.346768
C	2.128042	1.295088	2.466011
C	2.488449	2.131126	3.443132
H	2.278898	1.911640	4.485948

H	3.007285	3.062863	3.236852
C	2.396602	1.593988	1.004872
H	2.978587	2.527030	0.936623
H	3.012191	0.793327	0.570579
C	1.106795	1.753404	0.186184
H	0.444601	2.503602	0.628358
H	1.331881	2.018019	-0.854406
P	-0.148764	-0.201554	-2.480738
H	1.048932	-0.064319	-3.255757
H	-0.642684	-1.377115	-3.139227
H	-0.935318	0.746666	-3.214089