

Supporting Information

Catalyst-Controlled C–C σ Bond Cleavages in Metal Halide-Catalyzed Cycloisomerization of 3-Acylcyclopropenes via a Formal 1,1-Halometalation Mechanism: Insights from Quantum Chemical Calculations

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1. Complete Reference of Gaussian 09-----	S2
2. Results for Pd-Catalyzed Reactions-----	S3
3. Results for Cu-Catalyzed Reactions-----	S8
4. Energies for Key Transition States Calculated at the B3LYP Level-----	S10
5. Calculated Energy Values-----	S11
6. Cartesian Coordinates for All Species-----	S13

1. Complete Reference of Gaussian 09

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.02; Gaussian, Inc.: Wallingford, CT, **2009**.

2. Results for Pd-Catalyzed Reactions

2.1. Geometries for All Other Transition States in Scheme 1

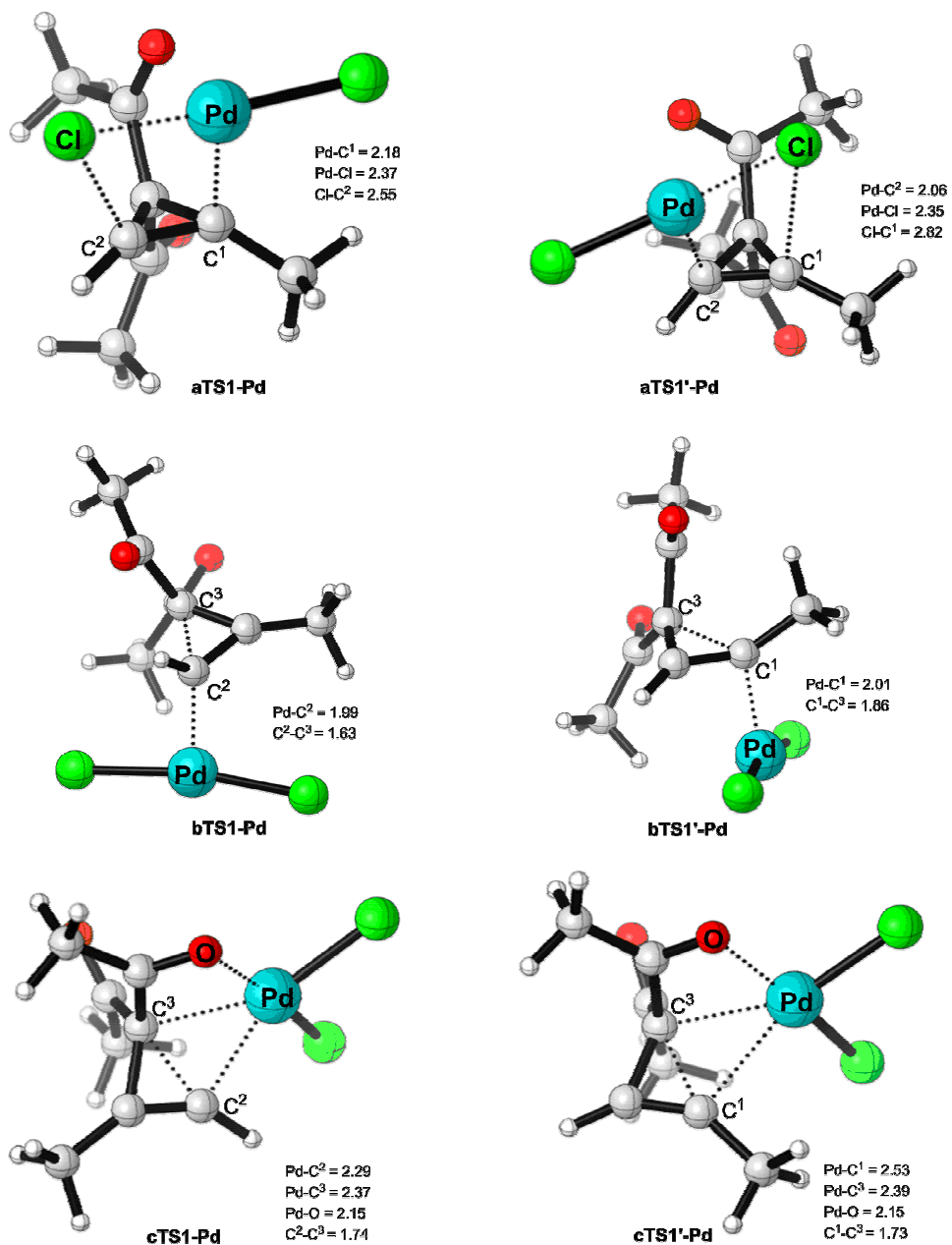


Figure S1.

2.2. Geometries for All Transition States and Intermediates in Figure 3

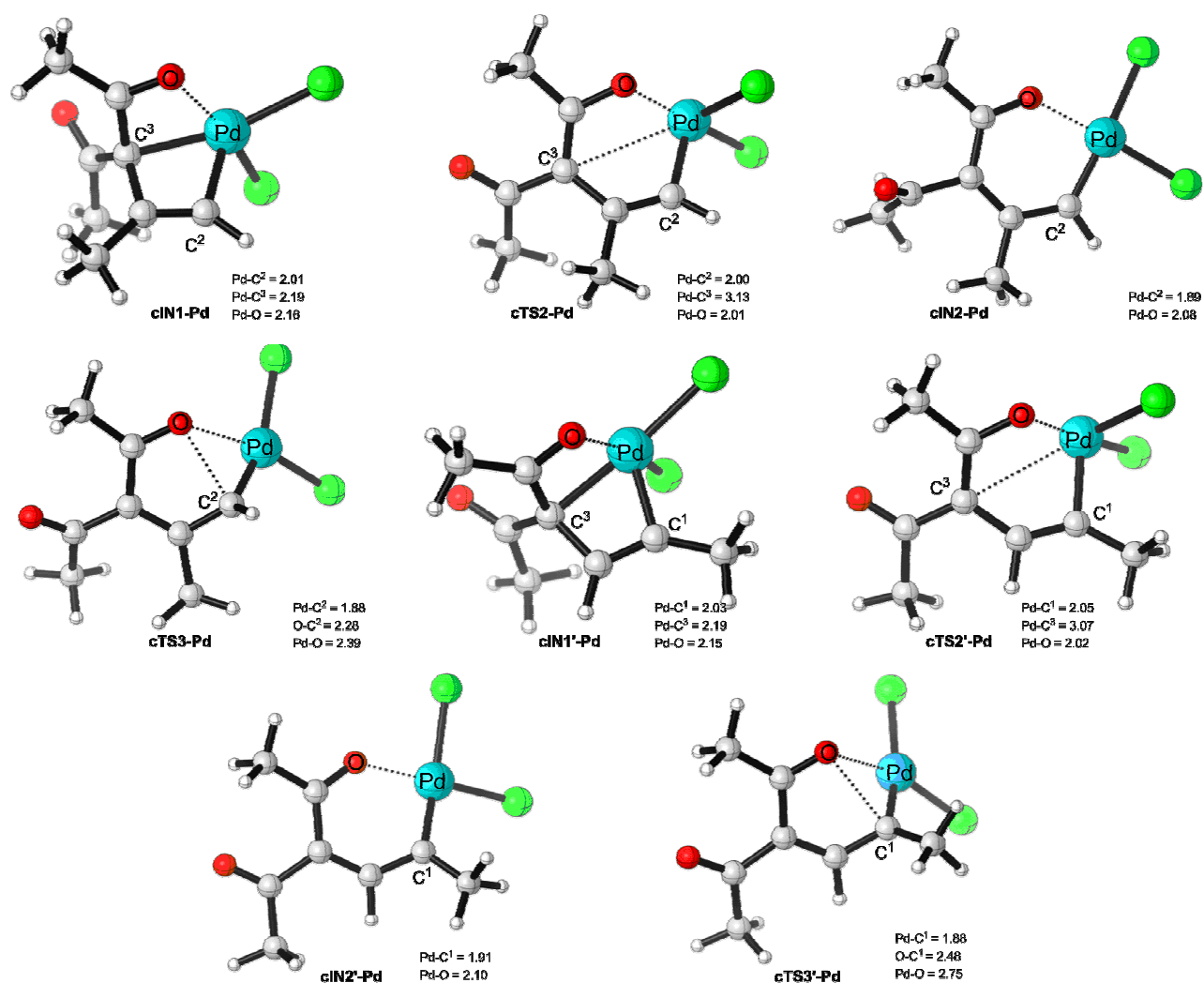


Figure S2.

2.3. Energy Profile for the Formation of 2,3,4-Trisubstituted Furan in PdCl₂-Catalyzed Reaction

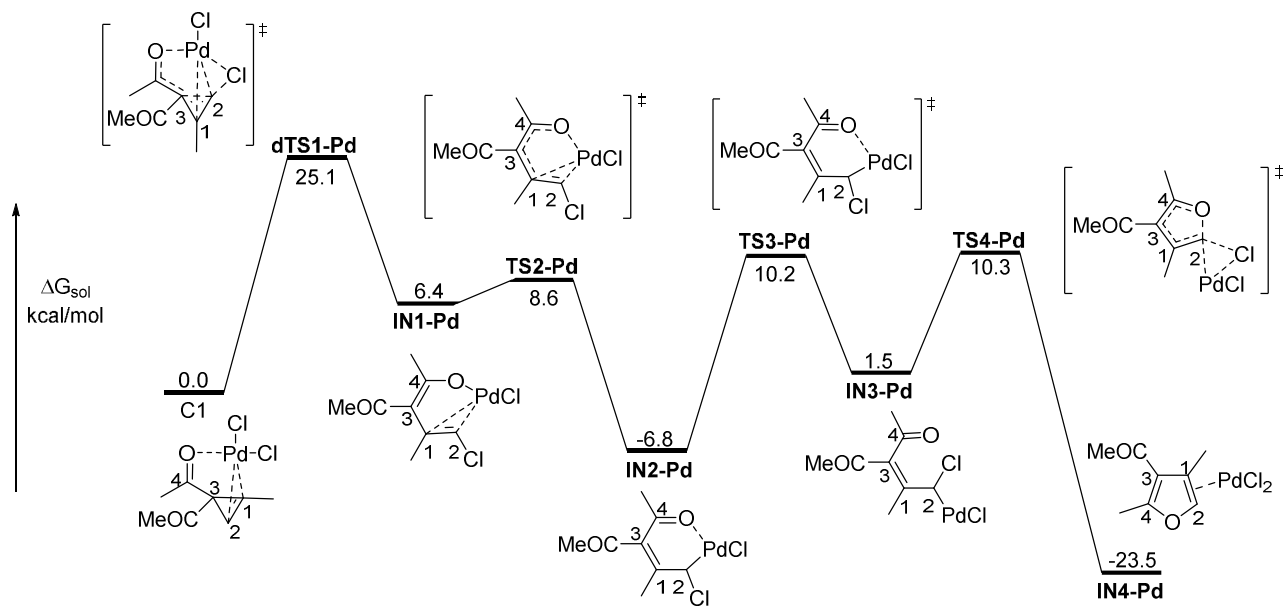


Figure S3.

2.4. Energy Profiles for the PdCl₂-Catalyzed Reaction Containing a CH₃CN Ligand (L = CH₃CN)

When one acetonitrile ligand is contained, no chelate complex like **C1** could be formed (Figure S4). Instead, the π -complex **C3-L** is formed with a relative energy of 10.9 kcal/mol. From this complex, the chlopalladation via **aTS1'-[Pd]** only requires a barrier of 6 kcal/mol to form **aIN1'-[Pd]** exergonically. This pathway could give rise to the experimentally observed major product 2,3,5-trisubstituted furan by the mechanism shown in Figure S4.

As the regioisomeric **aTS1-[Pd]** is much higher in energy, the 2,3,4-trisubstituted furan by-product is formed via the mechanism given in Figure S5. This mechanism starts with **bTS1-Pd**, which is 3.0 kcal/mol higher in energy than **aTS1'-[Pd]**.

Thus, in case of PdCl₂(CH₃CN)₂-catalyzed reactions, the major product is formed via Path a while the minor product is formed via Path b, different from that of the ligand-free reactions.

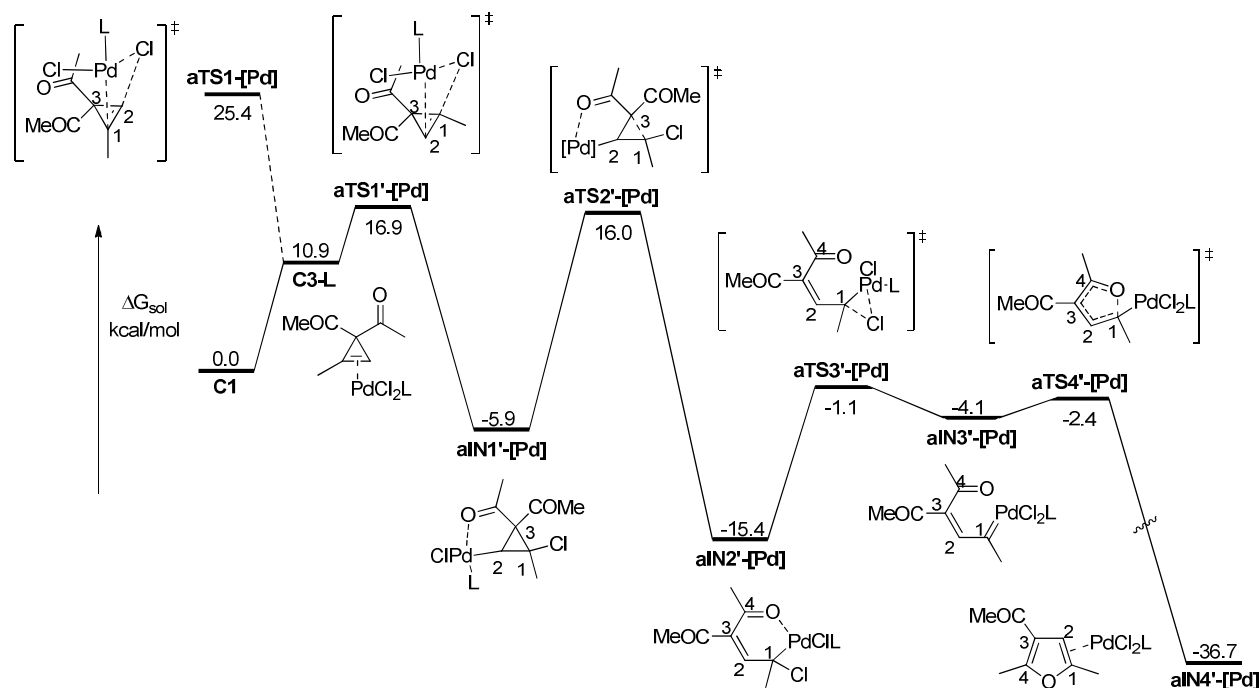


Figure S4.

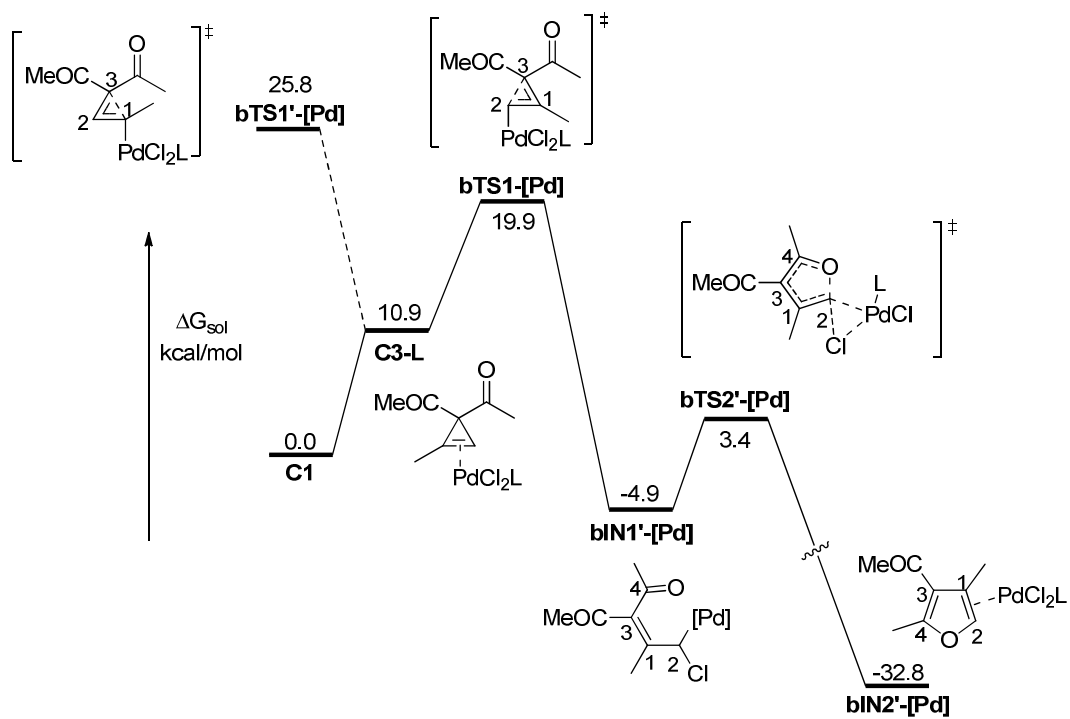


Figure S5.

3. Results for Cu-Catalyzed Reactions

3.1. Geometries for All Other Transition States in Scheme 1

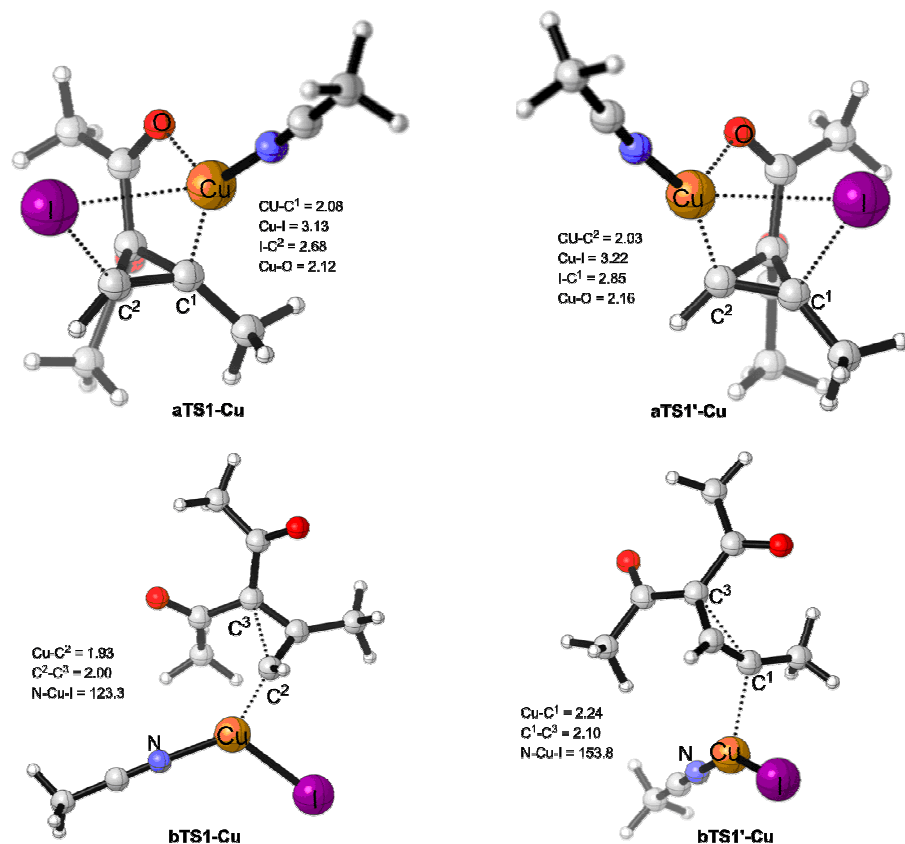


Figure S6.

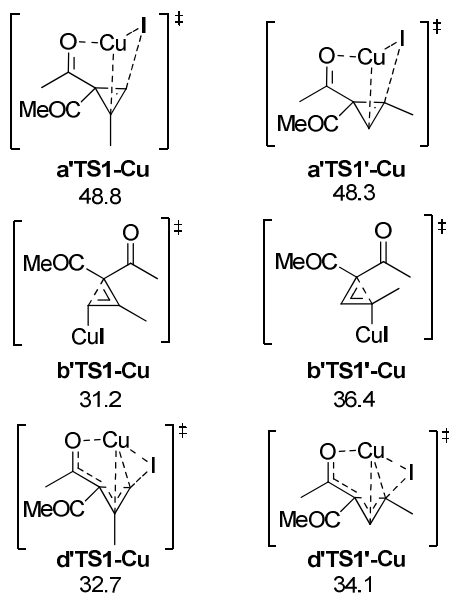
3.1. Difference between PdCl₂ and CuI in Path b

The above geometries in Figure S6 indicate the interaction between the catalyst and the substrate is weaker in **bTS1'-Cu** than that in **bTS1-Cu**, thus the catalyst is less distorted in **b-TS1'-Cu** and a slightly lower energy was calculated. However, when PdCl₂ is involved, the geometries in Figure S1 show the Pd-C¹ and Pd-C² distances are almost the same in **bTS1'-Pd** and **bTS1-Pd**, and much longer C¹-C³ breaking distance is required for the former TS. This suggests the **bTS1'-Pd** is a relatively late TS and stronger repulsive interaction between the PdCl₂ and the substrate is expected, thus making this TS unfavorable.

3.3. Energies for Key Transition States in the CuI-Catalyzed Reaction without a CH₃CN Ligand

The results in Scheme S1 indicate if no CH₃CN ligand is contained in the CuI catalyzed reactions, the TS are much higher in energies, indicating the reaction could be promoted by the CH₃CN solvent. Despite this fact, it was found that the **b'TS1-Cu** has the lowest energy for the opening of the less substituted C²-C³ σ bond whereas the **d'TS1'-Cu** is the lowest energy TS for opening of the more substituted C¹-C³ σ bond.

Scheme S1.

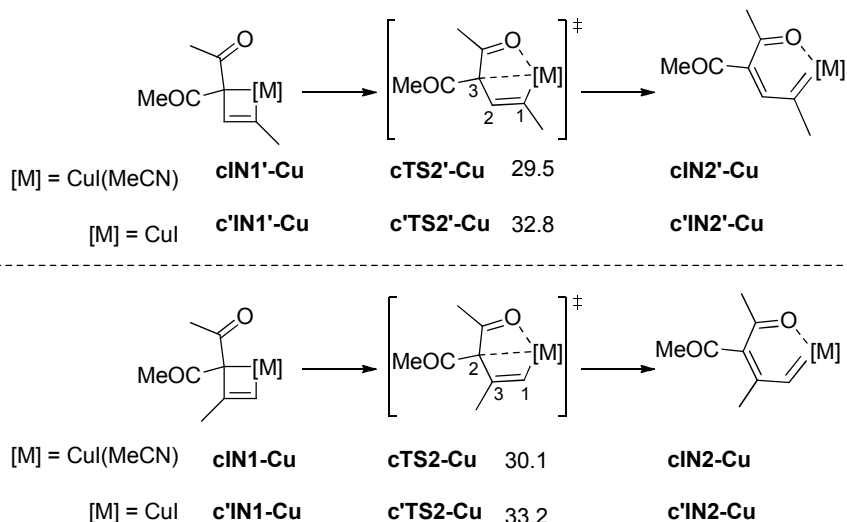


(All energies are relative to the energy sum of **C4** and **1a**)

3.4. Energies for Key Transition States in the CuI-Catalyzed Reaction via the Oxidative Addition Pathway

The results in Scheme S2 indicate the oxidative addition pathway (Path c) is unfavorable due to the high energies for the ring-opening of the four-membered ring intermediates.

Scheme S2.



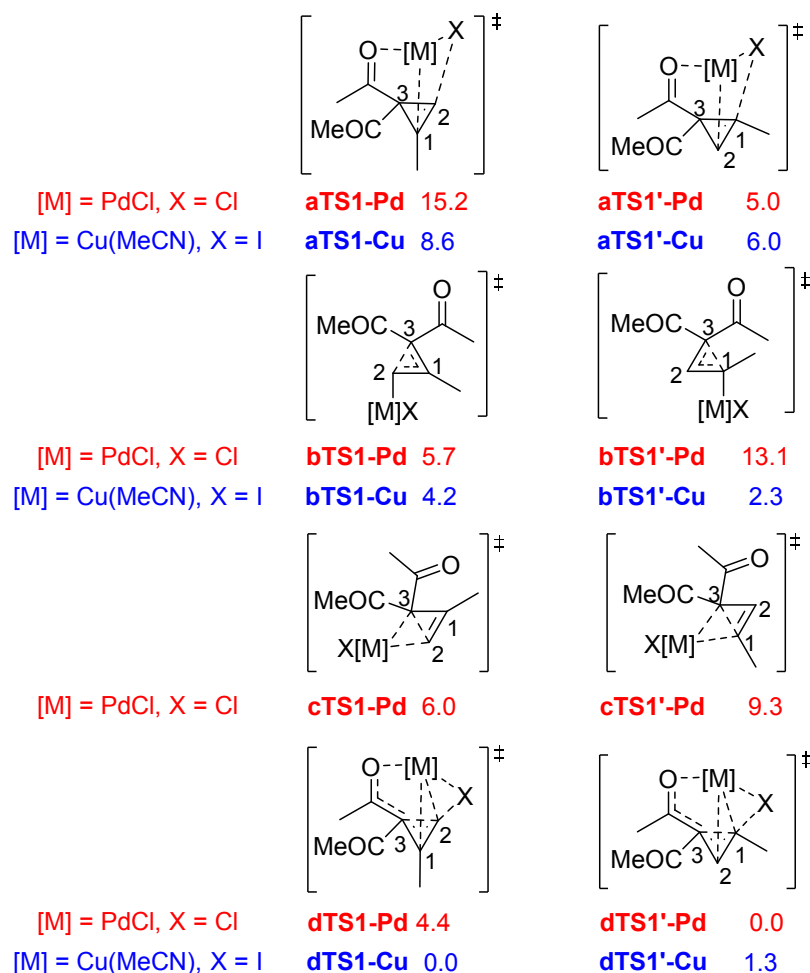
4. Energies for Key Transition States Calculated at the B3LYP Level

The values below were obtained by the following procedures:

Based on the geometry optimizations at the B3LYP/6-31+G(d)-SDD level, the single-point energies were recalculated at with a larger basis set combined by def2-TZVPPD for Pd, Cu, and I and 6-311+G(2d,2p) for all other atoms. The final energies are the single-point energies corrected by gas-phase Gibbs free energy correction, solvation correction, and dispersion correction using the B3LYP-D2 method developed by Grimme (Grimme, S. J. *Comput. Chem.* **2006**, 27, 1787.).

The relative energies are consistent with those of the CCSD(T)//B3LYP calculations. Path d is the most favorable for both PdCl₂- and CuI(CH₃CN)-catalyzed reactions and will lead to regiodivergent tri-substituted furan products.

Scheme S3.



5. Calculated Energy Values

Table S1.

Stationary point	CCSDT single-point energy (a.u.)	Thermal correction to Gibbs free energy (a.u.)	Solvation energy (a.u.)	Optimization energy (a.u.)
1a	-460.000072	0.121058	-461.257695	-461.247774
PdCl₂(CH₃CN)₂	-1311.862669	0.051547	-1313.964860	-1313.936892
CH₃CN	-132.398785	0.021448	-132.766043	-132.758528
C1	-1507.052400	0.119523	-1509.674075	-1509.647845
C2	-1507.033390	0.115782	-1509.671008	-1509.633084
C3	-1507.017969	0.115747	-1509.637616	-1509.613293
aTS1-Pd	-1506.995416	0.116469	-1509.618918	-1509.594361
aTS1'-Pd	-1507.005936	0.115136	-1509.633282	-1509.607372
bTS1-Pd	-1506.995710	0.113839	-1509.632324	-1509.605088
bTS1'-Pd	-1506.988694	0.114269	-1509.616890	-1509.590185
cTS1-Pd	-1507.013970	0.116152	-1509.633564	-1509.607624
cTS1'-Pd	-1507.009856	0.116843	-1509.627502	-1509.602511
d-TS1-Pd	-1507.014317	0.117905	-1509.636718	-1509.614065
dTS1'-Pd	-1507.017946	0.116749	-1509.644033	-1509.620417
IN1'-Pd	-1507.048744	0.119510	-1509.673616	-1509.649114
TS2'-Pd	-1507.047230	0.120461	-1509.672743	-1509.648711
IN2'-Pd	-1507.070604	0.120812	-1509.690045	-1509.666813
TS3'-Pd	-1507.037397	0.117455	-1509.662059	-1509.635389
IN3'-Pd	-1507.057397	0.118058	-1509.676780	-1509.652812
TS4'-Pd	-1507.042233	0.116542	-1509.665436	-1509.642276
IN4'-Pd	-1507.098151	0.120413	-1509.725024	-1509.701270
cIN1-Pd	-1507.031976	0.117145	-1509.648873	-1509.624215
cTS2-Pd	-1506.997577	0.119276	-1509.625692	-1509.600501
cIN2-Pd	-1507.033880	0.117571	-1509.670231	-1509.638948
cTS3-Pd	-1507.008777	0.116162	-1509.647594	-1509.617287

cIN1'-Pd	-1507.039002	0.117785	-1509.655818	-1509.631974
cTS2'-Pd	-1507.008768	0.118713	-1509.637758	-1509.613739
cIN2'-Pd	-1507.040788	0.118195	-1509.678901	-1509.649579
cTS3'-Pd	-1507.022373	0.114233	-1509.662242	-1509.632074
IN4-Pd	-1507.092025	0.121214	-1509.723994	-1509.698261
CuI	-1936.668876	-0.024739	-208.829987	-208.813992
C4	-2069.123348	0.013672	-341.645775	-341.626958
C5	-2201.532556	0.046695	-474.418470	-474.390168
C6	-2396.723503	0.113587	-670.129466	-670.110163
C7	-2396.711296	0.113630	-670.114620	-670.095475
aTS1-Cu	-2529.100921	0.155257	-802.863122	-802.840781
a'TS1-Cu	-2529.102664	0.155828	-802.866516	-802.842165
bTS1-Cu	-2529.093755	0.149368	-802.864743	-802.839216
bTS1'-Cu	-2529.093584	0.150554	-802.868026	-802.839714
dTS1-Cu	-2529.106092	0.149866	-802.871606	-802.849572
dTS1'-Cu	-2529.102952	0.150738	-802.869278	-802.848517
IN1-Cu	-2529.147812	0.156755	-802.908700	-802.887664
TS2-Cu	-2529.133826	0.158193	-802.896814	-802.876819
IN2-Cu	-2529.133153	0.156825	-802.896690	-802.877041
TS3-Cu	-2529.116604	0.154814	-802.890750	-802.868065

6. Cartesian Coordinates for All Species

1a

C	-2.70107100	-0.89143000	0.17389700
C	-1.52603400	-1.35612000	-0.06891600
C	-1.65408400	0.15668000	-0.24789200
H	-0.82445000	-2.16422900	-0.21201200
C	-4.13539400	-0.99042600	0.51449500
H	-4.73611600	-0.63910100	-0.33189800
H	-4.41274600	-2.02494200	0.74240800
H	-4.37870500	-0.36003600	1.37881600
C	-1.77292000	0.65569200	-1.68685500
C	-0.76089300	1.63251800	-2.24342300
H	-0.79704600	1.59744600	-3.33544300
H	-0.99876500	2.64389400	-1.89771700
H	0.25183500	1.41273600	-1.88628100
O	-2.66706100	0.20531300	-2.38987600
C	-1.11695100	1.09023200	0.80726600
O	-0.97484100	2.28591700	0.58654900
C	-0.79112000	0.51460700	2.17760800
H	-1.68014200	0.07623700	2.64691000
H	-0.04837400	-0.28902100	2.10104500
H	-0.40485200	1.31551500	2.81143800

PdCl₂(CH₃CN)₂

Pd	-1.76860900	2.29723400	1.68200800
Cl	-1.90488700	2.67657800	3.99276800
Cl	-1.63237600	1.91708700	-0.62829900
C	-4.88472300	1.95817400	1.56541000
N	-3.74061200	2.08318900	1.60438400
C	-6.33184900	1.79974900	1.51889500
H	-6.74128500	1.83180600	2.53354000
H	-6.77525000	2.60686900	0.92703600
H	-6.58588300	0.83963500	1.05849700
N	0.20336900	2.51129400	1.76069300
C	1.34744800	2.63550400	1.80308500
C	2.79455700	2.79221700	1.85592900
H	3.13918600	2.71488500	2.89196100
H	3.27458000	2.01168500	1.25707000
H	3.07669800	3.77170400	1.45665200

CH₃CN

C	-3.21987300	-0.02200300	-0.15272700
N	-2.05867800	-0.02222800	-0.15246600
C	-4.68190600	-0.02211600	-0.15262700

H	-5.06128900	0.46009400	0.75425600
H	-5.06141900	0.52214900	-1.02362700
H	-5.06121500	-1.04862900	-0.18842300

C1

C	-2.20068500	-0.46483100	0.47397500
C	-1.03054900	-0.30488200	1.10222800
C	-1.65999500	0.98459400	0.46515100
C	-2.31197300	1.93150400	1.42005900
C	-2.41183000	3.40996600	1.21409300
H	-1.41369200	3.85997700	1.24455500
H	-2.81317000	3.63982100	0.22135700
H	-3.04561400	3.83433100	1.99545800
O	-2.82036200	1.44715700	2.45313200
Cl	-3.72573200	-0.73697200	4.56818600
Cl	-2.32832900	-2.91000500	2.50850600
Pd	-2.61861600	-0.63493000	2.56482500
C	-0.98702200	1.49671200	-0.79351300
O	-0.63363400	2.66134400	-0.88069700
H	-2.77825800	-1.08415500	-0.19882900
C	0.34809900	-0.77214100	1.40266400
H	1.00237000	-0.58003000	0.54142600
H	0.76364300	-0.24469300	2.26655300
H	0.32909100	-1.84509000	1.61257400
C	-0.77668700	0.52262700	-1.93732600
H	-0.29421100	-0.40662200	-1.61482700
H	-1.74606000	0.24427900	-2.37262100
H	-0.16910800	1.00580900	-2.70490500

C2

C	-1.34011800	1.03129200	1.80561200
C	-2.19244100	1.95149200	1.50085900
C	-1.79937200	0.97953000	0.35885200
C	-0.89510100	1.52405600	-0.72574300
C	0.55054400	1.79010500	-0.39023100
H	0.63199400	2.51663800	0.42677100
H	1.03874100	0.86780000	-0.05017900
H	1.06115100	2.17713700	-1.27368500
O	-1.29340700	1.76225500	-1.86859900
Cl	-5.57783200	1.52539700	-2.85679800
Cl	-3.10724100	3.56237500	-3.70447600
Pd	-3.34500200	1.68881300	-2.42760300
C	-2.82974900	-0.04884700	-0.05538200
O	-3.43793200	0.00995600	-1.12708900
H	-0.69505300	0.54192200	2.52059900
C	-3.06663600	3.12162200	1.71015300

H	-4.10694300	2.87009900	1.47177800
H	-3.00670700	3.46803400	2.74686900
H	-2.77785400	3.93949700	1.03912300
C	-3.12615900	-1.18852500	0.88617900
H	-2.21465200	-1.76721400	1.08334300
H	-3.48209800	-0.81108400	1.85202500
H	-3.88763100	-1.83347300	0.44439300

C3

C	7.59232100	0.67903400	-5.63616900
C	7.25131000	1.48724200	-4.58086900
C	6.11104200	0.81065900	-5.31232200
C	5.41172800	1.80063200	-6.28060400
C	3.97511800	1.57013500	-6.68225000
O	6.04690700	2.76048600	-6.68205200
H	3.32686300	1.48110700	-5.80189500
H	3.64897200	2.41095400	-7.29770800
H	3.87781200	0.63034500	-7.23589200
Pd	8.43933700	-0.05173500	-3.75014900
Cl	9.72131500	1.66234700	-2.92256100
Cl	7.69152400	-2.17238100	-4.19879800
C	5.21510600	-0.31512000	-4.77929100
O	4.71739300	-1.08471700	-5.57687500
H	7.44554600	2.48780300	-4.21657000
C	8.43238500	0.49366900	-6.84374600
H	8.00329400	1.10889300	-7.64612600
H	9.46008600	0.81884200	-6.66105500
H	8.42430800	-0.55138300	-7.16629300
C	4.87716000	-0.32265900	-3.30618100
H	5.76075200	-0.17621400	-2.67908700
H	4.19225300	0.51386800	-3.10287400
H	4.38584700	-1.26228400	-3.04703100

aTS1-Pd

C	-3.00951200	-0.77886100	-0.09873600
C	-1.77039900	-1.33201800	-0.17933200
C	-1.78047700	0.14448200	-0.34713000
H	-1.12122000	-2.09751900	0.21765400
C	-4.11268400	-0.72739100	0.92598600
H	-4.88442600	-0.01542600	0.63460200
H	-4.57562600	-1.71243100	1.03541700
H	-3.69779300	-0.42701200	1.89783200
C	-1.57334000	0.80489000	-1.73011500
C	-0.41764800	1.76131500	-1.90778800
H	-0.19377400	1.84644500	-2.97304500
H	-0.69287000	2.74472600	-1.51260500

H	0.47004500	1.42530900	-1.36013400
O	-2.30219800	0.52916600	-2.66160900
C	-1.30463000	0.98800900	0.84043000
O	-1.46239900	2.19437200	0.81678600
Cl	-1.64293900	-2.69631400	-2.32555500
Pd	-3.65985200	-1.48797900	-2.05216800
Cl	-5.72688100	-0.51122800	-1.99038700
C	-0.66813400	0.28685000	2.02312900
H	0.25722700	-0.21425700	1.70805300
H	-0.43777800	1.01899100	2.79988000
H	-1.32831000	-0.48550800	2.43680000

aTS1'-Pd

C	-2.79528200	-1.04143700	-0.11005500
C	-1.63737500	-1.78450800	-0.17684700
C	-1.54444100	-0.25027000	-0.17826100
H	-1.19213500	-2.50392500	0.50559000
C	-4.19157800	-0.97823700	0.33451500
H	-4.75123000	-0.19064500	-0.17582500
H	-4.69603100	-1.93959000	0.21586200
H	-4.13805000	-0.72212000	1.40576400
C	-1.07470200	0.53794600	-1.42084200
C	-1.76604800	1.85768000	-1.67831000
H	-1.15916100	2.47449500	-2.34525400
H	-2.72275000	1.64019700	-2.17009400
H	-1.98646200	2.39752500	-0.75031400
O	-0.18616000	0.10225600	-2.11719600
C	-1.09076000	0.35231600	1.16443100
O	-1.77769700	0.22333100	2.16164700
Cl	-3.48995600	-1.14545900	-2.83913200
Pd	-1.84516700	-2.62700300	-2.04303200
Cl	-0.32262500	-4.24251700	-1.50068200
C	0.26465700	1.02155300	1.18599400
H	0.25891000	1.93403400	0.57629700
H	0.52316600	1.27859100	2.21524200
H	1.02511000	0.35844600	0.75651200

bTS1-Pd

C	7.96205500	-0.37473600	-4.73825100
C	7.81248600	0.47169700	-3.66153500
C	6.56528500	-0.23838400	-4.43057400
C	5.71993600	0.88321200	-5.11926500
C	4.40019300	0.47021900	-5.72324700
O	6.12937900	2.02056100	-5.14221100
H	3.72615100	0.10744200	-4.93695500
H	3.95367900	1.33733300	-6.21277400

H	4.53220800	-0.35178500	-6.43338700
Pd	8.67433600	0.13619800	-1.90168500
Cl	10.72278300	-0.60923800	-2.65775500
Cl	6.79437300	0.88476400	-0.78336300
C	5.83146900	-1.55580700	-4.11863800
O	5.56392900	-2.29701500	-5.04641000
H	7.62828800	1.55295100	-3.75554300
C	8.85341300	-1.25551600	-5.49051400
H	9.23721800	-0.66966600	-6.34352800
H	9.72408900	-1.51882700	-4.87800100
H	8.32861600	-2.13102400	-5.88310800
C	5.50247300	-1.85320000	-2.68271600
H	6.42461100	-1.96331800	-2.09902000
H	4.96889700	-1.01556200	-2.21893800
H	4.91665100	-2.77360500	-2.63012100

bTS1'-Pd

C	8.09653800	-0.96101300	-5.01793400
C	7.50242300	-0.21963500	-4.04005200
C	6.28711600	-0.78391500	-4.55539700
C	5.69986200	-0.10922000	-5.78735200
C	4.52474200	-0.72575800	-6.50484100
O	6.20503300	0.93649500	-6.17525200
H	3.63339300	-0.72766300	-5.86899000
H	4.33676000	-0.13278300	-7.40313400
H	4.71531000	-1.77275600	-6.75882100
Pd	9.11041100	-2.08055500	-3.69360800
Cl	10.54557100	-0.42280700	-2.98432600
Cl	8.02418200	-4.03876000	-4.23908500
C	5.44539400	-1.73259000	-3.71836700
O	4.53499100	-2.36105300	-4.22810300
H	7.83941600	0.33576500	-3.17073800
C	8.51571400	-1.07976900	-6.43917700
H	7.91455500	-0.42329100	-7.07506200
H	9.56279100	-0.75925400	-6.50289400
H	8.44967600	-2.11823000	-6.77349200
C	5.74646300	-1.82082800	-2.23894300
H	6.69850600	-2.33894600	-2.07548500
H	5.82744700	-0.82302500	-1.78928200
H	4.95070000	-2.38568100	-1.74924900

cTS1-Pd

C	-2.61268000	-0.64594900	0.20257400
C	-1.33522000	-0.86368900	0.16665600
C	-1.46196300	0.57416100	-0.24542600
C	-1.29985800	0.84151100	-1.74164400

C	0.03771900	0.91489700	-2.40076700
H	-0.07591500	0.89517200	-3.48721800
H	0.51525100	1.85263700	-2.09036400
H	0.68511800	0.09632300	-2.06621400
O	-2.35224900	0.96656400	-2.37874200
C	-0.95311500	1.66833700	0.68615900
O	-0.30574700	2.58197800	0.19889400
Cl	-4.86246800	1.39044100	1.25469700
Pd	-3.71676800	1.13599400	-0.72174600
Cl	-5.37990100	2.16753100	-1.88261100
C	-1.25758900	1.56296700	2.15816300
H	-2.34127200	1.63403500	2.31879600
H	-0.93316700	0.59921400	2.56852500
H	-0.75127200	2.37699900	2.68064700
C	-0.23399700	-1.81251700	0.47130300
H	0.32315100	-2.07685300	-0.43574900
H	0.47961400	-1.36422800	1.17358100
H	-0.63221800	-2.73171800	0.91109900
H	-3.55149700	-1.01582300	0.59930400

cTS1'-Pd

C	-2.57240500	-0.75341400	0.18960200
C	-1.28518700	-0.85919100	0.17138300
C	-1.52021500	0.56749400	-0.20729300
H	-0.43526500	-1.50663600	0.34263300
C	-3.84249100	-1.47198400	0.49062700
H	-4.49705500	-1.51805400	-0.38497500
H	-3.57584100	-2.49214200	0.79709800
H	-4.39698400	-0.97229600	1.28922300
C	-1.31956700	0.86366000	-1.69697100
C	0.03221000	0.85388600	-2.33094200
H	-0.05801900	0.91068600	-3.41807200
H	0.58648500	1.72345200	-1.95592600
H	0.59165200	-0.04317700	-2.04093700
O	-2.34842300	1.07834800	-2.34813400
C	-1.06833600	1.67603300	0.73455300
O	-0.48207400	2.62903900	0.24367100
Cl	-4.89074600	1.66549200	1.22045200
Pd	-3.73874700	1.29851400	-0.72890100
Cl	-5.34032200	2.36508800	-1.93496500
C	-1.32259300	1.52965500	2.21227100
H	-2.40249400	1.57049500	2.40493500
H	-0.95619200	0.56793600	2.58989700
H	-0.82682400	2.34857400	2.73739900

dTS1-Pd

C	-2.06145500	-0.44666500	0.15306900
C	-1.06195600	-0.66349400	1.03613100
C	-1.99178100	1.06132300	0.18419800
H	-0.62782600	-0.39863400	1.98703900
C	-3.13962800	-1.28335900	-0.46794200
H	-3.22064800	-1.06512400	-1.53781100
H	-2.94792500	-2.34796800	-0.32000600
H	-4.10135300	-1.02046200	-0.00686400
C	-1.11127100	1.66554800	-0.76841100
C	-1.14870200	3.12146400	-1.13486700
H	-2.14677900	3.41780500	-1.47061600
H	-0.93383700	3.73414200	-0.25272100
H	-0.40659800	3.30460900	-1.91501000
O	-0.22199100	0.97507100	-1.38482700
Cl	-0.22263700	-2.86458000	0.67627600
Cl	1.54041100	-1.55287900	-2.21638800
Pd	-0.07608500	-0.93974500	-0.70784600
C	-2.88667300	1.82618600	1.07799000
O	-3.03697800	3.03951900	0.95386100
C	-3.59465500	1.10154000	2.21647800
H	-3.77943300	0.03911400	2.03656200
H	-2.98028800	1.18373500	3.12321700
H	-4.54087900	1.61097300	2.41568900

dTS1'-Pd

C	-2.08071500	-0.38616600	0.46581200
C	-1.08402700	-0.80953400	1.28950500
C	-1.82908900	1.08195400	0.28581000
C	-2.29117600	1.92772000	1.32533800
C	-2.28235100	3.42874600	1.25164200
H	-1.25342300	3.79610500	1.17654500
H	-2.79558200	3.78004700	0.35163700
H	-2.76223400	3.82667300	2.14853000
O	-2.77981000	1.44694200	2.42091100
Cl	-3.90839000	-0.70709800	4.45825600
Cl	-2.11295300	-2.85664300	2.23445000
Pd	-2.66900700	-0.57381200	2.53186300
C	-1.19891400	1.55307300	-0.96044100
O	-0.99145100	2.74466400	-1.18295500
H	-2.75306300	-1.00528100	-0.12548400
C	0.34915100	-0.84646200	1.62022400
H	0.91688700	-0.28765100	0.86764700
H	0.54904900	-0.44372700	2.61789400
H	0.68323800	-1.89105400	1.60504100
C	-0.82857800	0.50260600	-1.99878900
H	-0.17525700	-0.27600600	-1.58469900

H	-1.72823200	-0.00057500	-2.37824100
H	-0.32039800	0.99324900	-2.83147300

IN1'-Pd

C	-1.92795400	-0.43626400	0.50367900
C	-1.10621200	-1.12524100	1.40728000
C	-1.77340900	1.01724800	0.22861300
C	-2.09991300	1.87348800	1.26372000
C	-1.93064000	3.36661600	1.28061500
H	-0.89293800	3.64657000	1.07726600
H	-2.53310400	3.81448600	0.48305100
H	-2.25091400	3.75540600	2.25070800
O	-2.64175400	1.41615400	2.37833000
Cl	-4.32589500	-0.67512400	4.25852100
Cl	-1.34626100	-2.89044300	1.49647400
Pd	-2.87974000	-0.55126900	2.49005600
C	-1.32793700	1.47727300	-1.09536000
O	-1.13131500	2.66537600	-1.35396400
H	-2.53077700	-1.03973000	-0.17543300
C	0.16683000	-0.65123900	2.04779000
H	0.22291200	0.43879100	2.01583500
H	0.23967400	-0.98810500	3.08590200
H	1.02246700	-1.06309100	1.49621200
C	-1.11754500	0.42061300	-2.17303000
H	-0.40500300	-0.34956700	-1.85092800
H	-2.06128900	-0.08707900	-2.41445400
H	-0.73961000	0.90690100	-3.07486000

TS2'-Pd

C	-1.88770500	-0.43271000	0.49051400
C	-1.10736800	-1.10674900	1.45832300
C	-1.79146700	0.99825600	0.21540200
C	-1.89352600	1.85706000	1.32023500
C	-1.53441700	3.31546700	1.33967600
H	-0.52487700	3.48525700	0.95564300
H	-2.21082500	3.85839700	0.66939700
H	-1.63815200	3.69973200	2.35725200
O	-2.38018800	1.42239200	2.44731800
Cl	-4.33299200	-0.68709900	4.27886400
Cl	-1.31186000	-2.87891500	1.49844000
Pd	-2.82220900	-0.55088200	2.55292000
C	-1.63243600	1.48688200	-1.16570800
O	-1.40944400	2.67115900	-1.41871100
H	-2.41711900	-1.06091000	-0.22380700
C	0.17795500	-0.64229900	2.08810500
H	0.25129800	0.44648100	2.05962800

H	0.25344700	-0.97781600	3.12667000
H	1.02527700	-1.06349200	1.53109300
C	-1.75333500	0.48030900	-2.30314600
H	-0.98210500	-0.29732600	-2.23444700
H	-2.73055600	-0.02028300	-2.29404000
H	-1.63882000	1.01298500	-3.24941400

IN2'-Pd

C	-1.77518800	-0.05023000	0.77377500
C	-1.58798200	-0.55096900	2.15639900
C	-1.60111400	1.22284500	0.29239200
C	-1.47127100	2.34562100	1.24124300
C	-0.73026800	3.61311200	0.93277100
H	0.23151800	3.41043800	0.45281600
H	-1.30620800	4.20393700	0.21136000
H	-0.59838400	4.18076300	1.85671200
O	-2.02426700	2.25423500	2.36123300
Cl	-4.34930900	-0.92362700	4.19901000
Cl	-1.88066200	-2.33515100	2.17513900
Pd	-3.00213200	0.55268800	3.11685900
C	-1.60518300	1.47990600	-1.18465800
O	-1.28997000	2.57750600	-1.62844500
H	-2.02454600	-0.82238700	0.05208000
C	-0.24494600	-0.28252000	2.84408300
H	-0.00217900	0.78222600	2.86596300
H	-0.26831900	-0.65643000	3.87006300
H	0.55014900	-0.81354300	2.30406300
C	-2.01137300	0.36406100	-2.13450900
H	-1.28255300	-0.45552900	-2.12184100
H	-2.99115300	-0.05559400	-1.87838400
H	-2.05130100	0.78129500	-3.14243100

TS3'-Pd

C	-1.55495700	-0.09099500	0.71281400
C	-1.36650900	-0.62112900	2.07574400
C	-1.55188200	1.21136500	0.30657200
C	-1.39854500	2.32357800	1.31804100
C	-0.79624500	3.65390800	0.93613200
H	0.04908600	3.54106700	0.25030200
H	-1.54325300	4.25687200	0.40898300
H	-0.49165600	4.16772500	1.85123500
O	-1.75143600	2.11280600	2.47385200
Cl	-4.92044300	0.51954100	4.10079700
Cl	-1.85508600	-2.41231700	2.13764700
Pd	-3.11310600	-0.44225400	3.01019500
C	-1.78177500	1.53185600	-1.14420500

O	-1.79758900	2.69522700	-1.52329800
H	-1.75973300	-0.84611300	-0.03956300
C	-0.10132100	-0.38488300	2.86828500
H	0.06735100	0.68787700	2.97789100
H	-0.18138100	-0.82668600	3.86506600
H	0.76246100	-0.82891400	2.35655200
C	-2.01348400	0.40749400	-2.14296000
H	-1.16313800	-0.28363700	-2.18375300
H	-2.90893100	-0.17414700	-1.89232200
H	-2.15207000	0.85841100	-3.12731100

IN3'-Pd

C	-1.33568700	-0.07124900	0.69071000
C	-1.60880700	-0.64243400	2.02100400
C	-1.17931500	1.22908200	0.34372400
C	-1.14184600	2.40543600	1.30964700
C	-2.39142000	3.23943300	1.42163100
H	-2.59706600	3.70996000	0.45272000
H	-3.25569200	2.60694800	1.66642000
H	-2.25451100	4.01080200	2.18372600
O	-0.12146500	2.62346800	1.93827800
Cl	-5.01358900	0.20521000	2.02815700
Cl	-1.13561300	-2.45230400	2.03575100
Pd	-3.42698000	-1.43688600	2.01561300
C	-1.01461700	1.62363300	-1.09739600
O	-0.90072400	2.81156800	-1.37040300
H	-1.33190000	-0.80679800	-0.10761400
C	-1.22660100	0.04049500	3.30977400
H	-1.81697500	0.95425400	3.42207000
H	-1.43728000	-0.60315200	4.16607800
H	-0.16617600	0.31812500	3.30826200
C	-0.98709400	0.56771100	-2.18706700
H	-0.18547500	-0.16181400	-2.02115300
H	-1.93614900	0.01983500	-2.23290700
H	-0.82034400	1.06962800	-3.14212600

TS4'-Pd

C	-1.33428800	0.02892900	0.82182600
C	-1.57162300	-0.49635500	2.17393800
C	-1.50218600	1.30069500	0.36852400
C	-2.04590400	2.32954700	1.32314600
C	-2.48061900	3.69874000	0.87092100
H	-1.61366300	4.29618700	0.57129300
H	-3.13033900	3.63695500	-0.00866900
H	-3.00712000	4.18034300	1.69754500
O	-2.16138900	1.98633600	2.49494400

Cl	-4.99133200	0.34326300	2.93717400
Cl	-1.57999800	-2.68840800	1.87256200
Pd	-3.36548700	-1.14930600	2.42193400
C	-1.13825700	1.63630000	-1.04983100
O	-0.96754600	2.80263500	-1.37651500
H	-1.00151500	-0.72670400	0.11799900
C	-0.60256300	-0.32397600	3.30891200
H	-0.64173300	0.72099100	3.62706700
H	-0.85753900	-0.96639800	4.15247700
H	0.41626200	-0.55221500	2.97304200
C	-0.96502200	0.52087600	-2.06860300
H	-0.06416700	-0.06955900	-1.85770600
H	-1.82027600	-0.16424600	-2.07566400
H	-0.85202300	0.97632200	-3.05441800

IN4'-Pd

C	-1.16544700	0.14035700	0.93018000
C	-1.40753900	0.36880500	2.32262900
C	-1.48510500	1.36421500	0.24276200
C	-1.90637100	2.25006100	1.21507400
C	-2.44593300	3.62642000	1.16971300
H	-2.24721500	4.07559500	0.19681400
H	-3.53234400	3.58414700	1.32988300
H	-2.01434400	4.23390200	1.97297700
O	-1.85134700	1.67367000	2.44700900
Cl	-4.70573600	0.43616700	1.56326900
Cl	-1.61166800	-2.93411600	1.60726600
Pd	-2.94583200	-1.04558300	1.60162300
C	-1.40119800	1.62352600	-1.21655400
O	-1.60559800	2.74051600	-1.67529700
H	-0.54910400	-0.66413300	0.54968500
C	-0.74927000	-0.16424600	3.55850800
H	0.12281900	0.46274500	3.79039200
H	-1.43448400	-0.11703600	4.41006000
H	-0.42873300	-1.19606200	3.41301800
C	-1.04578900	0.45161000	-2.10939300
H	-0.04680400	0.06564500	-1.86708000
H	-1.75495300	-0.37412400	-1.97289800
H	-1.05933300	0.77887300	-3.15074200

cIN1-Pd

C	0.13640200	-1.45654500	0.80154800
C	1.44238600	-1.32594600	0.69724100
C	1.61612000	0.12254200	0.24206400
C	1.59036300	0.27779600	-1.25202200
C	2.73409300	0.68170600	-2.11948400

H	2.50182300	0.46950800	-3.16606100
H	2.90536100	1.75623100	-1.98301300
H	3.65557100	0.17714700	-1.80935100
O	0.45847700	0.05708700	-1.73811400
C	2.37131700	1.12989300	1.05809800
O	2.84453300	2.11794100	0.50586200
Cl	-1.13626700	0.84413100	2.29693700
Pd	-0.56100000	0.31347100	0.15063800
Cl	-2.75489700	0.50586200	-0.60785800
C	2.50066700	0.90308000	2.54544300
H	1.51404200	0.73903200	2.99301200
H	3.11031900	0.01487500	2.75293700
H	2.97649800	1.77630600	2.99659200
C	2.55393600	-2.32476700	0.85815400
H	3.07569700	-2.48186100	-0.09507600
H	3.29770600	-1.98057000	1.58648300
H	2.16220500	-3.28919700	1.19615400
H	-0.61098100	-2.17417200	1.11662600

cTS2-Pd

C	-3.12286700	-0.85757000	0.13128100
C	-1.82206100	-0.62172400	0.26753600
C	-1.06705800	0.48127600	-0.38482900
C	-1.50298500	0.94370800	-1.63135400
C	-0.68167000	1.78000400	-2.58371600
H	-1.29457000	2.02396600	-3.45456900
H	-0.33710100	2.69708000	-2.09500300
H	0.21956200	1.24332000	-2.89215300
O	-2.70185700	0.68892900	-2.09705500
C	0.15598500	1.05023700	0.22799800
O	1.04080000	1.58183800	-0.44276700
Cl	-5.76581000	0.95468600	0.86182300
Pd	-4.17219700	0.61711800	-0.72393000
Cl	-5.40480900	-0.70582900	-2.07543000
C	0.29744200	1.06379000	1.74859500
H	-0.64948800	0.93537000	2.28105600
H	0.99742600	0.28329600	2.07045900
H	0.74057500	2.02471600	2.02640600
C	-1.05317400	-1.69629100	1.03613400
H	-0.18997200	-2.01440900	0.43855900
H	-0.68897500	-1.32559300	1.99711900
H	-1.68062900	-2.57066500	1.23042800
H	-3.76702000	-1.68741900	0.38889800

cIN2-Pd

C	-0.17510700	-1.28802300	0.64758700
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C	1.22112900	-1.07540400	0.93382100
C	2.01476900	-0.17798600	0.24750900
C	1.57674500	0.56061700	-0.95445900
C	2.55856600	1.42603900	-1.70173500
H	2.03139200	1.95375000	-2.49796300
H	3.03887200	2.15196500	-1.03419000
H	3.35593600	0.80799000	-2.13071700
O	0.42345800	0.48523600	-1.41360400
C	3.46529300	0.02271600	0.66253700
O	4.34774600	-0.49497600	0.00250500
Cl	-3.03921300	-1.68964700	0.13713100
Pd	-1.25384100	-0.50940000	-0.69740600
Cl	-2.55763800	0.73533700	-2.17978000
C	3.73623800	0.89833100	1.86426100
H	3.15950800	0.56633300	2.73524600
H	4.80432300	0.89374500	2.09499100
H	3.41386200	1.92677100	1.65053900
C	1.78578700	-1.91558700	2.06579900
H	1.48766600	-2.96145500	1.92864900
H	2.87628100	-1.89077800	2.12667200
H	1.36894700	-1.59170600	3.02837200
H	-0.68108600	-1.93222500	1.37074300

cTS3-Pd

C	-0.27161500	-1.56604000	0.29863400
C	0.97750000	-1.07675800	0.80819700
C	1.77525000	-0.23315300	0.06764600
C	1.26004000	0.03496500	-1.29100200
C	2.06110800	0.70748100	-2.36728000
H	1.42117300	0.86514600	-3.23707700
H	2.46057400	1.66230400	-2.00853400
H	2.93119400	0.09759400	-2.63109300
O	0.08972300	-0.31028900	-1.57451000
C	3.09252100	0.32330300	0.51445400
O	3.99257000	0.48448600	-0.29918200
Cl	-3.11650200	-0.73475900	1.74900500
Pd	-1.73101200	-0.43517700	-0.03755200
Cl	-3.10940100	0.96403000	-1.26446800
C	3.29473900	0.73319200	1.96361400
H	3.70241600	-0.10381600	2.54391700
H	4.03605700	1.53623700	1.98500900
H	2.37101800	1.06762500	2.44480700
C	1.24977500	-1.62806700	2.19551900
H	2.29674100	-1.92288200	2.30547900
H	1.01038200	-0.87358200	2.95285100
H	0.61908000	-2.49852400	2.40227200

H	-0.34324600	-2.61698200	-0.00891800
cIN1'-Pd			
C	0.33974300	-1.53289800	0.83975500
C	1.63389900	-1.29136200	0.77499800
C	1.83895900	0.13417600	0.29617200
C	1.80079300	0.27477500	-1.19173200
C	2.90215200	0.77804200	-2.06307300
H	2.68581300	0.53799600	-3.10705400
H	2.97836700	1.86443500	-1.93690300
H	3.86583500	0.36007000	-1.75309600
O	0.68751000	-0.03724300	-1.68387600
C	2.62292100	1.11868400	1.10658500
O	3.06756900	2.13179500	0.57655600
Cl	-0.87644800	0.88095700	2.31854600
Pd	-0.34210700	0.26592100	0.18015200
Cl	-2.56621900	0.16003100	-0.52496000
C	2.82243600	0.82280100	2.57400600
H	1.85033600	0.69549300	3.06507300
H	3.38319200	-0.11111000	2.71053000
H	3.36998100	1.64716000	3.03547800
C	-0.63937100	-2.57280000	1.21081600
H	-1.31959700	-2.79637300	0.38310300
H	-0.08755900	-3.48392700	1.48632800
H	-1.24130000	-2.24768000	2.06570800
H	2.44688600	-1.99400600	0.96995000
cTS2'-Pd			
C	-3.22858600	-0.76187000	0.22674400
C	-1.98909300	-0.33007700	0.42583600
C	-1.19371800	0.68325600	-0.29065000
C	-1.49495500	0.93812000	-1.63460000
C	-0.61104100	1.68119100	-2.60369000
H	-0.97670100	1.49581600	-3.61695700
H	-0.64608100	2.75666600	-2.39600500
H	0.43446400	1.38201600	-2.50459000
O	-2.60311600	0.50191900	-2.17778700
C	-0.03067500	1.30014200	0.37703000
O	0.67981700	2.13716400	-0.18047800
Cl	-5.92189000	1.19282000	0.42971800
Pd	-4.19635700	0.61716000	-0.94858500
Cl	-5.35877200	-0.76326100	-2.30686800
C	0.28994400	0.89046700	1.81140400
H	-0.56748000	1.03888400	2.47925700
H	0.57915800	-0.16735900	1.87171300
H	1.12657700	1.49932500	2.15951500

C	-4.06688100	-1.88317400	0.71171100
H	-4.31197400	-2.58214600	-0.09460800
H	-3.47851600	-2.42528700	1.46767400
H	-4.99949900	-1.53724300	1.16631600
H	-1.47992200	-0.85775200	1.23712000

cIN2'-Pd

C	-0.11510700	-1.03549400	0.91653400
C	1.15937600	-0.47726400	1.24415700
C	2.04329100	0.24465800	0.47517400
C	1.72019900	0.52631000	-0.94425000
C	2.74943500	0.93578800	-1.95978600
H	2.30796800	0.83602500	-2.95354300
H	3.04553800	1.97651500	-1.78897400
H	3.66256100	0.34028300	-1.87230800
O	0.54655700	0.42749100	-1.35207800
C	3.32648000	0.74330000	1.08011100
O	4.08271200	1.45212100	0.43017000
Cl	-3.17716400	-0.71568900	0.66591200
Pd	-1.21703600	-0.20953200	-0.41165000
Cl	-2.28006300	0.29402900	-2.43136000
C	3.66761900	0.38866600	2.51867600
H	2.90822100	0.76125200	3.21711800
H	3.75297300	-0.69526700	2.66120100
H	4.62428900	0.85548700	2.75978700
C	-0.51965300	-2.30414500	1.57697300
H	-0.69017000	-3.07274900	0.80967500
H	0.21418200	-2.68185300	2.29928000
H	-1.50862900	-2.16537200	2.04243300
H	1.46150800	-0.68631300	2.27143100

cTS3'-Pd

C	-0.27625200	-1.42521100	0.95386800
C	0.91376300	-0.63947800	1.15768200
C	1.70588300	-0.05015200	0.21722200
C	1.29358000	-0.27441200	-1.21361500
C	2.03803600	0.31705900	-2.37653500
H	1.49904100	0.07599100	-3.29454200
H	2.13815600	1.40129400	-2.26042300
H	3.06038700	-0.07396300	-2.41214900
O	0.28667300	-0.95837700	-1.41622200
C	2.90889100	0.75057700	0.60912800
O	3.70563400	1.12817900	-0.23918700
Cl	-2.92873800	-0.77222000	2.30515400
Pd	-1.76824500	-0.46938600	0.34069200
Cl	-3.24711100	0.59575700	-1.08161500

C	3.13201000	1.08542800	2.07522500
H	2.26178300	1.58695900	2.51482300
H	3.33472000	0.18227200	2.66478000
H	3.99965700	1.74422600	2.14353200
C	-0.33020700	-2.87166500	1.26716100
H	-1.00787600	-3.38958900	0.58096400
H	0.64720400	-3.36529800	1.29463400
H	-0.81444900	-2.94262200	2.25803000
H	1.15380600	-0.51830300	2.21669100

IN4'-Pd

C	-1.16544700	0.14035700	0.93018000
C	-1.40753900	0.36880500	2.32262900
C	-1.48510500	1.36421500	0.24276200
C	-1.90637100	2.25006100	1.21507400
C	-2.44593300	3.62642000	1.16971300
H	-2.24721500	4.07559500	0.19681400
H	-3.53234400	3.58414700	1.32988300
H	-2.01434400	4.23390200	1.97297700
O	-1.85134700	1.67367000	2.44700900
Cl	-4.70573600	0.43616700	1.56326900
Cl	-1.61166800	-2.93411600	1.60726600
Pd	-2.94583200	-1.04558300	1.60162300
C	-1.40119800	1.62352600	-1.21655400
O	-1.60559800	2.74051600	-1.67529700
H	-0.54910400	-0.66413300	0.54968500
C	-0.74927000	-0.16424600	3.55850800
H	0.12281900	0.46274500	3.79039200
H	-1.43448400	-0.11703600	4.41006000
H	-0.42873300	-1.19606200	3.41301800
C	-1.04578900	0.45161000	-2.10939300
H	-0.04680400	0.06564500	-1.86708000
H	-1.75495300	-0.37412400	-1.97289800
H	-1.05933300	0.77887300	-3.15074200

CuI

Cu	0.00000000	0.00000000	-1.55963600
I	0.00000000	0.00000000	0.84614200

C4

Cu	-2.31723200	-1.70670100	3.19606100
I	-3.34938700	-3.85113800	3.65370100
N	-1.52217200	-0.05467000	2.84429500
C	-1.02723200	0.96784400	2.62372500
C	-0.40359300	2.25513300	2.34555200
H	-0.93788500	3.05101000	2.87458100

H	0.63961300	2.24408400	2.67778600
H	-0.43313000	2.45957400	1.27032400
C5			
Cu	-6.16299000	-2.84554300	-3.35924100
I	-6.30903200	-4.35408000	-1.33094600
C	-3.05998000	-4.28713400	-6.37693800
H	-3.49973500	-4.57436500	-7.33752600
H	-2.63255800	-5.17671600	-5.90219300
H	-2.26007000	-3.56142400	-6.55609200
C	-4.08047900	-3.70671400	-5.51148400
N	-4.88758600	-3.26257700	-4.80922400
N	-7.32720600	-1.25365600	-3.48572800
C	-8.09572700	-0.40070500	-3.33178400
C	-9.07102700	0.66145100	-3.11277400
H	-9.56310700	0.51992800	-2.14465500
H	-8.57405100	1.63693600	-3.11915100
H	-9.82954900	0.64486900	-3.90205900
C6			
C	-4.13925600	-0.91977700	-0.91931200
C	-4.30311100	-2.08861500	-1.43145300
C	-2.94053500	-1.45778300	-1.74149100
H	-4.85727500	-3.00421900	-1.57377600
C	-4.55478200	0.29434400	-0.18708500
H	-4.61411100	1.15072200	-0.87059000
H	-5.54000400	0.14510300	0.26567200
H	-3.83418800	0.54880300	0.59917500
C	-2.75819100	-0.83218100	-3.10317800
C	-1.48828800	-0.13005000	-3.49059000
H	-1.69252500	0.54074400	-4.32871700
H	-1.05232000	0.41505900	-2.64803600
H	-0.74149500	-0.87466200	-3.78831700
O	-3.69201200	-0.82733600	-3.92323700
C	-1.71959200	-1.98872100	-1.02149800
O	-0.62355800	-2.01766600	-1.56126100
Cu	-5.43916200	-1.64646300	-3.95914100
I	-7.63624100	-2.67856000	-4.03840700
C	-1.90885100	-2.53331700	0.38416700
H	-2.36075600	-1.78884500	1.05027600
H	-2.57946100	-3.40133400	0.38040100
H	-0.93434100	-2.83337700	0.77397800
C7			
C	8.06861900	-0.23120700	-4.38968100
C	7.44019200	0.80224400	-3.82098200

C	6.55251500	-0.16863200	-4.59301900
C	6.14725400	0.35972700	-5.97398400
C	4.91904300	-0.18948600	-6.65845400
O	6.85437800	1.20629800	-6.49881900
H	4.89152700	0.17289400	-7.68816600
H	4.91387500	-1.28688600	-6.64750000
H	4.01826700	0.13352700	-6.12459700
C	5.53952300	-1.04549500	-3.86282500
O	4.41390200	-0.61176100	-3.68459100
H	7.46925300	1.86976800	-3.63513800
C	9.27791200	-0.73831800	-5.09246400
H	10.18587400	-0.26336400	-4.70957200
H	9.37519300	-1.82458500	-4.99998400
H	9.17890000	-0.49141500	-6.15803000
C	5.94216300	-2.43843300	-3.42805700
H	6.26930700	-3.02035600	-4.30042300
H	6.78603600	-2.41805200	-2.72615100
H	5.09437300	-2.93224600	-2.94858500
Cu	8.19877600	-0.28999100	-2.27042200
I	8.98840500	-1.06440200	-0.11034900

aTS1-Cu

C	-3.04649400	-0.51636200	0.00137500
C	-2.33959200	-1.51482300	-0.61247000
C	-1.61160900	-0.19239000	-0.53502400
H	-1.97548800	-2.50265700	-0.36989900
C	-3.61767000	-0.39599900	1.39627400
H	-3.92827300	0.62991700	1.61630000
H	-4.50215800	-1.03823900	1.48358100
H	-2.90907000	-0.70745300	2.17876800
C	-1.54385400	0.69475500	-1.76414400
C	-0.21519300	1.07387700	-2.36197100
H	-0.36917800	1.42819700	-3.38337800
H	0.24777400	1.86146600	-1.75862600
H	0.47150900	0.21983500	-2.36003300
O	-2.58415900	1.06339500	-2.31013900
C	-0.46528500	-0.06678800	0.44091200
O	0.12378400	0.99980300	0.56346600
Cu	-4.28830900	0.03959900	-1.56940400
I	-3.06555000	-2.45220600	-3.02017100
N	-6.07304700	0.23500600	-2.13801200
C	-7.14846100	0.29244200	-2.56308400
C	-8.49907200	0.35217800	-3.10833900
H	-9.23431200	0.38007800	-2.29741800
H	-8.61592200	1.24901900	-3.72549700
H	-8.68672800	-0.53104900	-3.72792400

C	-0.06891900	-1.26704000	1.28219400
H	0.34405800	-2.05425300	0.63707100
H	0.69057000	-0.96037500	2.00492400
H	-0.92332000	-1.70209000	1.81258000

aTS1'-Cu

C	-2.80031400	-0.64505600	0.42767900
C	-2.28228100	-1.70851900	-0.26098700
C	-1.57821100	-0.32993900	-0.41089100
H	-1.86803600	-2.62092700	0.16359000
C	-3.24541600	-0.29707300	1.81118300
H	-3.40171300	0.77659300	1.93518900
H	-4.18100300	-0.81186000	2.04108500
H	-2.48636200	-0.63820300	2.52979800
C	-1.76096300	0.34145700	-1.77091300
C	-1.41808900	1.79499400	-1.96146300
H	-2.14564700	2.23532100	-2.64848800
H	-1.41152700	2.34184300	-1.01566300
H	-0.41704900	1.87042500	-2.39956500
O	-2.21784500	-0.31174100	-2.70586800
C	-0.22793500	-0.08514500	0.21661400
O	0.64459400	0.49029300	-0.42292200
Cu	-3.34449100	-2.00062100	-1.96964200
I	-5.14582100	0.40073300	-0.80669200
N	-4.43907100	-3.02821500	-3.11186800
C	-5.18491700	-3.55463400	-3.82321100
C	-6.13694700	-4.20232800	-4.71688300
H	-5.79538200	-4.11755900	-5.75366200
H	-6.23736400	-5.26196100	-4.46028000
H	-7.11553800	-3.71944100	-4.62536700
C	0.08168500	-0.59997500	1.61289600
H	1.16602000	-0.68457300	1.71582200
H	-0.27654500	0.12521300	2.35489400
H	-0.38781400	-1.56281100	1.83389200

bTS1-Cu

C	7.88545700	0.62313200	-4.82415400
C	7.97353200	0.83454900	-3.47295700
C	6.73259300	-0.19464700	-4.65790400
C	5.50631700	0.21193600	-5.44508700
C	4.36240800	-0.76105600	-5.62914600
O	5.47138800	1.33065300	-5.94471000
H	3.69670300	-0.36668500	-6.40046700
H	4.71649000	-1.76023900	-5.90649800
H	3.81670900	-0.87678500	-4.68695600
C	6.71113800	-1.43551500	-3.81082100

O	5.68178800	-1.81283400	-3.26456100
Cu	8.93845900	0.08086700	-1.97482300
I	11.22316900	1.12692300	-2.47693800
N	8.57050400	-0.96439400	-0.37324800
C	8.38347200	-1.55364700	0.60456900
C	8.15192800	-2.29414000	1.83863700
H	7.25071800	-2.90857600	1.74455300
H	9.00811200	-2.94249500	2.05145200
H	8.02136600	-1.59517100	2.67114500
H	7.73556300	1.85506900	-3.14276700
C	8.48459100	1.30124400	-6.00269400
H	8.29030400	2.37992100	-5.96709300
H	9.57422400	1.16971900	-5.94967100
H	8.10431900	0.90337400	-6.94571600
C	7.94509800	-2.33035600	-3.81514100
H	8.88348200	-1.80082500	-3.99286100
H	7.99852800	-2.89356400	-2.88024500
H	7.80886800	-3.05407700	-4.63159500

bTS1'-Cu

C	8.22830000	-0.95529500	-4.70850100
C	7.41460100	-0.18338900	-4.02646300
C	6.15561000	-0.60205300	-4.66441700
C	5.83023700	-0.04305500	-5.99618200
C	4.44104600	-0.22505100	-6.57900900
O	6.67703000	0.58790400	-6.63939900
H	3.65692800	0.04576300	-5.86538200
H	4.37487000	0.39786200	-7.47479400
H	4.26352500	-1.27463500	-6.83638700
C	5.26580800	-1.50994900	-3.91630600
O	4.21846300	-1.96319900	-4.38355700
H	7.59597000	0.40694800	-3.13232600
C	8.70974800	-1.49569200	-5.98947700
H	8.13142100	-1.05960100	-6.81543500
H	9.75221300	-1.17655200	-6.11685700
H	8.68300300	-2.59066100	-6.01813400
C	5.65657200	-1.86866700	-2.48471700
H	6.60003600	-2.42506900	-2.45034400
H	5.79559800	-0.96769300	-1.87287400
H	4.86037900	-2.47782000	-2.05045900
Cu	9.58922600	-1.88580600	-3.19083500
I	11.10303300	0.04477500	-2.98426300
C	8.52524700	-6.24138200	-2.50876600
H	9.14812400	-6.87125900	-3.15220400
H	7.47093300	-6.43207300	-2.73429000
H	8.71965600	-6.49889900	-1.46251600

C	8.83778800	-4.83669900	-2.73895800
N	9.08770700	-3.72113100	-2.91953100

dTS1-Cu

C	-3.94077500	-1.20640500	-0.84811300
C	-4.13910800	-2.47405300	-1.15517200
C	-2.57800700	-1.27684100	-1.44003400
H	-3.70694300	-3.45579300	-1.03967000
C	-4.79250700	-0.03245700	-0.51757300
H	-4.86772300	0.63520700	-1.38640000
H	-5.79435600	-0.35091000	-0.21878000
H	-4.33524500	0.54754600	0.29432900
C	-2.52273900	-1.11097600	-2.89282100
C	-1.23053500	-0.75792100	-3.59200100
H	-1.45759500	-0.48806100	-4.62652700
H	-0.70355700	0.05530200	-3.08485300
H	-0.54627500	-1.61344500	-3.57086100
O	-3.55331100	-1.24401900	-3.60068900
C	-1.39012400	-1.43054200	-0.58241800
O	-0.24130700	-1.42745600	-1.02897300
Cu	-5.21444600	-2.52331300	-2.90532000
I	-6.98390900	-3.36067600	-1.17577600
C	-6.63705900	-3.47116500	-7.18797400
H	-6.13565700	-4.36286500	-7.57773000
H	-6.44342500	-2.63139800	-7.86291100
H	-7.71503300	-3.65799300	-7.14851200
C	-6.13595800	-3.16338900	-5.85348900
N	-5.74162500	-2.92096200	-4.79414500
C	-1.61817600	-1.61065700	0.91469100
H	-2.27108000	-0.82968900	1.32276100
H	-2.10004100	-2.57276700	1.12944400
H	-0.65029800	-1.58013500	1.42020100

dTS1'-Cu

C	-3.99357200	-1.51934500	-1.23430900
C	-3.68991800	-2.77565100	-1.27701400
C	-2.64839600	-0.94938000	-1.52703700
C	-1.74830200	-0.88360200	-0.39830700
C	-0.40253000	-0.20140100	-0.51411400
H	0.08111500	-0.22535200	0.46570000
H	0.22289900	-0.70194800	-1.26052700
H	-0.50684200	0.83007700	-0.86516900
O	-2.03522200	-1.37039700	0.73261400
C	-2.33270300	-0.47150300	-2.87705600
O	-1.24898200	0.03747900	-3.18127300
Cu	-3.56270300	-2.16985600	1.86254600

I	-5.27066700	-3.85845100	0.91482300
C	-3.27649900	-0.58038800	6.12222200
H	-4.09761800	0.11731000	6.31662100
H	-2.32525100	-0.06311700	6.28402400
H	-3.35061700	-1.41737500	6.82424200
C	-3.35507300	-1.07106000	4.75091300
N	-3.42058200	-1.46324400	3.66357000
C	-2.90936500	-3.96791100	-1.61298800
H	-2.32775700	-3.79046300	-2.52661100
H	-2.23289900	-4.23423200	-0.79297400
H	-3.57751300	-4.81727600	-1.78819900
H	-4.90451300	-1.01972500	-0.91937000
C	-3.41557500	-0.61594400	-3.94361100
H	-3.59915700	-1.67080700	-4.18424600
H	-4.37251200	-0.19653600	-3.60873400
H	-3.08402200	-0.09856500	-4.84676900

IN1-Cu

C	-3.83404100	-1.53662800	-1.63056400
C	-4.23450300	-2.81564400	-1.67339400
C	-2.35154900	-1.28351400	-1.64737100
H	-3.55179600	-3.65475500	-1.73510800
C	-4.73729200	-0.33194100	-1.51843800
H	-4.45650700	0.41546400	-2.27010500
H	-5.79756400	-0.57531600	-1.63060500
H	-4.59672400	0.14469800	-0.53889700
C	-1.75591800	-0.88596300	-2.84851000
C	-0.31243600	-0.45495100	-2.96280100
H	-0.15293500	-0.05170700	-3.96685400
H	-0.04597100	0.28302200	-2.20170300
H	0.35820700	-1.30533700	-2.79650100
O	-2.39958300	-0.84027200	-3.98435900
C	-1.59785800	-1.40608000	-0.39670100
O	-0.37521000	-1.22993700	-0.31203300
Cu	-3.95691400	-1.66857000	-4.49682500
I	-6.27047300	-3.52943600	-1.46758000
C	-7.64516600	-3.57444300	-6.07330800
H	-7.43160700	-4.21133100	-6.93781800
H	-8.38202300	-2.81717900	-6.36013800
H	-8.05903800	-4.18918000	-5.26723900
C	-6.42291100	-2.93057300	-5.61296700
N	-5.45343800	-2.42577900	-5.23586200
C	-2.35603100	-1.78852400	0.87712500
H	-3.30813600	-1.25737600	0.98644800
H	-2.58573700	-2.86158400	0.88086200
H	-1.71265900	-1.56999700	1.73293200

TS2-Cu

C	-2.49357900	-0.61660400	0.02041600
C	-2.80176500	-1.45074600	-1.06195700
C	-1.56859400	0.48908900	-0.11581600
H	-2.04916400	-1.65388700	-1.81845000
C	-3.23040100	-0.80218400	1.33255600
H	-3.10261300	0.05053600	2.00092500
H	-4.30155600	-0.92822600	1.14092900
H	-2.90423600	-1.71266300	1.85055800
C	-1.37779100	1.12808800	-1.39322100
C	-0.43836200	2.30361400	-1.58101300
H	-0.24233800	2.40423100	-2.65204200
H	-0.89805900	3.22573700	-1.20945600
H	0.49803200	2.18667300	-1.02992300
O	-1.99415500	0.76180600	-2.44363200
C	-0.88606900	1.03774800	1.07658500
O	-0.55422800	2.22190400	1.17753000
Cu	-3.85397500	-0.15815300	-2.25998300
I	-3.95209700	-3.29951600	-0.78383500
N	-5.41893400	0.38334700	-3.15259900
C	-6.37762800	0.71796200	-3.70872800
C	-7.58596100	1.13716000	-4.40794500
H	-8.47308600	0.81994300	-3.84997900
H	-7.59993200	2.22713400	-4.51105600
H	-7.61346300	0.68636800	-5.40535600
C	-0.44694200	0.09415400	2.20145700
H	-0.65745500	-0.96168200	2.01784000
H	0.63629200	0.21840000	2.31477700
H	-0.90198900	0.39875900	3.15099700

IN2-Cu

C	-2.48082700	-0.73351500	0.08193000
C	-2.84471700	-1.58669400	-0.99567300
C	-1.65033800	0.41321500	-0.11178800
H	-2.09478700	-1.79158400	-1.75603400
C	-3.09087500	-0.98305100	1.44614100
H	-2.97939700	-0.13089600	2.11801600
H	-4.16008000	-1.19247900	1.33621100
H	-2.65558700	-1.87153400	1.92057200
C	-1.48300600	0.99367300	-1.43201800
C	-0.61550700	2.21672200	-1.66928300
H	-0.38080600	2.25608400	-2.73643400
H	-1.15374900	3.12752600	-1.38542400
H	0.30486200	2.20514600	-1.07936600
O	-2.06188800	0.52273600	-2.44962600

C	-1.04845500	1.11584800	1.05258200
O	-0.94825600	2.34181600	1.10643300
Cu	-4.01641100	-0.45018100	-2.13266400
I	-3.79617500	-3.54246600	-0.57041200
N	-5.45160200	0.30636900	-3.08577800
C	-6.31316800	0.78493700	-3.69212000
C	-7.39970000	1.38637600	-4.45514000
H	-7.81199700	2.23937800	-3.90640100
H	-7.02798600	1.73388400	-5.42455600
H	-8.19430500	0.65134000	-4.61990200
C	-0.39938300	0.30204700	2.17430200
H	-0.53545800	-0.77754400	2.08771800
H	0.67638700	0.51562400	2.13836200
H	-0.76060300	0.64682600	3.14946700

TS3-Cu

C	-2.39476700	-0.33035100	-0.11217300
C	-2.83255400	-0.83420200	-1.39333400
C	-1.34159100	0.58044900	-0.04967900
H	-2.14933600	-1.41174100	-2.00526000
C	-3.19919500	-0.66207100	1.12764500
H	-3.03565400	0.05676400	1.93254900
H	-4.26481600	-0.67535800	0.88476100
H	-2.95937100	-1.66911500	1.48800600
C	-0.77624700	1.03299700	-1.32578100
C	0.36169400	2.02971900	-1.39878900
H	0.75171500	2.03467700	-2.41940100
H	0.00263100	3.03029900	-1.13574000
H	1.16320800	1.79106100	-0.69178500
O	-1.24364400	0.57079800	-2.37929900
C	-0.83868000	1.17270400	1.22892300
O	-0.59599100	2.37247700	1.31517000
Cu	-4.49367400	-0.44217200	-2.21001800
I	-4.36255100	-3.05080900	-1.08818200
N	-6.00972900	0.17758000	-3.13318200
C	-6.95039600	0.51448000	-3.71538500
C	-8.13483000	0.93582800	-4.45204200
H	-8.54572400	1.84850100	-4.00839500
H	-7.87206500	1.13478000	-5.49612100
H	-8.89518000	0.14869300	-4.41903700
C	-0.49585700	0.26604700	2.40742800
H	-0.76715500	-0.78042800	2.25774700
H	0.59002800	0.32561000	2.55492900
H	-0.96308300	0.64638500	3.32256100