

## Supporting Information

# Bis(CBT)palladium(II) Derivatives (CBT=*m*-carborane-1-thiolate): Synthesis, Molecular Structure and Physicochemical Properties of *cis*-[(bipy)Pd(CBT)<sub>2</sub>] and *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>]

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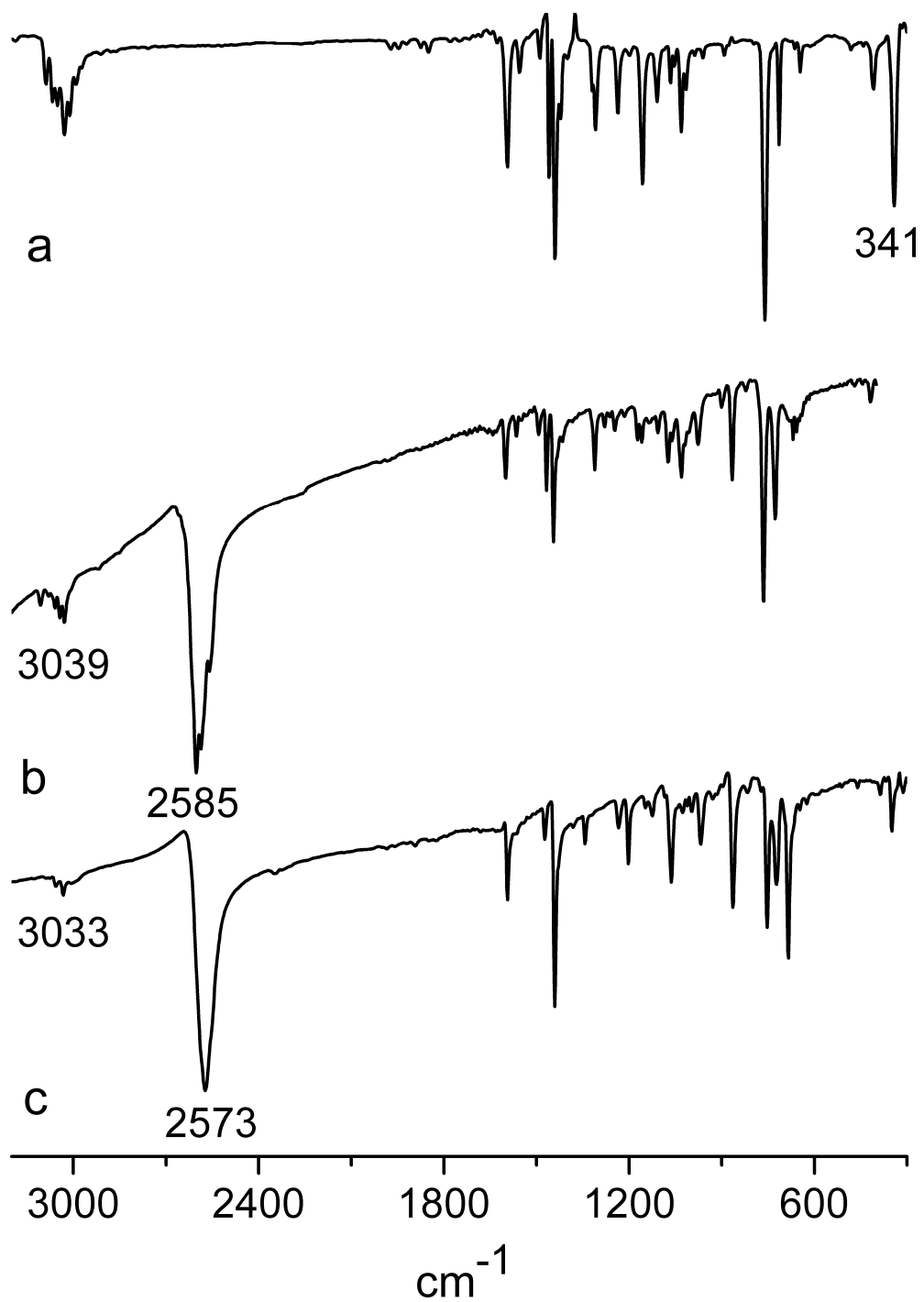
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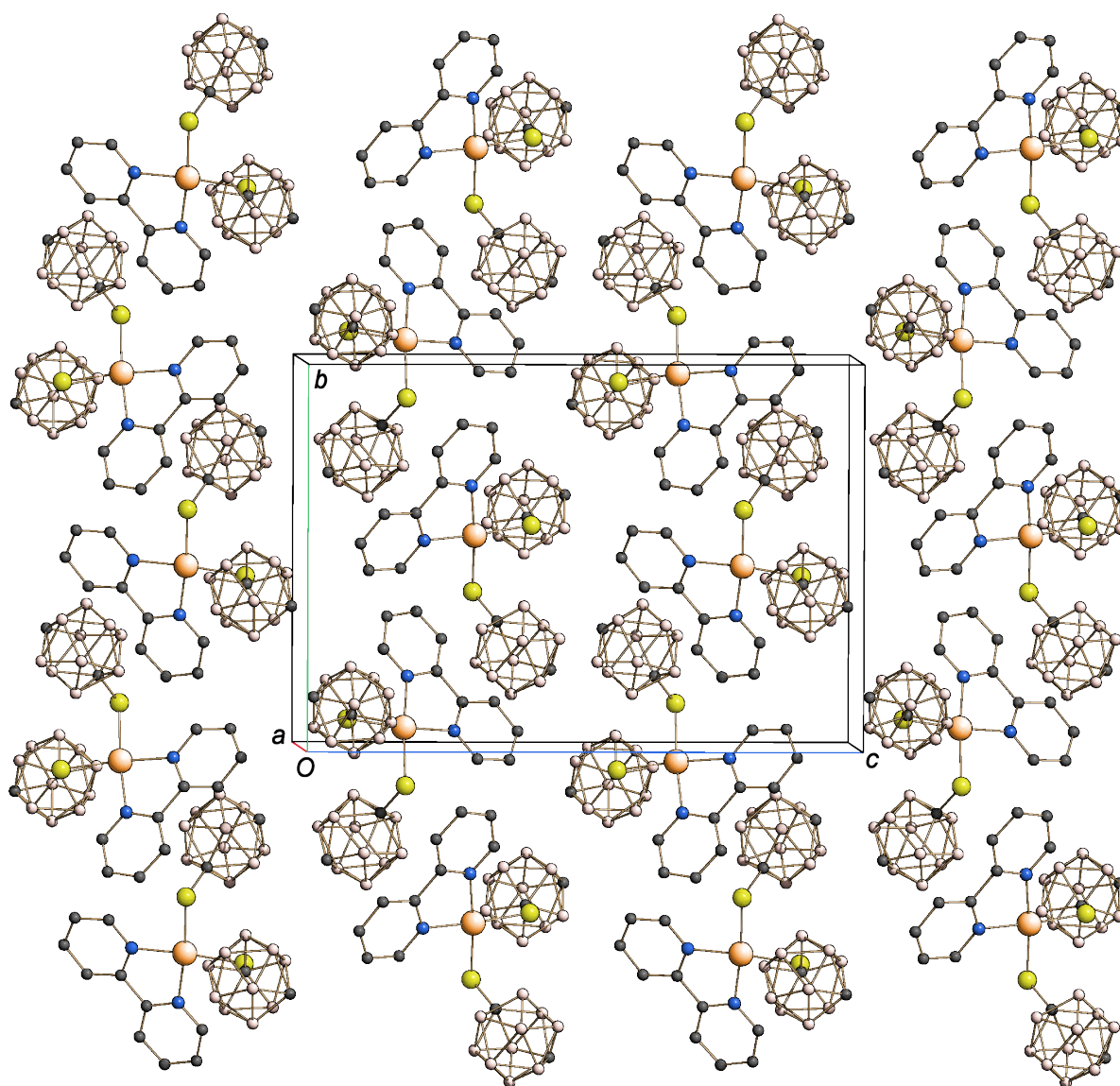
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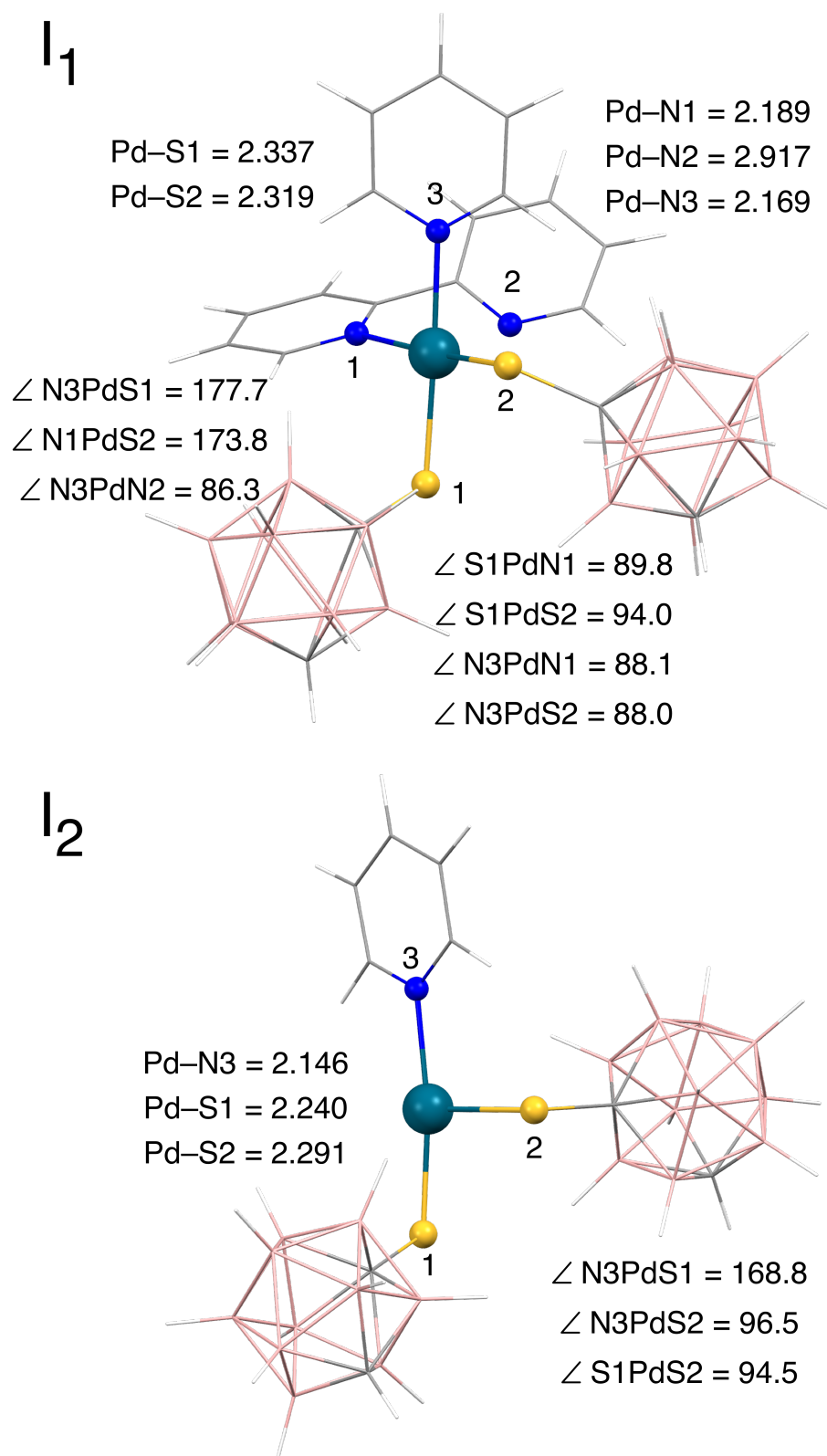
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**Figure S1.** IR spectra of *cis*-[(bipy)PdCl<sub>2</sub>] (a), *cis*-[(bipy)Pd(CBT)<sub>2</sub>] (b) and *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] (c).

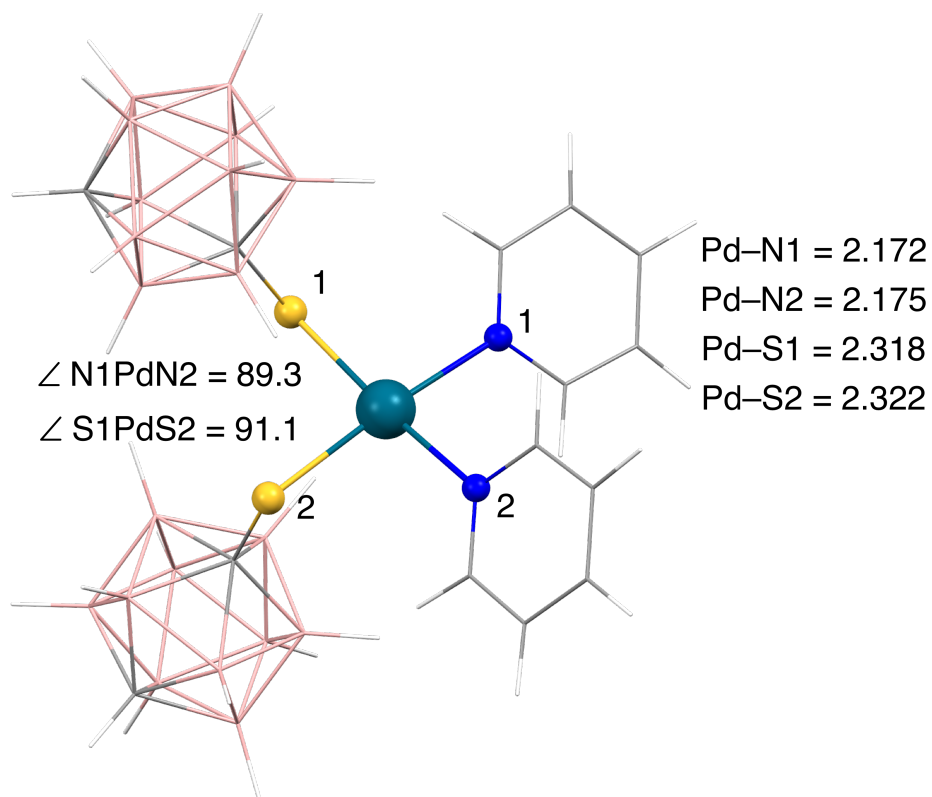


**Figure S2.** Crystal structure of the *cis*-[(bipy)Pd(CBT)<sub>2</sub>] complex approximately viewed along the *a* axis. Hydrogen atoms are omitted for clarity.

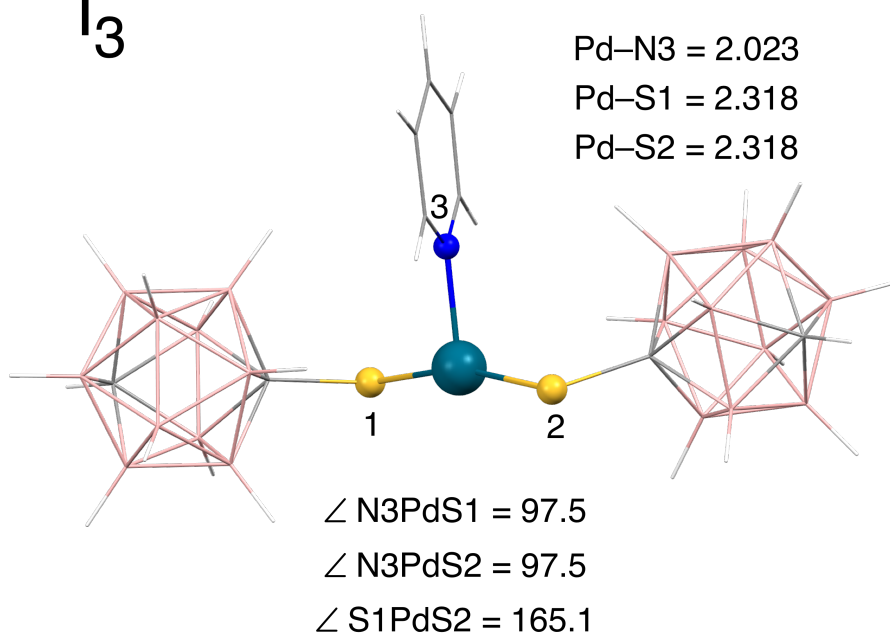


**Figure S3.** DFT/ZORA/CAMY-B3LYP/TZP optimized structures of the **I<sub>1</sub>** and **I<sub>2</sub>** species involved in the *cis*-[(bipy)Pd(CBT)<sub>2</sub>] → *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] conversion reaction with bond lengths in angstroms and angles in degrees.

*cis*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>]



I<sub>3</sub>



**Figure S4.** DFT/ZORA/CAMY-B3LYP/TZP optimized structures of the *cis*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] and I<sub>3</sub> species involved in the *cis*-[(bipy)Pd(CBT)<sub>2</sub>] → *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] conversion reaction with bond lengths in angstroms and angles in degrees.

**Cartesian Coordinates of the *cis*-[(bipy)Pd(CBT)<sub>2</sub>] and *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] complexes optimized in the gas-phase at DFT/ZORA/CAMY-B3LYP/TZ2P level of theory.**

***cis*-[(bipy)Pd(CBT)<sub>2</sub>]**

Pd	0.078542	-0.003828	-0.003126
S	1.728966	1.607723	-0.009858
S	1.664447	-1.673440	0.012818
N	-1.606853	-1.309344	0.032514
N	-1.565860	1.354366	-0.034265
C	-1.461246	2.679409	-0.038861
H	-0.448340	3.060209	-0.044626
C	-2.567796	3.508012	-0.033915
H	-2.435416	4.579212	-0.039455
C	-3.823138	2.933363	-0.023949
H	-4.712655	3.546972	-0.020911
C	-3.931609	1.554926	-0.014698
H	-4.904944	1.092263	-0.000806
C	-2.781323	0.780877	-0.018845
C	-2.804099	-0.699028	0.001729
C	-3.977606	-1.436855	-0.008130
H	-4.935963	-0.944542	-0.035773
C	-3.911774	-2.817990	0.015702
H	-4.819723	-3.403957	0.009012
C	-2.675095	-3.430587	0.047202
H	-2.575571	-4.505134	0.067872
C	-1.543015	-2.636838	0.054314
H	-0.542595	-3.049203	0.076240
C	2.253364	1.845634	-1.717913
C	3.668485	3.396470	-3.298941
H	4.292197	4.271247	-3.375060
C	2.190188	-1.905862	1.721133
C	4.237677	-2.060236	3.365046
H	5.303500	-1.959565	3.483642
B	3.823578	2.471146	-1.896798
H	4.495569	2.785595	-0.987329
B	3.477995	0.825745	-2.393771
H	3.892533	-0.061920	-1.747452
B	1.817028	0.806962	-3.008536
H	1.120828	-0.115387	-2.784494
B	1.148714	2.442847	-2.902772
H	0.024854	2.619047	-2.599085
B	2.386818	3.469134	-2.212579

H	2.200130	4.376210	-1.490222
B	4.423993	1.878522	-3.442261
H	5.588200	1.822145	-3.607937
B	3.180997	0.834143	-4.138452
H	3.458472	-0.096361	-4.808181
B	1.737436	1.833852	-4.452297
H	0.993441	1.608920	-5.340398
B	2.101213	3.488146	-3.950583
H	1.730912	4.489795	-4.447433
B	3.355337	2.497920	-4.712371
H	3.821312	2.850389	-5.734885
B	1.868447	-0.769844	2.967541
H	1.264238	0.207573	2.718415
B	1.080675	-2.355211	2.958948
H	-0.064343	-2.428427	2.690286
B	2.208190	-3.535687	2.289785
H	1.836943	-4.389969	1.570271
B	3.692314	-2.680183	1.894127
H	4.396754	-2.922169	0.987348
B	3.487062	-0.971395	2.317681
H	4.066673	-0.188737	1.666224
B	3.251161	-0.866544	4.057495
H	3.737223	0.034969	4.638010
B	1.752644	-1.719317	4.461732
H	1.066509	-1.364507	5.354031
B	1.967908	-3.435606	4.042656
H	1.434066	-4.306108	4.634282
B	3.592206	-3.633426	3.371528
H	4.309550	-4.559032	3.493582
B	3.312780	-2.511118	4.717426
H	3.851110	-2.699124	5.747853

***trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>]**

Pd	0.000000	0.000000	0.000000
S	-0.020610	2.374207	0.020556
S	0.020610	-2.374207	-0.020556
N	2.057158	0.018582	-0.138454
N	-2.057158	-0.018582	0.138454
C	2.668822	0.744959	-1.077389
C	-2.668822	-0.744959	1.077389
H	2.032700	1.321430	-1.729229
H	-2.032700	-1.321430	1.729229
C	4.042635	0.779272	-1.202656
C	-4.042635	-0.779272	1.202656

H	4.489422	1.375446	-1.983562
H	-4.489422	-1.375446	1.983562
C	4.815253	0.056397	-0.312308
C	-4.815253	-0.056397	0.312308
H	5.893809	0.072672	-0.379154
H	-5.893809	-0.072672	0.379154
C	4.180461	-0.686253	0.666330
C	-4.180461	0.686253	-0.666330
H	4.737943	-1.265076	1.386746
H	-4.737943	1.265076	-1.386746
C	2.801469	-0.688892	0.715343
C	-2.801469	0.688892	-0.715343
H	2.268205	-1.278076	1.443618
H	-2.268205	1.278076	-1.443618
C	0.094970	2.898050	1.736597
C	-0.094970	-2.898050	-1.736597
C	-1.078248	4.137438	3.741900
C	1.078248	-4.137438	-3.741900
H	-1.969407	4.627277	4.097008
H	1.969407	-4.627277	-4.097008
B	-1.292748	2.814451	2.721497
B	1.292748	-2.814451	-2.721497
H	-2.340941	2.462615	2.325482
H	2.340941	-2.462615	-2.325482
B	0.083501	1.774692	3.036880
B	-0.083501	-1.774692	-3.036880
H	-0.003136	0.623967	2.800448
H	0.003136	-0.623967	-2.800448
B	1.548520	2.681944	2.636017
B	-1.548520	-2.681944	-2.636017
H	2.450154	2.128061	2.119865
H	-2.450154	-2.128061	-2.119865
B	1.071262	4.282146	2.061007
B	-1.071262	-4.282146	-2.061007
H	1.635721	4.797667	1.167550
H	-1.635721	-4.797667	-1.167550
B	-0.683545	4.361237	2.115070
B	0.683545	-4.361237	-2.115070
H	-1.366372	4.940270	1.356212
H	1.366372	-4.940270	-1.356212
B	-0.717389	2.603475	4.370762
B	0.717389	-2.603475	-4.370762
H	-1.438165	2.106502	5.158392
H	1.438165	-2.106502	-5.158392



B	1.050027	2.515008	4.324039
B	-1.050027	-2.515008	-4.324039
H	1.650224	1.849909	5.092109
H	-1.650224	-1.849909	-5.092109
B	1.660661	4.074130	3.720977
B	-1.660661	-4.074130	-3.720977
H	2.697972	4.522886	4.059069
H	-2.697972	-4.522886	-4.059069
B	0.268286	5.114248	3.389876
B	-0.268286	-5.114248	-3.389876
H	0.195129	6.280569	3.532038
H	-0.195129	-6.280569	-3.532038
B	0.255108	4.024700	4.790368
B	-0.255108	-4.024700	-4.790368
H	0.175010	4.477432	5.874413
H	-0.175010	-4.477432	-5.874413

**Cartesian Coordinates of the *cis*-[(bipy)Pd(CBT)<sub>2</sub>] and *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] complexes optimized in CHCl<sub>3</sub> at DFT/ZORA/CAMY-B3LYP/COSMO/TZ2P level of theory.**

***cis*-[(bipy)Pd(CBT)<sub>2</sub>]**

Pd	0.094417	0.001550	-0.001226
S	1.761742	1.607229	-0.006515
S	1.691237	-1.672119	0.002252
N	-1.576211	-1.296749	0.025115
N	-1.524328	1.365309	-0.017241
C	-1.417696	2.691679	-0.010722
H	-0.408493	3.076833	-0.019335
C	-2.521458	3.522246	0.010321
H	-2.385806	4.592652	0.015818
C	-3.778804	2.951006	0.024066
H	-4.665979	3.566667	0.039761
C	-3.890631	1.572935	0.020828
H	-4.864840	1.113147	0.036544
C	-2.743847	0.795813	0.001643
C	-2.772597	-0.680061	0.005974
C	-3.948831	-1.411543	-0.009021
H	-4.904063	-0.913735	-0.025680
C	-3.890985	-2.792988	-0.005436
H	-4.801654	-3.373430	-0.017328
C	-2.657025	-3.412846	0.011371
H	-2.563112	-4.487734	0.012867

C	-1.521286	-2.626221	0.026729
H	-0.527845	-3.050444	0.037864
C	2.288307	1.839833	-1.713278
C	3.622507	3.436305	-3.322563
H	4.188426	4.347797	-3.416755
C	2.221256	-1.911464	1.707333
C	4.272644	-2.077832	3.349100
H	5.339406	-1.985205	3.465668
B	3.814783	2.565447	-1.892384
H	4.452490	2.946738	-0.983569
B	3.586647	0.887068	-2.343555
H	4.051288	0.047377	-1.666175
B	1.941901	0.738759	-2.976693
H	1.306361	-0.222986	-2.739896
B	1.165047	2.328420	-2.928388
H	0.027985	2.437004	-2.645372
B	2.322716	3.454892	-2.255831
H	2.063916	4.367625	-1.564304
B	4.476503	1.968885	-3.408917
H	5.644582	1.980230	-3.557669
B	3.317211	0.825297	-4.088451
H	3.666141	-0.104234	-4.727824
B	1.817753	1.714962	-4.449215
H	1.104280	1.413867	-5.341092
B	2.063862	3.402517	-3.994770
H	1.632586	4.359337	-4.529194
B	3.390032	2.477587	-4.709152
H	3.845517	2.825531	-5.738428
B	1.911860	-0.772373	2.951058
H	1.314800	0.210061	2.704346
B	1.110814	-2.350040	2.947532
H	-0.034774	-2.415907	2.682233
B	2.229546	-3.538340	2.280011
H	1.850356	-4.393713	1.565797
B	3.718871	-2.695654	1.881767
H	4.419035	-2.947107	0.973952
B	3.527822	-0.987527	2.301116
H	4.111327	-0.209418	1.647639
B	3.295343	-0.877036	4.038472
H	3.785684	0.022995	4.618352
B	1.792421	-1.716648	4.445856
H	1.110747	-1.354625	5.339988
B	1.993908	-3.432354	4.030978
H	1.454567	-4.297890	4.626793

B	3.614116	-3.643904	3.359107
H	4.321651	-4.576953	3.483144
B	3.346085	-2.518055	4.701097
H	3.880760	-2.708463	5.733465

***trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>]**

Pd	0.000000	0.000000	0.000000
S	-0.014001	2.376597	0.021128
S	0.014001	-2.376597	-0.021128
N	2.051188	0.013886	-0.125319
N	-2.051188	-0.013886	0.125319
C	2.664128	0.650596	-1.127280
C	-2.664128	-0.650596	1.127280
H	2.031423	1.155887	-1.838792
H	-2.031423	-1.155887	1.838792
C	4.038220	0.673460	-1.250463
C	-4.038220	-0.673460	1.250463
H	4.487314	1.193423	-2.082479
H	-4.487314	-1.193423	2.082479
C	4.808180	0.033115	-0.295842
C	-4.808180	-0.033115	0.295842
H	5.886324	0.040932	-0.362398
H	-5.886324	-0.040932	0.362398
C	4.170655	-0.616584	0.746050
C	-4.170655	0.616584	-0.746050
H	4.725970	-1.128398	1.516781
H	-4.725970	1.128398	-1.516781
C	2.791696	-0.612657	0.793349
C	-2.791696	0.612657	-0.793349
H	2.258594	-1.124579	1.577964
H	-2.258594	1.124579	-1.577964
C	0.105124	2.899150	1.737561
C	-0.105124	-2.899150	-1.737561
C	-1.093338	4.050236	3.782457
C	1.093338	-4.050236	-3.782457
H	-2.005266	4.476837	4.165231
H	2.005266	-4.476837	-4.165231
B	-1.246791	2.720149	2.759716
B	1.246791	-2.720149	-2.759716
H	-2.278352	2.298602	2.391512
H	2.278352	-2.298602	-2.391512
B	0.205742	1.773832	3.029355
B	-0.205742	-1.773832	-3.029355
H	0.190197	0.620575	2.791573

H	-0.190197	-0.620575	-2.791573
B	1.593859	2.777724	2.594411
B	-1.593859	-2.777724	-2.594411
H	2.516443	2.288362	2.050692
H	-2.516443	-2.288362	-2.050692
B	0.991647	4.342857	2.043627
B	-0.991647	-4.342857	-2.043627
H	1.496543	4.902235	1.139831
H	-1.496543	-4.902235	-1.139831
B	-0.761063	4.305052	2.148625
B	0.761063	-4.305052	-2.148625
H	-1.499179	4.841352	1.410455
H	1.499179	-4.841352	-1.410455
B	-0.611773	2.541622	4.388197
B	0.611773	-2.541622	-4.388197
H	-1.270965	1.991793	5.194369
H	1.270965	-1.991793	-5.194369
B	1.154209	2.573177	4.292420
B	-1.154209	-2.573177	-4.292420
H	1.819859	1.948210	5.041502
H	-1.819859	-1.948210	-5.041502
B	1.640275	4.169425	3.682491
B	-1.640275	-4.169425	-3.682491
H	2.654923	4.686867	3.994561
H	-2.654923	-4.686867	-3.994561
B	0.173657	5.114088	3.398046
B	-0.173657	-5.114088	-3.398046
H	0.032380	6.273363	3.547867
H	-0.032380	-6.273363	-3.547867
B	0.272993	4.021824	4.789385
B	-0.272993	-4.021824	-4.789385
H	0.198617	4.462549	5.879266
H	-0.198617	-4.462549	-5.879266

**Cartesian Coordinates of the species involved in the *cis*-[(bipy)Pd(CBT)<sub>2</sub>] → *trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>] conversion upon reaction with pyridine optimized in the gas-phase at DFT/ZORA/CAMY-B3LYP/TZP level of theory.**

***cis*-[(bipy)Pd(CBT)<sub>2</sub>]**

Pd	0.000251	0.705880	-0.001735
S	-1.092897	-0.925887	-1.237178
S	1.081648	-0.919036	1.247431
N	0.909612	2.369819	0.976374

N	-0.885677	2.375447	-0.993132
C	-1.764247	2.291857	-1.989740
H	-2.039362	1.284345	-2.276296
C	-2.282988	3.413352	-2.612572
H	-2.994419	3.298478	-3.417293
C	-1.871571	4.660318	-2.180942
H	-2.254800	5.559989	-2.642573
C	-0.956528	4.746427	-1.146035
H	-0.623067	5.712715	-0.801593
C	-0.473785	3.582808	-0.564066
C	0.511032	3.579903	0.542195
C	1.009350	4.740673	1.116057
H	0.686183	5.709107	0.767814
C	1.928131	4.649054	2.147476
H	2.324080	5.546493	2.602682
C	2.327706	3.399765	2.582631
H	3.042895	3.280189	3.383297
C	1.792765	2.280802	1.968504
H	2.058721	1.271788	2.258550
C	-2.526891	-1.444438	-0.266675
C	-4.779956	-2.790763	-0.379352
H	-5.450075	-3.371972	-0.991602
C	2.520340	-1.443145	0.287257
C	3.837567	-3.489759	-0.707090
H	3.851440	-4.554422	-0.874944
B	-3.128405	-2.982925	-0.664592
H	-2.696169	-3.633859	-1.541914
B	-2.361319	-2.721491	0.890493
H	-1.295437	-3.176546	1.081863
B	-2.750573	-1.067286	1.389713
H	-1.939848	-0.415119	1.941217
B	-3.766888	-0.318316	0.147434
H	-3.631535	0.815285	-0.144636
B	-3.997767	-1.500319	-1.121747
H	-4.081763	-1.265207	-2.270420
B	-3.872377	-3.620054	0.797510
H	-3.989354	-4.787724	0.905152
B	-3.635510	-2.434727	2.083676
H	-3.500837	-2.762513	3.209854
B	-4.502519	-0.946162	1.624639
H	-4.978503	-0.218967	2.424430
B	-5.272651	-1.224932	0.060973
H	-6.308350	-0.808116	-0.317514
B	-5.192210	-2.530395	1.253102

H	-6.194768	-2.984875	1.674577
B	2.709820	-1.101253	-1.384076
H	1.883260	-0.482101	-1.947841
B	3.756251	-0.338109	-0.176427
H	3.613430	0.805948	0.070562
B	4.021534	-1.485757	1.136979
H	4.047969	-1.129594	2.259437
B	3.146521	-2.957159	0.735797
H	2.617454	-3.667357	1.507294
B	2.338765	-2.724173	-0.825342
H	1.327058	-3.293190	-0.991857
B	3.579846	-2.482651	-2.047438
H	3.417225	-2.953785	-3.115126
B	4.459283	-0.997981	-1.653604
H	4.902500	-0.304950	-2.501235
B	5.273981	-1.241043	-0.091417
H	6.298799	-0.720021	0.179547
B	4.885801	-2.868448	0.479088
H	5.582510	-3.600565	1.085076
B	5.159436	-2.569076	-1.247992
H	6.053550	-3.108778	-1.794301

### TS<sub>1</sub>

Pd	0.264975	0.409479	-0.231291
S	-1.610076	-0.166978	-1.453214
S	0.027824	-1.473011	1.073580
N	2.803757	0.708052	-0.636777
N	0.631318	2.218165	-1.422527
C	-0.384673	2.847945	-2.017914
H	-1.350453	2.380863	-1.900451
C	-0.226526	3.999544	-2.767021
H	-1.089955	4.464294	-3.220432
C	1.046215	4.512197	-2.928565
H	1.218542	5.398716	-3.523722
C	2.104886	3.856995	-2.328538
H	3.113247	4.212759	-2.472271
C	1.874622	2.715451	-1.567685
C	3.005072	1.993830	-0.928451
C	4.213923	2.628787	-0.655904
H	4.345282	3.681669	-0.855246
C	5.245874	1.894794	-0.097693
H	6.192513	2.368091	0.125513
C	5.043112	0.553286	0.172193
H	5.822292	-0.061694	0.599616

C	3.799628	0.007027	-0.107625
H	3.590061	-1.032863	0.101868
C	-3.078162	0.192332	-0.448347
C	-5.684215	0.514727	-0.619713
H	-6.546088	0.533661	-1.266664
C	0.618878	-2.966905	0.240251
C	0.079722	-5.151527	-1.124406
H	-0.660265	-5.704557	-1.679711
B	-4.477107	-0.603991	-0.993002
H	-4.498049	-1.275823	-1.956656
B	-3.765455	-1.044195	0.547952
H	-3.205343	-2.072338	0.641561
B	-3.089793	0.434155	1.250186
H	-2.077375	0.399713	1.845824
B	-3.400107	1.781082	0.145863
H	-2.598867	2.631283	-0.011280
B	-4.252719	1.141211	-1.240053
H	-4.135164	1.511732	-2.349733
B	-5.508515	-0.825343	0.414908
H	-6.313275	-1.685867	0.391462
B	-4.649184	-0.186597	1.817644
H	-4.783453	-0.656542	2.892291
B	-4.419656	1.562814	1.568620
H	-4.385474	2.331272	2.465330
B	-5.143192	1.992839	0.017778
H	-5.697928	2.993534	-0.267037
B	-5.913894	0.778159	1.047788
H	-7.001452	0.978916	1.455775
B	1.708169	-2.960500	-1.082791
H	2.043500	-1.931950	-1.545777
B	2.243955	-3.475131	0.518726
H	2.945519	-2.777300	1.160135
B	0.891842	-4.275910	1.325632
H	0.688667	-4.113000	2.473944
B	-0.467250	-4.284114	0.212282
H	-1.597519	-4.193001	0.515363
B	0.034425	-3.469919	-1.276205
H	-0.790695	-2.902217	-1.882253
B	1.330236	-4.412220	-2.004072
H	1.360753	-4.512727	-3.177853
B	2.706996	-4.419545	-0.894875
H	3.818829	-4.450847	-1.293979
B	2.199795	-5.234278	0.603241
H	2.948433	-5.847440	1.280381

B	0.513267	-5.731374	0.409445
H	0.002909	-6.703473	0.837242
B	1.632975	-5.818008	-0.963970
H	1.865223	-6.863289	-1.456884
N	1.039192	1.556517	1.739636
C	0.605878	2.800414	1.951987
C	0.865219	3.499219	3.118232
C	1.609801	2.882506	4.110698
C	2.057377	1.589748	3.897581
C	1.745066	0.963027	2.702239
H	0.019945	3.246852	1.159258
H	0.480876	4.501793	3.242439
H	1.828815	3.397490	5.036511
H	2.631766	1.062365	4.646130
H	2.042183	-0.059148	2.507155

**Imaginary Frequency:  $i67.9 \text{ cm}^{-1}$**

**I<sub>1</sub>**

Pd	-0.227634	-0.564006	0.361486
S	1.456649	-0.007949	-1.159794
S	-0.128000	1.471787	1.467072
N	-2.239527	-0.933652	-1.717912
N	-0.298778	-2.587965	-0.470631
C	0.751916	-3.367055	-0.197456
H	1.533903	-2.917047	0.393974
C	0.861578	-4.672451	-0.637006
H	1.739182	-5.249629	-0.384814
C	-0.157886	-5.192741	-1.413046
H	-0.103902	-6.202234	-1.797599
C	-1.244936	-4.390704	-1.703320
H	-2.043101	-4.755065	-2.332595
C	-1.299569	-3.089283	-1.212744
C	-2.473308	-2.229854	-1.522879
C	-3.748796	-2.781602	-1.615894
H	-3.911097	-3.831641	-1.419262
C	-4.810725	-1.954015	-1.939042
H	-5.813190	-2.354009	-2.011621
C	-4.565443	-0.610374	-2.160453
H	-5.361077	0.073606	-2.420137
C	-3.262852	-0.148398	-2.033522
H	-3.030167	0.897251	-2.189516
C	3.097535	-0.131431	-0.403320
C	5.638563	0.454577	-0.779979
H	6.365116	0.929987	-1.418623



C	-0.628265	2.851286	0.409474
C	0.052715	5.177906	-0.619623
H	0.844786	5.890869	-0.781294
B	4.133813	1.201682	-0.653362
H	3.830427	2.142155	-1.287376
B	3.570132	0.823822	0.958690
H	2.778666	1.522261	1.469680
B	3.438565	-0.941259	1.062440
H	2.545090	-1.417684	1.669816
B	3.938007	-1.647257	-0.477169
H	3.389412	-2.580390	-0.939709
B	4.349812	-0.321471	-1.540973
H	4.172995	-0.294992	-2.702132
B	5.266849	1.213122	0.692629
H	5.792326	2.228926	0.977072
B	4.831381	-0.114263	1.773121
H	4.987625	-0.037191	2.941068
B	5.060544	-1.640398	0.883468
H	5.373958	-2.645494	1.420547
B	5.623769	-1.243694	-0.741620
H	6.380190	-1.852375	-1.410135
B	6.183279	-0.299500	0.648169
H	7.332864	-0.283791	0.908479
B	-0.959990	2.729189	-1.267674
H	-0.859378	1.691397	-1.808023
B	-2.259313	3.038712	-0.108564
H	-3.036971	2.184319	0.130604
B	-1.619226	4.026075	1.202616
H	-1.939701	3.835017	2.319273
B	0.071863	4.341030	0.843846
H	0.930165	4.438856	1.639346
B	0.481628	3.545490	-0.684123
H	1.585211	3.174994	-0.811419
B	-0.484667	4.281117	-1.954779
H	0.005783	4.447718	-3.013089
B	-2.190162	3.964567	-1.604589
H	-2.977394	3.812690	-2.473968
B	-2.597392	4.771798	-0.073994
H	-3.676093	5.195364	0.155105
B	-1.141538	5.575391	0.521365
H	-1.076042	6.596369	1.106186
B	-1.494426	5.540197	-1.217533
H	-1.668860	6.552636	-1.795421
N	-1.769361	-1.163579	1.763859

C	-1.662728	-2.319906	2.426846
C	-2.601903	-2.742416	3.348426
C	-3.707491	-1.942513	3.589004
C	-3.821354	-0.746381	2.903263
C	-2.828301	-0.386015	2.009149
H	-0.790332	-2.919540	2.211573
H	-2.459014	-3.679824	3.866571
H	-4.461935	-2.244491	4.302902
H	-4.660358	-0.083764	3.059879
H	-2.858564	0.554997	1.482461

## TS<sub>2</sub>

Pd	-0.082001	0.601409	0.403472
S	-1.327745	-0.643038	-1.125669
S	0.606322	-1.301942	1.535562
N	-0.689434	2.424669	-0.608095
C	-1.927129	2.891152	-0.402659
H	-2.541861	2.323184	0.279247
C	-2.416939	4.020735	-1.027125
H	-3.426645	4.347417	-0.825062
C	-1.597187	4.694655	-1.915543
H	-1.947574	5.577649	-2.432722
C	-0.321049	4.211440	-2.137375
H	0.349020	4.696408	-2.832432
C	0.107945	3.072617	-1.469384
C	-2.933801	-1.028002	-0.385013
C	-5.095074	-2.498284	-0.696087
H	-5.587993	-3.257717	-1.280921
C	1.742376	-2.274144	0.517434
C	2.283550	-4.657706	-0.458343
H	1.937461	-5.667926	-0.605187
B	-3.429641	-2.656907	-0.492048
H	-2.792559	-3.488823	-1.022155
B	-3.092707	-1.948564	1.071617
H	-2.126818	-2.273344	1.652303
B	-3.586840	-0.248455	0.988879
H	-2.936093	0.565881	1.544447
B	-4.242095	0.085454	-0.616255
H	-4.030341	1.101473	-1.171557
B	-4.130569	-1.399822	-1.535149
H	-3.912541	-1.476617	-2.686944
B	-4.537457	-2.930576	0.848120
H	-4.687163	-4.032543	1.237919
B	-4.629809	-1.435034	1.783196

H	-4.791065	-1.446070	2.952961
B	-5.341933	-0.179873	0.738423
H	-6.004243	0.699993	1.167351
B	-5.672799	-0.905688	-0.836157
H	-6.569001	-0.669042	-1.564283
B	-5.919647	-1.844900	0.645100
H	-7.000847	-2.235187	0.905909
B	1.998878	-2.036939	-1.162238
H	1.424039	-1.186142	-1.730484
B	3.268016	-1.656505	0.010746
H	3.526867	-0.526729	0.229373
B	3.166634	-2.807243	1.341640
H	3.336887	-2.465087	2.455618
B	1.842371	-3.906539	0.984367
H	1.126112	-4.390919	1.779135
B	1.121323	-3.436699	-0.565645
H	-0.023915	-3.644413	-0.703504
B	2.342760	-3.639027	-1.812819
H	2.010471	-4.042369	-2.868908
B	3.676698	-2.530435	-1.462950
H	4.306817	-2.035558	-2.332329
B	4.400664	-3.011530	0.087738
H	5.546562	-2.857672	0.330818
B	3.505554	-4.407084	0.696801
H	3.931450	-5.321703	1.305768
B	3.822973	-4.238676	-1.040815
H	4.473257	-5.051916	-1.593386
N	0.991309	1.804568	1.868579
C	0.411067	2.893264	2.385285
C	1.020246	3.684888	3.340403
C	2.291109	3.345301	3.776271
C	2.894627	2.220288	3.243370
C	2.211074	1.470641	2.301659
H	-0.576980	3.132252	2.020228
H	0.499484	4.546488	3.732812
H	2.796949	3.943952	4.521829
H	3.881178	1.908308	3.554875
H	2.629731	0.566552	1.888064
C	1.483027	2.544373	-1.725376
C	2.571886	3.011460	-0.999964
C	3.829823	2.519785	-1.308503
C	3.949572	1.586210	-2.322802
C	2.802314	1.189217	-2.993155
N	1.590696	1.659095	-2.712659

H	2.433202	3.738305	-0.211605
H	4.700149	2.857936	-0.762298
H	4.907966	1.164587	-2.590362
H	2.856904	0.457210	-3.789618

**Imaginary Frequency:  $i38.9 \text{ cm}^{-1}$**

**I<sub>2</sub>**

Pd	-0.147633	-0.540614	0.338617
S	1.542457	0.065567	-1.157400
S	-0.095358	1.498051	1.442774
C	-2.320647	-0.868037	-1.965980
N	-0.278337	-2.533644	-0.552833
C	0.759843	-3.346443	-0.319579
H	1.620705	-2.893975	0.145649
C	0.751550	-4.689173	-0.639320
H	1.621514	-5.293439	-0.426744
C	-0.383199	-5.222749	-1.227782
H	-0.430433	-6.270892	-1.490837
C	-1.452949	-4.388818	-1.482657
H	-2.360887	-4.750024	-1.940566
C	-1.372333	-3.041300	-1.146214
C	-2.517746	-2.151362	-1.469826
N	-3.730266	-2.685306	-1.304501
C	-4.785175	-1.933147	-1.597578
H	-5.755281	-2.392234	-1.446116
C	-4.688920	-0.632956	-2.072615
H	-5.582895	-0.065899	-2.291528
C	-3.428711	-0.094428	-2.267418
H	-3.303733	0.910746	-2.645971
C	3.170435	-0.101395	-0.383146
C	5.712859	0.514847	-0.674883
H	6.449663	1.030061	-1.269416
C	-0.614623	2.864510	0.375526
C	0.015802	5.223314	-0.612007
H	0.787614	5.963850	-0.745335
B	4.203622	1.248833	-0.532379
H	3.906421	2.224379	-1.114107
B	3.610368	0.771511	1.042918
H	2.805253	1.435272	1.578271
B	3.485160	-0.997566	1.037846
H	2.581150	-1.511655	1.596799
B	4.015926	-1.608106	-0.532356
H	3.477547	-2.511977	-1.060392

B	4.443072	-0.218453	-1.506665
H	4.286333	-0.122087	-2.666999
B	5.309842	1.182132	0.833574
H	5.824876	2.180578	1.189093
B	4.859776	-0.210068	1.823461
H	4.992528	-0.202798	2.996627
B	5.112731	-1.679232	0.847871
H	5.419723	-2.713758	1.329065
B	5.704799	-1.183386	-0.739553
H	6.476313	-1.747866	-1.428837
B	6.233524	-0.322408	0.715376
H	7.377674	-0.318685	0.998160
B	-0.899921	2.753028	-1.310488
H	-0.750915	1.730802	-1.868309
B	-2.238598	3.002757	-0.183362
H	-2.990588	2.118262	0.024170
B	-1.664846	3.997339	1.153678
H	-2.006601	3.783122	2.259584
B	0.024334	4.371885	0.842849
H	0.857963	4.487992	1.661673
B	0.499952	3.607017	-0.682030
H	1.617645	3.271877	-0.784258
B	-0.457625	4.325433	-1.969849
H	0.054244	4.517924	-3.013442
B	-2.160573	3.948268	-1.667589
H	-2.918508	3.779885	-2.559474
B	-2.633576	4.724310	-0.140329
H	-3.730979	5.109784	0.064664
B	-1.220713	5.568720	0.501216
H	-1.203646	6.584429	1.098158
B	-1.527263	5.541628	-1.246264
H	-1.719743	6.553933	-1.818247
N	-1.690680	-1.170599	1.718172
C	-1.573564	-2.338075	2.360228
C	-2.516811	-2.791349	3.262000
C	-3.637206	-2.013365	3.503469
C	-3.761820	-0.806308	2.839218
C	-2.764969	-0.414098	1.963976
H	-0.691232	-2.922235	2.142611
H	-2.367686	-3.737992	3.760890
H	-4.396755	-2.341861	4.199903
H	-4.614253	-0.161203	2.995814
H	-2.805852	0.534666	1.452377
H	-1.322109	-0.492090	-2.128314

**I<sub>3</sub>**

Pd	-0.088508	0.905684	-0.583988
S	-1.411073	-0.743244	-1.324802
S	0.767925	-0.318599	1.152488
C	-2.971887	-0.631343	-0.418510
C	-4.795461	-1.954265	0.923788
H	-5.091064	-2.897716	1.353234
C	2.233550	-1.164499	0.521299
C	3.266330	-3.270488	-0.655166
H	3.077017	-4.187412	-1.189345
B	-3.154286	-1.571592	0.988872
H	-2.325360	-2.300756	1.386924
B	-3.107598	0.183840	1.086280
H	-2.160595	0.705632	1.550773
B	-3.882269	0.826894	-0.372020
H	-3.428815	1.783761	-0.890612
B	-4.397707	-0.533938	-1.377454
H	-4.292683	-0.496851	-2.549197
B	-3.952480	-2.013182	-0.533453
H	-3.597834	-3.008423	-1.046695
B	-4.323196	-0.717129	1.986748
H	-4.317990	-0.910946	3.148601
B	-4.776200	0.775840	1.149194
H	-5.049125	1.755858	1.748165
B	-5.577853	0.329110	-0.375346
H	-6.423806	0.989693	-0.866589
B	-5.611757	-1.437173	-0.477202
H	-6.457160	-2.111994	-0.943645
B	-5.847114	-0.628587	1.083799
H	-6.865688	-0.768449	1.659295
B	3.209056	-0.539621	-0.745762
H	2.884677	0.455831	-1.284064
B	3.789014	-0.532637	0.921686
H	3.842907	0.486211	1.511075
B	3.138778	-1.966191	1.738809
H	2.764520	-1.909716	2.854022
B	2.183508	-2.869268	0.568271
H	1.205815	-3.472878	0.807769
B	2.219722	-1.983113	-0.965306
H	1.273949	-2.066906	-1.654286
B	3.881785	-1.957329	-1.542270
H	4.074410	-2.071111	-2.698872
B	4.863118	-1.061025	-0.374812

H	5.792689	-0.419705	-0.718871
B	4.819795	-1.941799	1.171084
H	5.718561	-1.933108	1.936112
B	3.819051	-3.386886	0.947003
H	3.973013	-4.445011	1.440783
B	4.879527	-2.825844	-0.359151
H	5.747851	-3.526195	-0.738105
N	1.088311	2.667087	-0.240893
C	1.119208	3.573918	-1.225386
C	1.805425	4.767183	-1.117787
C	2.487406	5.038397	0.058018
C	2.456202	4.102486	1.076777
C	1.749275	2.927956	0.890473
H	0.574958	3.327305	-2.128010
H	1.801413	5.464079	-1.943320
H	3.034969	5.963681	0.175300
H	2.975122	4.268243	2.009814
H	1.707285	2.156430	1.646846

### TS<sub>3</sub>

Pd	-0.124416	-0.072033	-0.128005
S	-1.819810	-0.899408	-1.406450
S	1.435388	-0.724509	1.445924
C	-3.389132	-0.673769	-0.539884
C	-5.697891	-1.742136	0.083656
H	-6.329213	-2.614524	0.036132
C	3.031560	-0.815131	0.607708
C	4.963279	-2.397174	-0.208657
H	5.311936	-3.411746	-0.313915
B	-4.042417	-2.010428	0.274808
H	-3.548525	-3.075851	0.265821
B	-3.464168	-0.620203	1.178948
H	-2.464478	-0.724750	1.792519
B	-3.787368	0.821210	0.203022
H	-2.992216	1.690442	0.175945
B	-4.570444	0.317990	-1.306404
H	-4.300713	0.834857	-2.328919
B	-4.733409	-1.428863	-1.258462
H	-4.643891	-2.146826	-2.183490
B	-5.010390	-1.350333	1.589637
H	-5.224299	-2.032663	2.525684
B	-4.852429	0.409974	1.553736
H	-4.883275	1.051130	2.544613

B	-5.536079	0.992961	0.014811
H	-6.054142	2.048673	-0.088389
B	-6.118768	-0.410974	-0.888818
H	-7.063903	-0.472930	-1.589000
B	-6.291193	-0.356577	0.873288
H	-7.369868	-0.379799	1.346533
B	3.202609	-0.503881	-1.070373
H	2.252663	-0.209118	-1.701943
B	3.891531	0.598968	0.136381
H	3.394613	1.651404	0.316201
B	4.416536	-0.356260	1.526110
H	4.261710	0.037488	2.624381
B	4.059979	-2.043472	1.172924
H	3.725134	-2.849177	1.958906
B	3.315970	-2.135849	-0.434954
H	2.531799	-2.991998	-0.609097
B	4.490483	-1.575486	-1.616115
H	4.538543	-2.117924	-2.660535
B	4.846258	0.124761	-1.270880
H	5.103829	0.884524	-2.137408
B	5.603243	0.210686	0.337620
H	6.401335	1.032953	0.620689
B	5.699259	-1.432735	0.984926
H	6.549969	-1.887755	1.660534
B	5.969214	-1.135782	-0.744252
H	7.015722	-1.394887	-1.219112
N	0.528716	1.859795	0.003697
C	0.800951	2.517867	-1.130827
C	1.164807	3.848835	-1.133759
C	1.241095	4.527393	0.071662
C	0.952516	3.844692	1.239871
C	0.606514	2.508592	1.171793
H	0.721199	1.952752	-2.047001
H	1.381522	4.336638	-2.072738
H	1.521754	5.571312	0.098525
H	0.999536	4.329342	2.204063
H	0.399877	1.930845	2.058218

**Imaginary Frequency:  $i61.4 \text{ cm}^{-1}$**

**$I_4$**

Pd	0.000000	0.000000	0.675138
S	-0.913041	2.109618	0.976511
S	0.913041	-2.109618	0.976511



C	0.405450	3.304228	0.672946
C	1.007150	5.853389	0.538547
H	0.650956	6.867596	0.618299
C	-0.405450	-3.304228	0.672946
C	-1.007150	-5.853389	0.538547
H	-0.650956	-6.867596	0.618299
B	0.335759	4.725091	1.598533
H	-0.545075	4.969278	2.336063
B	1.613693	3.555879	1.882745
H	1.576182	2.902966	2.860706
B	2.014274	2.830366	0.322061
H	2.267653	1.678786	0.273268
B	0.987947	3.557191	-0.928166
H	0.545205	2.910488	-1.807180
B	-0.046234	4.730660	-0.138938
H	-1.155847	4.972784	-0.437818
B	2.000307	5.269242	1.791421
H	2.260206	5.967593	2.703514
B	3.052171	4.090513	1.001794
H	4.135247	3.856964	1.408206
B	2.665117	4.086011	-0.738407
H	3.474067	3.850887	-1.565892
B	1.382495	5.270267	-1.013269
H	1.235824	5.965432	-1.953101
B	2.651698	5.599474	0.176820
H	3.358400	6.528753	0.018801
B	-0.335759	-4.725091	1.598533
H	0.545075	-4.969278	2.336063
B	-1.613693	-3.555879	1.882745
H	-1.576182	-2.902966	2.860706
B	-2.014274	-2.830366	0.322061
H	-2.267653	-1.678786	0.273268
B	-0.987947	-3.557191	-0.928166
H	-0.545205	-2.910488	-1.807180
B	0.046234	-4.730660	-0.138938
H	1.155847	-4.972784	-0.437818
B	-2.000307	-5.269242	1.791421
H	-2.260206	-5.967593	2.703514
B	-3.052171	-4.090513	1.001794
H	-4.135247	-3.856964	1.408206
B	-2.665117	-4.086011	-0.738407
H	-3.474067	-3.850887	-1.565892
B	-1.382495	-5.270267	-1.013269
H	-1.235824	-5.965432	-1.953101

B	-2.651698	-5.599474	0.176820
H	-3.358400	-6.528753	0.018801
N	0.000000	0.000000	-1.347735
C	-1.133455	0.233539	-2.021833
C	-1.167938	0.236023	-3.401850
C	0.000000	0.000000	-4.106304
C	1.133455	-0.233539	-2.021833
C	1.167938	-0.236023	-3.401850
H	-2.015678	0.426533	-1.433449
H	-2.104065	0.427260	-3.905345
H	0.000000	0.000000	-5.187585
H	2.015678	-0.426533	-1.433449
H	2.104065	-0.427260	-3.905345

***trans*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>]**

Pd	0.000000	0.000000	0.000000
S	1.637704	1.736611	0.019826
S	-1.637704	-1.736611	-0.019826
N	1.503036	-1.425122	0.022175
N	-1.503036	1.425122	-0.022175
C	2.502007	-1.349377	0.908716
C	-2.502007	1.349377	-0.908716
H	2.481844	-0.509227	1.584133
H	-2.481844	0.509227	-1.584133
C	3.524286	-2.277926	0.947439
C	-3.524286	2.277926	-0.947439
H	4.305000	-2.175607	1.686893
H	-4.305000	2.175607	-1.686893
C	3.530456	-3.309977	0.025200
C	-3.530456	3.309977	-0.025200
H	4.324457	-4.044283	0.023940
H	-4.324457	4.044283	-0.023940
C	2.500891	-3.381790	-0.897214
C	-2.500891	3.381790	0.897214
H	2.459799	-4.165464	-1.639422
H	-2.459799	4.165464	1.639422
C	1.500849	-2.429825	-0.861020
C	-1.500849	2.429825	0.861020
H	0.668228	-2.468501	-1.545154
H	-0.668228	2.468501	1.545154
C	2.162524	1.973486	-1.689317
C	-2.162524	-1.973486	1.689317
C	2.197162	3.577913	-3.775657

C	-2.197162	-3.577913	3.775657
H	1.863082	4.511880	-4.197577
H	-1.863082	-4.511880	4.197577
B	1.113798	2.764816	-2.773129
B	-1.113798	-2.764816	2.773129
H	0.068810	3.199178	-2.455968
H	-0.068810	-3.199178	2.455968
B	1.494200	1.065803	-2.985102
B	-1.494200	-1.065803	2.985102
H	0.661303	0.263750	-2.756374
H	-0.661303	-0.263750	2.756374
B	3.170993	0.819473	-2.476890
B	-3.170993	-0.819473	2.476890
H	3.464654	-0.162212	-1.895794
H	-3.464654	0.162212	1.895794
B	3.820964	2.371912	-1.939372
B	-3.820964	-2.371912	1.939372
H	4.534212	2.440304	-1.005714
H	-4.534212	-2.440304	1.005714
B	2.550056	3.571419	-2.124944
B	-2.550056	-3.571419	2.124944
H	2.368865	4.491946	-1.418199
H	-2.368865	-4.491946	1.418199
B	1.504418	2.149181	-4.373553
B	-1.504418	-2.149181	4.373553
H	0.679349	2.202509	-5.213506
H	-0.679349	-2.202509	5.213506
B	2.779931	0.935796	-4.196056
B	-2.779931	-0.935796	4.196056
H	2.842947	0.003709	-4.918657
H	-2.842947	-0.003709	4.918657
B	4.223847	1.749376	-3.549623
B	-4.223847	-1.749376	3.549623
H	5.320850	1.398664	-3.809782
H	-5.320850	-1.398664	3.809782
B	3.832112	3.458629	-3.324205
B	-3.832112	-3.458629	3.324205
H	4.547204	4.383359	-3.471900
H	-4.547204	-4.383359	3.471900
B	3.190331	2.572944	-4.720569
B	-3.190331	-2.572944	4.720569
H	3.486283	2.914966	-5.808818
H	-3.486283	-2.914966	5.808818

*cis*-[(py)<sub>2</sub>Pd(CBT)<sub>2</sub>]

Pd	-0.012421	0.887900	-0.001299
S	1.092089	-0.731913	1.242184
S	-1.084898	-0.742283	-1.252814
N	0.751102	2.445989	1.310386
C	1.977069	2.431995	1.842960
H	2.611936	1.611666	1.546890
C	2.406137	3.393065	2.741706
H	3.411034	3.340594	3.135419
C	1.531061	4.393115	3.126629
H	1.835367	5.151207	3.835596
C	0.253311	4.399660	2.590195
H	-0.472098	5.151122	2.866867
C	-0.093309	3.415516	1.684688
C	2.424975	-1.393087	0.209358
C	4.598440	-2.871729	0.305928
H	5.261390	-3.454781	0.924212
C	-2.402303	-1.435284	-0.221168
C	-3.487412	-3.640446	0.718178
H	-3.399783	-4.709441	0.825408
B	2.954213	-2.938833	0.679368
H	2.528437	-3.503994	1.617196
B	2.126950	-2.728515	-0.852112
H	1.029328	-3.129809	-0.965470
B	2.589527	-1.137427	-1.478002
H	1.800516	-0.468625	-2.038750
B	3.712465	-0.381379	-0.338426
H	3.668543	0.777401	-0.126959
B	3.934444	-1.489798	0.996099
H	4.090816	-1.186805	2.120934
B	3.583666	-3.714211	-0.769612
H	3.623200	-4.891445	-0.803920
B	3.353790	-2.600577	-2.119663
H	3.143119	-2.989834	-3.214036
B	4.333318	-1.145914	-1.801429
H	4.810983	-0.501402	-2.668430
B	5.163160	-1.373508	-0.260447
H	6.239587	-0.999383	0.041381
B	4.942796	-2.743465	-1.358197
H	5.892842	-3.287694	-1.794780
B	-2.535040	-1.199454	1.475152
H	-1.745234	-0.536205	2.039030
B	-3.706415	-0.474541	0.365901
H	-3.682221	0.691391	0.187547
B	-3.941006	-1.567600	-0.997653

H	-4.057377	-1.155465	-2.094816
B	-2.921867	-2.973629	-0.723238
H	-2.375715	-3.592811	-1.558548
B	-2.055005	-2.752053	0.807503
H	-0.993767	-3.241907	0.894249
B	-3.245615	-2.686526	2.099540
H	-2.987778	-3.196740	3.129815
B	-4.271515	-1.268976	1.833615
H	-4.726504	-0.661843	2.739011
B	-5.143783	-1.501167	0.301571
H	-6.221985	-1.058690	0.109576
B	-4.646839	-3.054234	-0.378929
H	-5.308050	-3.812838	-0.992089
B	-4.853306	-2.872020	1.373740
H	-5.666758	-3.517465	1.931426
N	-0.819185	2.422283	-1.310186
C	0.005598	3.398564	-1.709789
C	-0.369478	4.366731	-2.620958
C	-1.656038	4.336182	-3.135344
C	-2.511073	3.329746	-2.723366
C	-2.054188	2.384927	-1.820940
H	0.998639	3.391216	-1.283688
H	0.340892	5.124162	-2.919500
H	-1.982352	5.080993	-3.848597
H	-3.521597	3.258675	-3.099251
H	-2.673485	1.560013	-1.504965
H	-1.078666	3.389919	1.242018