

## Supporting Information

### **C–N bond Metathesis: Mechanistic insight into Palladium-Catalyzed Ring-Closing Using Amino Species**

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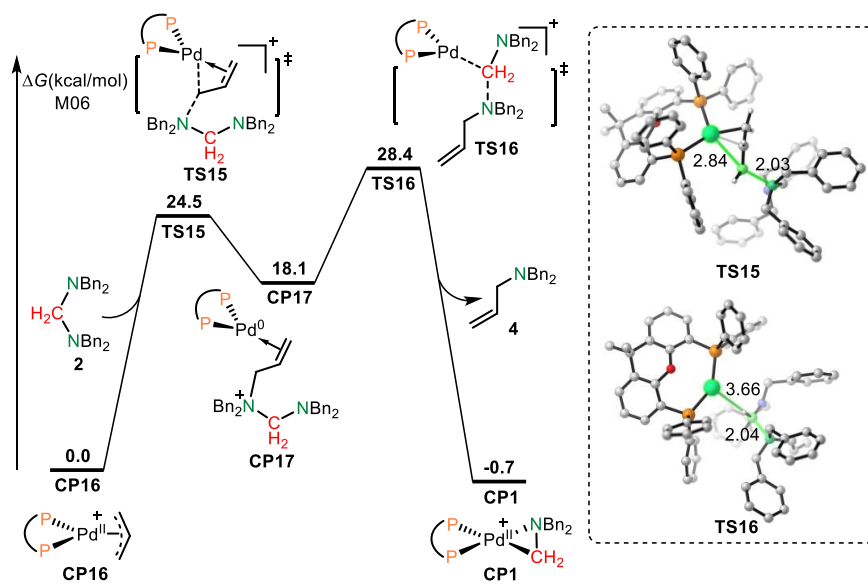
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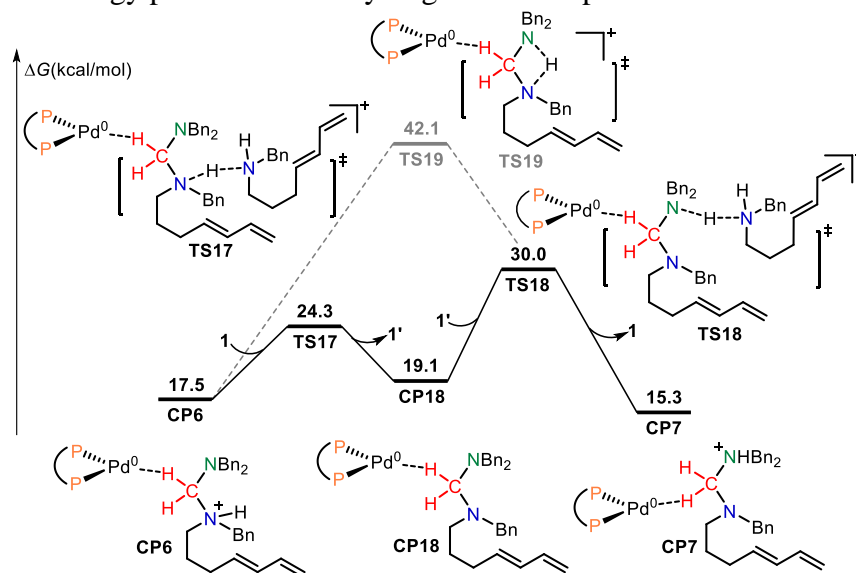
1. The calculated potential energy profiles for formation of active intermediate **CP1**.



**Figure S1.** The calculated potential energy profiles for formation of active intermediate **CP1** from allyl palladium complex.

The calculated potential energy profiles for formation of active intermediate **CP1** from allyl palladium complex are shown in Figure S1. The  $S_N2$  type reductive elimination of allyl palladium complex **CP16** with aminal occurs via transition state **TS15** to form amino cation Pd(0) intermediate **CP17**. The subsequent oxidative addition of **CP17** onto the Pd(0) center occurs via transition state **TS16** with an energy barrier of 10.3 kcal/mol to generate Huang-complex (Xantphos)Pd-(CH<sub>2</sub>NBn<sub>2</sub>)<sup>+</sup> **CP1** with concomitant release of an amine. The overall activation free energy for this transformation is 28.4 kcal/mol, while the palladacycle-complex **CP1** was generated with an exothermic energy of 0.7 kcal/mol.

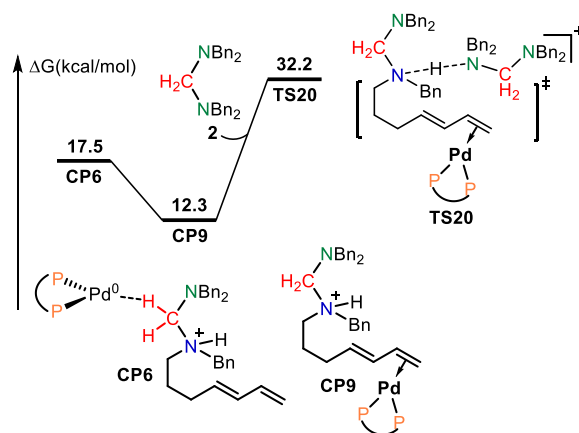
## 2. The calculated free energy profiles for the hydrogen transfer process from **CP6**.



**Figure S2.** The calculated free energy profiles for the hydrogen transfer process from **CP6**.

The calculated free energy profiles for the substrate **1** promoted rapid hydrogen transfer process from **CP6** are shown in Figure S2. The intermolecular hydrogen transfer from **CP6** to substrate **1** occurs via transition state **TS17** with an energy barrier of 6.8 kcal/mol, where complex **CP18** and **1'** were generated. The following intermolecular hydrogen transfer from **1'** to the terminal amino in **CP18** gives the amino cation intermediate **CP7** via transition state **TS18** with an activation free energy of 30.0 kcal/mol. The free energy of **TS18** is 9.6 kcal/mol higher than that of **TS8**, which is indicated that substrate **1** promoted rapid hydrogen transfer process from **CP6** is unfavorable. The direct

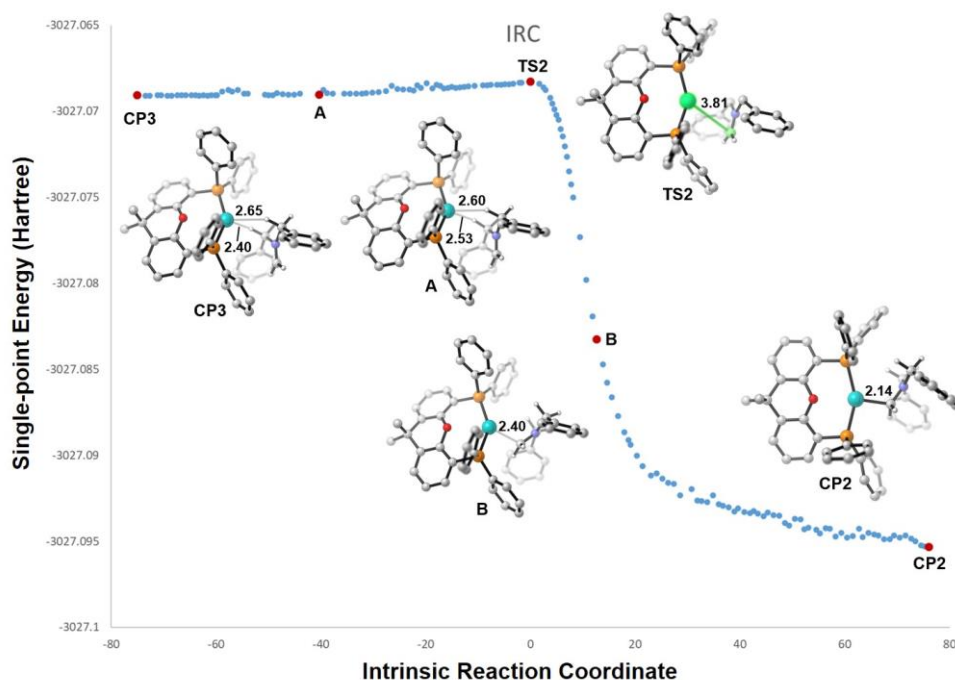
intramolecular hydrogen transfer of **CP6** has also been calculated. The calculated results showed that the free energy of the direct intramolecular hydrogen transfer transition state **TS19** is 21.7 kcal/mol higher than that of transition state **TS8**.



**Figure S3.** The calculated free energy profiles for the hydrogen transfer process promoted by aminal **2**.

The hydrogen transfer process promoted by aminal **2** has also been calculated. The calculated aminal **2** promoted hydrogen transfer process occurs via transition state **TS20** with a free energy barrier of 19.9 kcal/mol, which is 11.8 kcal/mol higher than that of **TS8**. The calculated results showed that this hydrogen transfer process is also unfavorable.

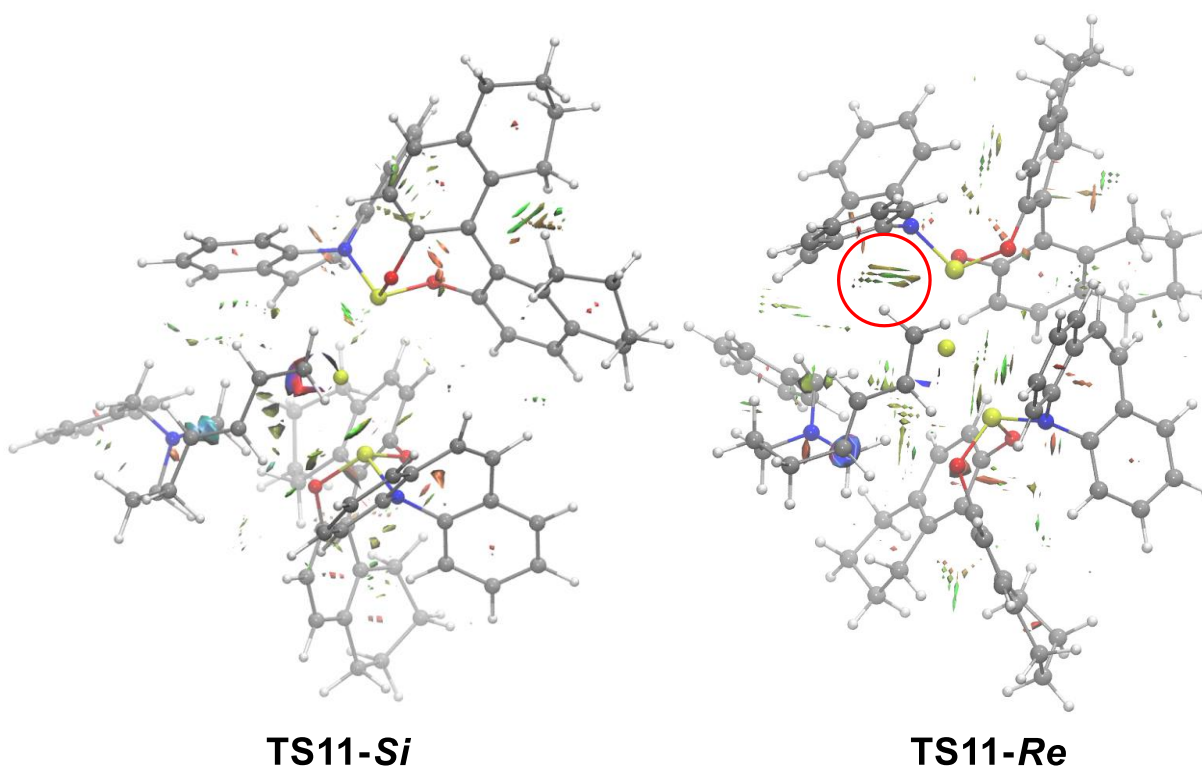
### 3. Intrinsic reaction coordinate (IRC) calculation of transition state **TS3**.



**Figure S4.** Intrinsic reaction coordinate (IRC) calculation of transition state **TS3**. The abscissa values are the IRCs; the ordinate values are the Single-point energies. The geometry information of some selected points on IRC profiles are given. The values of bond lengths are given by ångstrom. Hydrogen atoms are omitted for clarity.

We performed intrinsic reaction coordinate (IRC) calculation to further confirm which two intermediates are linked by the transition state **TS2**. The IRC calculation of transition state **TS2** clearly revealed that intermediates **CP2** and **CP3** are linked by that transition state. In **CP3**, the Pd(0) is bonded to imine cations by two hydrogen bonds.

#### 4. Higher resolution NCI plots copies for **TS11-Si** and **TS11-Re**.



**Figure S5.** Higher resolution NCI plots copies for **TS11-Si** and **TS11-Re**.

#### 5. Complete reference for 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, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.;

Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; 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, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian 09, revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

## 6. Benchmarks for some frequently used calculation methods.

We performed benchmarks for some frequently used calculation methods. The calculated results shown that the relative free energies between **CP1** and **CP2**, calculated by most methods tested, stays roughly the same. The calculated results indicated that this method used herein is reliable. Thus, a commonly used combination of computational methods, M06 with the SMD solvation model for single point calculations and B3LYP for geometry optimization, was chosen in the present study.

Method for Geometry Optimization	Method for energy calculation	CP1	CP2
B3-LYP/SDD-6-31G(d)	B3-LYP/SDD-6-311+G(d)/SMD	0.0	1.5
B3-LYP/SDD-6-31G(d)	B3-LYP-D3/SDD-6-311+G(d)/SMD	0.0	10.5
B3-LYP/SDD-6-31G(d)	M06/SDD-6-311+G(d)/SMD	0.0	10.7
B3-LYP/SDD-6-31G(d)	M06-L/SDD-6-311+G(d)/SMD	0.0	9.0
B3-LYP/SDD-6-31G(d)	M11/SDD-6-311+G(d)/SMD	0.0	15.4
B3-LYP/SDD-6-31G(d)	M11-L/SDD-6-311+G(d)/SMD	0.0	8.5
B3-LYP-D3/SDD-6-31G(d)	B3-LYP-D3/SDD-6-311+G(d)/SMD	0.0	not got
BP86/SDD-6-31G(d)	BP86/SDD-6-311+G(d)/SMD	0.0	-0.3
M06/SDD-6-31G(d)	M06/SDD-6-311+G(d)/SMD	0.0	not got
M06-L/SDD-6-31G(d)	M06-L/SDD-6-311+G(d)/SMD	0.0	12.2
M11/SDD-6-31G(d)	M11/SDD-6-	0.0	15.8

	311+G(d)/SMD		
M11-L/SDD-6-31G(d)	M11-L/SDD-6-311+G(d)/SMD	0.0	12.0
wB97xd/SDD-6-31G(d)	wB97xd/SDD-6-311+G(d)/SMD	0.0	17.3
B3-LYP-D3/SDD-6-31G(d) in solvent	B3-LYP-D3/SDD-6-311+G(d)/SMD	0.0	11.5
BP86/SDD-6-31G(d)/SMD in solvent	BP86/SDD-6-311+G(d)/SMD	0.0	1.8
M06/SDD-6-31G(d) /SMD in solvent	M06 SDD-6-311+G(d)/SMD	0.0	8.9
M06-L/SDD-6-31G(d) /SMD in solvent	M06-L SDD-6-311+G(d)/SMD	0.0	10.5
M11/SDD-6-31G(d) /SMD in solvent	M11 SDD-6-311+G(d)/SMD	0.0	15.3
M11-L/SDD-6-31G(d) /SMD in solvent	M11-L SDD-6-311+G(d)/SMD	0.0	11.6
wB97xd/SDD-6-31G(d) /SMD in solvent	wB97xd SDD-6-311+G(d)/SMD	0.0	18.9

## 7. B3-LYP and M06 absolute calculation energies, enthalpies, and free energies.

**Table S1.** B3-LYP and M06 absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-M06})}^1$	$H_{(\text{corr-M06})}^2$	$G_{(\text{corr-M06})}^3$	$E_{(\text{solv-M06-L})}^4$	IF <sup>5</sup>
<b>CP1</b>	-3027.109567	0.928553	0.784786	-3025.981620	-
<b>TS1</b>	-3027.095707	0.927005	0.779600	-3025.958443	-90.9
<b>CP2</b>	-3027.098831	0.928026	0.778727	-3025.958569	-
<b>TS2</b>	-3027.068278	0.926896	0.777279	-3025.937679	-41.1
<b>CP3</b>	-3027.069124	0.927442	0.776498	-3025.938967	-
<b>CP4</b>	-635.730059	0.289290	0.231355	-635.446527	-
Pd <sup>0</sup>	-2391.306824	0.636487	0.523833	-2390.466712	-
<b>1</b>	-599.628510	0.315521	0.253209	-599.303820	-
<b>TS3</b>	-1235.373261	0.606118	0.505437	-1234.759633	-39.2
<b>CP5</b>	-1235.386170	0.609965	0.514058	-1234.784787	-

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<b>TS4</b>	-3626.705176	1.244916	1.052061	-3625.252259	-25.2
<b>CP6</b>	-3626.721577	1.247660	1.059509	-3625.279144	-
<b>TS5</b>	-3626.713659	1.246048	1.054247	-3625.263658	-64.9
<b>CP7</b>	-3626.716524	1.248384	1.056380	-3625.279381	-
<b>TS6</b>	-3626.715787	1.246490	1.055064	-3625.267183	-99.5
<b>CP8</b>	-3029.484080	0.973552	0.820365	-3028.339957	-
HNBn <sub>2</sub>	-597.248356	0.269956	0.214043	-596.939236	-
<b>CP9</b>	-3626.726338	1.248158	1.061985	-3625.289811	-
<b>TS7</b>	-4226.365413	1.561689	1.335213	-4224.608744	-1154.6
<b>1'</b>	-600.014918	0.330869	0.267844	-599.757196	-
<b>CP10</b>	-3626.315871	1.233216	1.044416	-3624.842235	-
<b>TS8</b>	-4226.362144	1.562002	1.337628	-4224.603229	-1151.3
<b>CP11</b>	-3626.723419	1.248119	1.060761	-3625.292000	-
<b>TS9</b>	-3626.686929	1.242701	1.057866	-3625.246886	-1673.3
<b>CP12</b>	-3029.458439	0.973226	0.822966	-3028.329313	-
<b>TS10</b>	-3029.422595	0.972255	0.822925	-3028.294287	-227.0
<b>CP13</b>	-3029.448288	0.973653	0.824652	-3028.321895	-
<b>TS11</b>	-3029.445793	0.972467	0.825014	-3028.323091	-51.1
<b>CP14</b>	-3029.491779	0.974996	0.827157	-3028.358698	-
<b>TS12</b>	-3029.403559	0.971874	0.824372	-3028.269555	-328.3
<b>TS13</b>	-4262.062292	1.527553	1.316754	-4260.317570	-254.5
<b>CP15</b>	-4262.064778	1.529579	1.319302	-4260.325776	-
<b>TS14</b>	-4262.075937	1.527672	1.30936	-4260.311599	-58.7
<b>3</b>	-1235.001352	0.596480	0.503187	-1234.357240	-
<b>TS11-Si</b>	-4486.660755	1.520162	1.314645	-4484.903353	-52.0
<b>TS11-Re</b>	-4486.657888	1.520809	1.318718	-4484.903796	-129.7
<b>CP16</b>	-2508.447768	0.713898	0.595662	-2507.577740	-
<b>TS15</b>	-3741.037656	1.265963	1.079310	-3739.533856	-207.1
<b>2</b>	-1232.605325	0.549145	0.458391	-1231.969940	-
<b>CP17</b>	-3741.044161	1.268467	1.084219	-3739.548940	-

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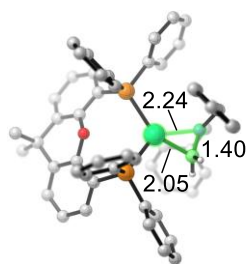


<b>TS16</b>	-3741.019842	1.266795	1.073457	-3739.521770	-41.1
<b>4</b>	-713.947944	0.334927	0.271212	-713.569076	-
<b>TS17</b>	-4226.344933	1.562357	1.332527	-4224.591853	-1021.2
<b>CP18</b>	-3626.300036	1.233215	1.040127	-3624.818341	-
<b>TS18</b>	-4226.341208	1.562735	1.333738	-4224.584049	-1209.1
<b>TS19</b>	-3626.676775	1.243425	1.054147	-3625.234543	-1688.2
<b>TS20</b>	-4859.319397	1.795948	1.547085	-4857.254753	-1375.0

<sup>1</sup>The electronic energy calculated by B3-LYP. <sup>2</sup>The thermal correction to enthalpy calculated by B3-LYP. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3-LYP. <sup>4</sup>The electronic energy calculated by M06 in dichloroethane solvent. <sup>5</sup>The B3-LYP calculated imaginary frequencies for the transition states.

## 8. B3-LYP geometries for all the optimized compounds and transition states.

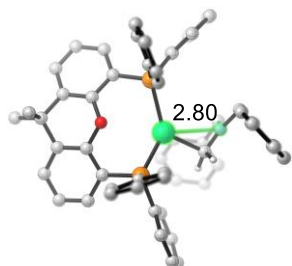
### CP1



Pd	0.79949600	0.39353300	0.47252500	C	3.37085800	-4.47075500	2.73819000
P	0.33084200	-2.03500600	0.16563600	C	3.42505700	-4.54594500	1.34664000
P	-0.65560300	1.69712200	-0.86929000	C	2.49402300	-3.85598500	0.56394400
O	-2.16315700	-0.88024600	-0.63811900	C	-0.50037700	3.50072400	-0.48569800
N	2.43920600	0.82469500	1.93245000	C	-0.74307300	3.92016400	0.83541100
C	-1.33177900	-2.65858600	0.66881600	C	-0.64347400	5.26680500	1.18121300
C	-1.57706300	-3.77637800	1.47820400	C	-0.28894400	6.21513300	0.21684500
C	-2.88682300	-4.13944900	1.79394100	C	-0.04481400	5.80825000	-1.09438800
C	-3.96658400	-3.40894400	1.29389000	C	-0.15402000	4.45936400	-1.44771000
C	-3.76611200	-2.30281500	0.45968500	C	-0.27564600	1.58763100	-2.66840800
C	-2.44156000	-1.95764100	0.17783900	C	-1.27484100	1.47428200	-3.64488400
C	-4.88192000	-1.50551200	-0.22881200	C	-0.93410600	1.41201700	-4.99840700
C	-4.40186400	-0.05286900	-0.36513000	C	0.40348200	1.47499900	-5.39065600
C	-3.03705700	0.18201500	-0.57729700	C	1.40599100	1.59184000	-4.42349600
C	-2.48724200	1.46238300	-0.73904800	C	1.07049900	1.63788700	-3.07047400
C	-3.37760400	2.54888600	-0.75080300	C	1.91201000	1.92973000	1.25247500
C	-4.74303600	2.34777500	-0.56270800	C	2.12677200	0.64109600	3.39130000
C	-5.24561200	1.06219000	-0.35508900	C	0.81369500	1.21989800	3.86156100
C	-5.08838900	-2.09029900	-1.65646200	C	-0.39961600	0.54615400	3.65697700
C	-6.21064700	-1.59896100	0.54225700	C	-1.60190600	1.09363100	4.10739500
C	0.50178900	-2.70515200	-1.54314500	C	-1.60694700	2.32094800	4.77605300
C	0.02936300	-3.98494300	-1.88060100	C	-0.40421600	2.99574700	4.99463200
C	0.18529200	-4.47362200	-3.17712500	C	0.79661900	2.44646400	4.53973500
C	0.80850100	-3.69005400	-4.15290700	C	3.84208600	0.36180600	1.65346900
C	1.27439500	-2.41597800	-3.82748600	C	4.32148600	0.52165700	0.23232500
C	1.12198900	-1.92572000	-2.52810500	C	4.12489600	-0.50096000	-0.70519400
C	1.49796300	-3.07003800	1.16351400	C	4.59310200	-0.36478900	-2.01331800
C	1.45565200	-3.00051400	2.56885700	C	5.26665200	0.79696900	-2.39852200
C	2.37715200	-3.69982300	3.34874300	C	5.47732600	1.81863300	-1.46901800
				C	5.01109800	1.67792000	-0.16074100
				H	-0.74855000	-4.35668100	1.86959500
				H	-3.06835800	-5.00234100	2.42764100
				H	-4.97382400	-3.71911000	1.54964400
				H	-2.99966300	3.55512500	-0.88944800
				H	-5.41893700	3.19744000	-0.56976400
				H	-6.31062400	0.93359500	-0.19569100
				H	-5.40636400	-3.13701800	-1.59549600
				H	-5.85984100	-1.52385200	-2.18982100
				H	-4.16506400	-2.04745500	-2.24259300

H	-6.12408700	-1.19313900	1.55574100
H	-7.00346900	-1.05679800	0.01921100
H	-6.54534400	-2.63785700	0.61305300
H	-0.46427200	-4.59913100	-1.13311800
H	-0.18334600	-5.46450000	-3.42711100
H	0.92332300	-4.07127800	-5.16371800
H	1.74273900	-1.79315700	-4.58425700
H	1.47335500	-0.92949100	-2.28269700
H	0.68299400	-2.41600300	3.06130100
H	2.31579500	-3.64736900	4.43243700
H	4.09041000	-5.01333200	3.34435200
H	4.18721000	-5.15027000	0.86272800
H	2.54105900	-3.94102200	-0.51676700
H	-1.02265000	3.19343200	1.59458900
H	-0.84019100	5.57410500	2.20453800
H	-0.20749200	7.26403100	0.48721400
H	0.22421400	6.53935200	-1.85159000
H	0.02507400	4.16249500	-2.47547200
H	-2.31962300	1.43756400	-3.35370800
H	-1.71773600	1.32036400	-5.74509900
H	0.66474600	1.43400500	-6.44431900
H	2.45005600	1.64193400	-4.71995400
H	1.85930800	1.71223700	-2.32602600
H	1.33209600	2.62842600	1.84572100
H	2.56027900	2.37757300	0.50493400
H	2.94788000	1.10510700	3.95421700
H	2.17445600	-0.43601900	3.57454300
H	-0.40932100	-0.41153400	3.14433200
H	-2.53223900	0.55662200	3.94582500
H	-2.54165500	2.74169400	5.13545100
H	-0.39727600	3.94214500	5.52773000
H	1.73143500	2.97164200	4.72283000
H	3.87859400	-0.68889900	1.95606900
H	4.50039500	0.92401700	2.33006600
H	3.62313100	-1.41487100	-0.40062300
H	4.44140300	-1.17095600	-2.72547100
H	5.64378100	0.89803500	-3.41239600
H	6.01718600	2.71613600	-1.75678200
H	5.19960300	2.46627000	0.56493800

### TS1

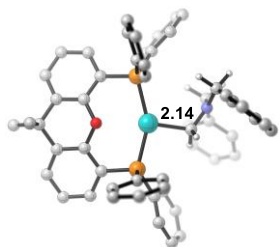


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P	-0.39337900	-2.08146200	-0.59149000
O	2.29599100	-0.72691800	-0.22519800
N	-2.72197600	1.33134600	1.23458400
C	2.78476200	1.44750200	0.63744700
C	3.69481200	2.30878600	1.26917600
C	4.94879400	1.85484500	1.66826700
C	5.32527300	0.53634000	1.41704700
C	4.46306900	-0.35300500	0.76713700
C	3.19382900	0.11968800	0.40637200
C	4.86540700	-1.76929500	0.34372400
C	3.61310200	-2.65064200	0.39049000

C	2.38022200	-2.08338000	0.03997400
C	1.20254100	-2.84764300	-0.07582900
C	1.28300900	-4.22145200	0.20117200
C	2.48840900	-4.80127300	0.58721200
C	3.63921300	-4.01995600	0.67722700
C	5.35976000	-1.71035300	-1.13198000
C	6.00033700	-2.33195400	1.21845900
C	1.45729800	2.62734500	-1.64046500
C	2.46419900	3.57002700	-1.91060200
C	2.70884400	3.98419700	-3.21884200
C	1.95946300	3.45568400	-4.27482100
C	0.96611600	2.51093800	-4.01814200
C	0.71493900	2.09872600	-2.70656600
C	0.80170400	3.53872400	1.06537200
C	0.86177800	3.46930700	2.46994600
C	0.51182400	4.56924100	3.25316300
C	0.07778400	5.75271900	2.64879300
C	0.00275100	5.82867100	1.25804200
C	0.36299900	4.73173200	0.46951000
C	-1.66838200	-3.28765800	-0.03970400
C	-1.94854600	-3.37540400	1.33647400
C	-2.92385300	-4.25547400	1.80388200
C	-3.64079000	-5.04988200	0.90494600
C	-3.37460300	-4.96327900	-0.46213200
C	-2.39324700	-4.08836900	-0.93525700
C	-0.40286100	-2.19121900	-2.43049300
C	0.44580400	-3.05520300	-3.13859900
C	0.38528800	-3.11658100	-4.53274800
C	-0.52555000	-2.32428300	-5.23333200
C	-1.37610100	-1.46249100	-4.53601800
C	-1.31026800	-1.38981700	-3.14470000
C	-2.51423900	0.11705000	0.65707700
C	-2.49013200	1.59437700	2.67812400
C	-2.29779600	0.36815100	3.53914300
C	-1.01239800	-0.10698900	3.83439300
C	-0.83728200	-1.22683300	4.65025700
C	-1.94958700	-1.88469400	5.18161900
C	-3.23527900	-1.41878800	4.89402000
C	-3.40632000	-0.29858400	4.07894900
C	-3.10600900	2.53796700	0.45981700
C	-3.80932800	2.25787900	-0.84858300
C	-3.17639600	2.52437900	-2.06864200
C	-3.83718700	2.29119700	-3.27805800
C	-5.13684000	1.78305200	-3.27769100
C	-5.77796400	1.51581800	-2.06409100
C	-5.11992400	1.75691100	-0.85880400
H	3.41194700	3.33747900	1.46539200
H	5.63791600	2.53064600	2.16557100
H	6.31175700	0.20535400	1.72109200
H	0.39186500	-4.83471500	0.12318000
H	2.53392000	-5.86315000	0.80867200
H	4.57224900	-4.49114900	0.96443000
H	6.24280900	-1.06656200	-1.21012200
H	5.62818800	-2.71332300	-1.48199700
H	4.58739700	-1.31120100	-1.79712400
H	5.71116500	-2.39648100	2.27274700
H	6.29608500	-3.32821800	0.87826800
H	6.89458400	-1.70754500	1.14181200
H	3.06111100	3.97858700	-1.10036900
H	3.48808600	4.71492700	-3.41623500
H	2.15667000	3.77657000	-5.29377800
H	0.39088700	2.08544400	-4.83567000
H	-0.04670800	1.34930900	-2.50885500
H	1.20607100	2.55910200	2.95451600

H	0.58135000	4.50272800	4.33544100	C	-1.01144900	-4.10635400	-4.12690300
H	-0.19480500	6.60889300	3.25891200	C	-0.51684800	-2.81282100	-3.95744500
H	-0.32720100	6.74625100	0.77895700	C	-0.38313700	-2.27768200	-2.67358600
H	0.31495000	4.81460000	-0.61160800	C	0.08984100	-3.52116300	1.23223500
H	-1.39687300	-2.76430500	2.04707100	C	-0.11182700	-3.41314900	2.62059400
H	-3.12628100	-4.31341800	2.86942100	C	0.50711100	-4.30221100	3.49823700
H	-4.40387700	-5.73186300	1.26906300	C	1.34518500	-5.30725500	3.00637300
H	-3.92691600	-5.57995300	-1.16555700	C	1.55697900	-5.41811300	1.63224300
H	-2.19056700	-4.03728800	-1.99995200	C	0.93541400	-4.53113200	0.74869200
H	1.15471600	-3.68142700	-2.60629200	C	0.59189600	3.65132200	0.46680900
H	1.05021000	-3.78727500	-5.06954000	C	1.08793200	3.43622000	1.76421600
H	-0.57168100	-2.37661900	-6.31735800	C	1.81737500	4.43221300	2.41323100
H	-2.08863500	-0.84314600	-5.07379400	C	2.06650300	5.64789600	1.77195100
H	-1.96599700	-0.70483900	-2.61341200	C	1.58369200	5.86644000	0.48008800
H	-2.58794200	-0.72759500	1.33648600	C	0.85050100	4.87419000	-0.17311600
H	-3.01663400	-0.01507500	-0.29793900	C	-0.44156500	2.74731900	-2.11376700
H	-3.36499700	2.15511300	3.03103200	C	-1.61389200	3.19004900	-2.74337900
H	-1.62745100	2.26536700	2.76944400	C	-1.61291000	3.47926700	-4.11053800
H	-0.14458100	0.40606200	3.42784300	C	-0.44491400	3.33591900	-4.85967700
H	0.16520400	-1.57725400	4.87954200	C	0.72884700	2.89779000	-4.23951200
H	-1.81468200	-2.74789600	5.82726600	C	0.72994700	2.59869200	-2.87836900
H	-4.10338600	-1.91731900	5.31575100	C	2.18808300	0.22868500	0.12124500
H	-4.40884300	0.06776600	3.86967400	C	2.99474100	-1.29550400	1.88111500
H	-2.21486500	3.15449500	0.29209700	C	3.29266900	-0.17269800	2.85537600
H	-3.76774200	3.11628100	1.11664200	C	2.37645300	0.14916200	3.86372800
H	-2.16582100	2.92501700	-2.07379900	C	2.66402600	1.14796300	4.79899400
H	-3.33900700	2.51661400	-4.21697700	C	3.87366800	1.84048200	4.72910600
H	-5.65418600	1.60602400	-4.21630500	C	4.79337200	1.53031100	3.72191200
H	-6.79419500	1.13226600	-2.05782800	C	4.50540500	0.52945700	2.79532000
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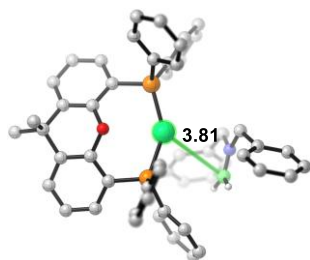
## CP2



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P	-0.37264900	2.30945900	-0.32721800	C	4.21100900	-1.09737700	-4.17731900
O	-2.50091600	0.17441300	0.01130500	C	5.35817000	-0.32103900	-4.01270100
N	2.93748700	-0.86791500	0.47067500	C	5.81722900	-0.02773800	-2.72485100
C	-2.39059300	-2.13099600	0.66814000	C	5.13357000	-0.51231500	-1.61091200
C	-3.04079300	-3.25988600	1.19092600	H	-2.48731800	-4.18353500	1.31996000
C	-4.37604700	-3.20507200	1.57442300	H	-4.86006400	-4.08367800	1.98961500
C	-5.09408800	-2.02198200	1.41478800	H	-6.13782800	-1.99959000	1.70522900
C	-4.50005500	-0.87625000	0.87558500	H	-1.89479200	4.63737400	0.64032600
C	-3.14248000	-0.94853800	0.53082300	H	-4.23502800	4.93680200	1.39703700
C	-5.28332800	0.40045300	0.55867100	H	-5.78285000	3.02430500	1.40250800
C	-4.33394500	1.59167100	0.70831200	H	-6.39994800	-0.52805500	-1.08350300
C	-2.98954200	1.43610600	0.34614300	H	-6.27854700	1.24226800	-1.20468700
C	-2.09675900	2.52306100	0.28378800	H	-4.88134200	0.22400800	-1.60484100
C	-2.56875000	3.78728300	0.66665900	H	-6.27987200	0.59306700	2.50852100
C	-3.88366300	3.95691400	1.08913200	H	-7.09685300	1.44428800	1.18099300
C	-4.75478200	2.86903600	1.09693500	H	-7.21901300	-0.29408100	1.28972800
C	-5.73687200	0.33039500	-0.92994700	H	-1.55174500	-4.92678400	-0.87294000
C	-6.53471200	0.54430100	1.44466300	H	-1.76920900	-5.86928500	-3.13896500
C	-0.74880300	-3.03070600	-1.54697900	H	-1.11312800	-4.52477500	-5.12415500
C	-1.25622900	-4.32853100	-1.72931300	H	-0.23578500	-2.21708500	-4.82133600
C	-1.38045300	-4.86309200	-3.01082700	H	-0.00339700	-1.26748600	-2.54218200
				H	-0.76345100	-2.63928300	3.01745300
				H	0.33294700	-4.21153000	4.56670300
				H	1.82610600	-5.99980800	3.69093600
				H	2.20192800	-6.19971800	1.24062100
				H	1.10340300	-4.63918900	-0.31806200
				H	0.90534900	2.49131500	2.27006300
				H	2.20101200	4.24892200	3.41224400
				H	2.63989700	6.42104600	2.27538700
				H	1.77735900	6.80979500	-0.02251500
				H	0.48216300	5.05222700	-1.17854100
				H	-2.52779900	3.31407200	-2.17169500

H	-2.52751900	3.82145800	-4.58647000
H	-0.44699000	3.56468600	-5.92150700
H	1.64288300	2.78549500	-4.81565100
H	1.64979400	2.25726900	-2.41041200
H	2.24434400	1.02815600	0.85852700
H	2.38914000	0.55559600	-0.89894300
H	3.78250700	-2.05421900	1.94244300
H	2.05669900	-1.78741500	2.16569700
H	1.43809500	-0.39714900	3.92703000
H	1.94809300	1.37608900	5.58394600
H	4.10605800	2.60961300	5.46054600
H	5.73989600	2.06082900	3.66754800
H	5.22953500	0.28507200	2.02179500
H	2.34831400	-2.38492600	-0.88831200
H	3.89107400	-2.62215800	-0.07570700
H	2.62994900	-2.18232700	-3.19192300
H	3.84948400	-1.33213100	-5.17473900
H	5.89504600	0.05171600	-4.88042700
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H	5.49552100	-0.28361200	-0.61173100

## TS2

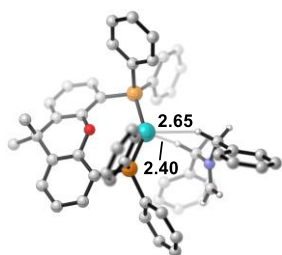


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C	4.04085800	2.05880000	0.83815600
C	5.14139400	1.61878000	1.56817100
C	5.32497800	0.25575400	1.79918900
C	4.41712900	-0.68626900	1.30732100
C	3.30263100	-0.21600000	0.59640500
C	4.60202500	-2.20342300	1.42879700
C	3.21168800	-2.82505300	1.60465900
C	2.14610900	-2.26298600	0.88490000
C	0.84857600	-2.81527400	0.89477500
C	0.64612200	-3.96826200	1.67134900
C	1.68071500	-4.52983300	2.41351300
C	2.95280700	-3.95885600	2.37906500
C	5.20658100	-2.73070100	0.09382300
C	5.55444500	-2.57974900	2.57682600
C	2.26573900	2.00224400	-2.33893800
C	3.60804100	2.30252000	-2.61904700
C	4.02927700	2.49543600	-3.93573300
C	3.11676400	2.39669700	-4.98851400
C	1.77943900	2.09735200	-4.72173400
C	1.35914800	1.89422600	-3.40627500
C	1.39881500	3.47987500	0.01696100
C	1.09021000	3.65890000	1.37850100
C	0.83385000	4.93017300	1.89110200
C	0.86539000	6.04617800	1.04834900
C	1.16299600	5.87912300	-0.30390900
C	1.43175000	4.60615200	-0.81760800

C	-2.04960400	-2.57439400	0.82914900
C	-2.13902000	-2.29166800	2.20552700
C	-3.32459100	-2.51552000	2.90685100
C	-4.45224100	-3.01104600	2.24399000
C	-4.37863700	-3.28831300	0.87775700
C	-3.18791200	-3.07524400	0.17565500
C	-0.55712300	-3.13509400	-1.62403200
C	-0.71699800	-4.53031600	-1.57787200
C	-0.70272100	-5.28293300	-2.75152000
C	-0.52002700	-4.65463400	-3.98705600
C	-0.34986600	-3.27112400	-4.04423000
C	-0.36936600	-2.51553500	-2.86893900
C	-3.60707600	0.54966900	0.79849900
C	-2.66735400	2.70751400	1.47860100
C	-2.70320100	2.25205700	2.91186800
C	-1.65613400	1.47330100	3.42929400
C	-1.67684400	1.06774700	4.76381100
C	-2.74168300	1.43584300	5.59127600
C	-3.78724400	2.20944100	5.08261100
C	-3.76812000	2.61579900	3.74742800
C	-2.96710300	2.12122600	-0.94712200
C	-3.86723000	1.43751700	-1.94092800
C	-3.41261400	0.31402600	-2.64613400
C	-4.24318200	-0.31826500	-3.57372100
C	-5.53179000	0.16780700	-3.80253900
C	-5.98989900	1.29031800	-3.10621700
C	-5.16128800	1.92363100	-2.18096000
H	3.90498700	3.12212700	0.66912500
H	5.85956900	2.33652500	1.95321000
H	6.19233900	-0.07132400	2.36134700
H	-0.34085100	-4.41706200	1.71384400
H	1.49920200	-5.41578800	3.01467700
H	3.75097500	-4.41356500	2.95488200
H	6.19051500	-2.28076600	-0.07945300
H	5.32462600	-3.81919800	0.13605200
H	4.56527900	-2.48963100	-0.75927600
H	5.18532600	-2.23229600	3.54778000
H	5.69202000	-3.66365900	2.62652200
H	6.54746800	-2.15242300	2.41104600
H	4.32961000	2.37936800	-1.81203400
H	5.07223900	2.72241900	-4.13854500
H	3.44821500	2.54683400	-6.01213700
H	1.06578100	2.01256100	-5.53676400
H	0.32243200	1.63995200	-3.19951100
H	1.07274700	2.79945000	2.04462200
H	0.61427100	5.05088800	2.94871500
H	0.66588600	7.03701500	1.44651000
H	1.19833400	6.74100200	-0.96474400
H	1.67517000	4.49591300	-1.86943200
H	-1.27214100	-1.90440200	2.73393600
H	-3.36586800	-2.30549200	3.97238800
H	-5.37434600	-3.18861800	2.79006900
H	-5.24470800	-3.68500800	0.35477100
H	-3.14565200	-3.31065100	-0.88327000
H	-0.85173400	-5.03419300	-0.62543400
H	-0.82854900	-6.36096500	-2.70204600
H	-0.50409900	-5.24448000	-4.89927300
H	-0.19435800	-2.77886400	-5.00039300
H	-0.21849100	-1.43920700	-2.90610000
H	-3.65300100	0.25850800	1.84051700
H	-3.92159200	-0.13397600	0.01898700
H	-3.26414000	3.61320700	1.32877600
H	-1.64374200	2.92414000	1.15261200
H	-0.83068400	1.18667000	2.78095500

H	-0.85794000	0.47457400	5.16076400
H	-2.75257800	1.12660100	6.63243100
H	-4.61178000	2.50344300	5.72517300
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H	-3.08659000	3.20781900	-0.96872400
H	-2.40552300	-0.05631300	-2.46558500
H	-3.87967200	-1.18495400	-4.11827900
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### CP3

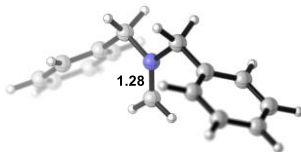


Pd	0.01327700	0.24019600	-0.40333000
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P	-0.73089800	-1.91049600	0.02916900
O	2.27110800	-1.33308700	0.12553400
N	-3.14079200	1.84376300	0.53218300
C	3.27855100	0.84642900	0.17025400
C	4.35742100	1.64797800	0.57881100
C	5.42112300	1.11203100	1.29963200
C	5.43745400	-0.24682400	1.61227900
C	4.39683800	-1.09076100	1.21275900
C	3.32404500	-0.52125900	0.51112000
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C	2.94435500	-3.04205500	1.66970800
C	1.93101100	-2.38813300	0.95243300
C	0.57636500	-2.77555300	1.02656300
C	0.26156500	-3.85820600	1.86422400
C	1.24527800	-4.50623100	2.60572100
C	2.57498000	-4.09748100	2.50821100
C	4.88299000	-3.28279400	0.10458500
C	5.32933900	-3.03806300	2.56490000
C	2.42670900	1.57114900	-2.53144700
C	3.77941200	1.53000000	-2.90237300
C	4.14259400	1.54053700	-4.25065200
C	3.16261400	1.59925800	-5.24348700
C	1.81335500	1.64187000	-4.88526300
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C	1.57929300	3.70362400	1.03321800
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C	-1.27514100	1.49584300	4.84263800
C	-2.11258900	2.36267200	5.54749500
C	-2.91882800	3.27174400	4.85622100
C	-2.88726500	3.31264900	3.46268100
C	-3.07756100	2.04116300	-0.95356400
C	-4.22427300	1.45587900	-1.72948300
C	-4.09904300	0.19574600	-2.33243400
C	-5.15683400	-0.33883200	-3.06988400
C	-6.34707000	0.37829800	-3.20731600
C	-6.47904200	1.63547000	-2.61101300
C	-5.42164800	2.17301600	-1.87776600
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H	3.33001100	-4.61981800	3.08494100
H	5.90987000	-2.97307700	-0.11928000
H	4.86301700	-4.37352300	0.20692100
H	4.24974000	-3.00782300	-0.74439900
H	5.03396900	-2.59775700	3.52330000
H	5.33782900	-4.12651400	2.67177800
H	6.36089500	-2.74351300	2.35207700
H	4.55203400	1.48497600	-2.14144700
H	5.19340700	1.50325400	-4.52424400
H	3.44896000	1.60714000	-6.29142200
H	1.04572500	1.68292000	-5.65329800
H	0.39727500	1.63272100	-3.26046200
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H	1.29918900	5.28066100	2.46933200
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H	2.44400100	6.51120900	-1.49152800
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H	-1.46073400	-1.59512300	2.86779500
H	-3.57336000	-1.81239900	4.11510000
H	-5.64237100	-2.58156800	2.95731500
H	-5.55385000	-3.14528000	0.53422500
H	-3.43768700	-2.95192600	-0.71283000
H	-1.15207200	-4.85578900	-0.44786300
H	-1.31694200	-6.19165900	-2.51354100
H	-1.12596800	-5.09254500	-4.73514600
H	-0.76091000	-2.63633400	-4.87333000
H	-0.58952400	-1.28910500	-2.79062200
H	-3.91867300	0.90892200	2.17365000
H	-4.73026000	0.56016500	0.50555000
H	-1.95155000	3.51520300	0.86913800
H	-1.10941100	1.94404500	0.85060200
H	-0.59121000	0.86493400	2.89169800
H	-0.63723000	0.79847600	5.37807600
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H	-2.10932100	1.58667300	-1.23290900
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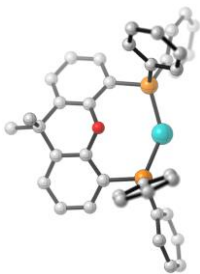
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### CP4



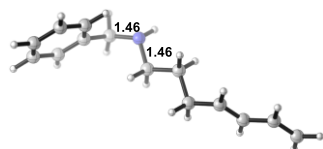
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C -2.54230200 -0.00019900 0.52326400  
C -3.14481800 1.21243500 0.15416100  
C -4.33260000 1.21136400 -0.57705900  
C -4.92566300 0.00038600 -0.94355300  
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C 1.26884800 -0.00070700 1.31885300  
C 2.54230400 -0.00029800 0.52326100  
C 3.14471300 1.21240900 0.15419200  
C 4.33247600 1.21146000 -0.57703900  
C 4.92566300 0.00053700 -0.94356000  
C 4.33287700 -1.21080200 -0.57778000  
C 3.14509800 -1.21258100 0.15344300  
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H 0.94735100 0.00005600 -1.31101600  
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H -1.18720500 0.88291800 1.96047600  
H -2.69480300 2.15679400 0.45254200  
H -4.79947600 2.15259000 -0.85041500  
H -5.85433100 0.00061500 -1.50621900  
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H 1.18723300 0.88236400 1.96082400  
H 1.18718800 -0.88452100 1.95982000  
H 2.69463900 2.15671800 0.45264800  
H 4.79924900 2.15273200 -0.85041000  
H 5.85432300 0.00088100 -1.50623800  
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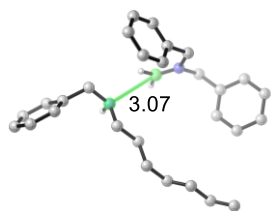


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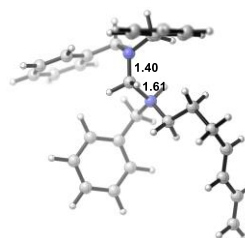
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H	-0.15743000	-1.41576100	-1.04365800
H	0.48960900	0.14653100	-0.53652200
N	0.86501700	-1.36434500	0.84096600
H	0.40178500	-2.18232300	1.23246200
C	2.17372500	-1.76512700	0.32348400
H	2.61995500	-2.43981100	1.06724300
H	2.10340400	-2.34260900	-0.61852200
C	3.10858200	-0.58664000	0.10470700
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C	3.16213000	0.46424100	1.03066600
C	4.86242500	0.50322000	-1.18003000
H	3.92392000	-1.35526900	-1.73469300
C	4.05547000	1.52092100	0.85409300
H	2.48666600	0.44481600	1.88087500
C	4.91142800	1.54305800	-0.25060700
H	5.51801600	0.51449300	-2.04711500
H	4.08473600	2.32958800	1.58029400
H	5.60712500	2.36688700	-0.38733600

**TS3**

N	-1.41160200	-2.01668500	-1.26912200
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C	-0.28016900	-3.12712700	0.71625800
C	0.57027000	-4.18649900	0.36557400
C	1.73703300	-4.42259000	1.09213900
C	2.06013300	-3.60525200	2.17864600
C	1.21610800	-2.55075900	2.53692400
C	0.05075200	-2.31085400	1.80736500
C	-2.67436400	-1.80989000	-2.05653800
C	-3.77166500	-1.15346300	-1.25235700
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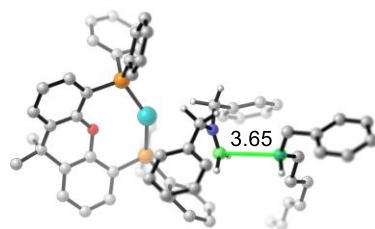
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H	2.38482100	-5.25051100	0.82055800
H	2.96176700	-3.79781600	2.75251700
H	1.45623700	-1.92606200	3.39210900
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H	-2.39664400	-1.21741900	-2.93224800
H	-2.98168000	-2.80319300	-2.39844700
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H	-6.79740400	-1.86745500	0.14180300
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H	3.43573500	-1.26012200	-1.19268100
C	4.57931000	0.39548300	-0.43639300
C	5.24459100	0.70244600	-1.63241300
C	5.08880100	0.90673100	0.76448300
C	6.38452800	1.50638100	-1.63079900
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C	6.23048200	1.71112000	0.77132300
H	4.59493300	0.66530400	1.70344500
C	6.87924800	2.01419600	-0.42684900
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**CP5**

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C	-3.44173300	-0.78438700	-0.97567200
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H	0.37912400	4.45930400	-1.25875300
H	-3.51475700	1.09148100	-2.00596500
H	-2.27003500	0.00921000	-2.59530300
H	-3.17731400	-2.13578600	-2.63800100
H	-4.38189700	-4.01196800	-1.56595600
H	-5.35130300	-3.73480200	0.70842100
H	-5.11208200	-1.56174100	1.89450800
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C	6.44391100	-0.76711600	-0.73304800
H	6.58979500	-0.55997100	-1.79320400
C	7.19594000	-1.70145100	-0.13292300
H	7.08670100	-1.92896300	0.92525800
H	7.95175100	-2.26095100	-0.67499600
C	5.42368300	0.01684500	-0.04979700
H	5.29255200	-0.18368400	1.01532100
C	4.66651600	0.96210300	-0.63501400
H	4.81296100	1.17255200	-1.69656900
C	3.62191900	1.78722900	0.06582500
H	3.85641000	2.85499200	-0.03997000
H	3.62993900	1.57329000	1.14237800
C	2.19229400	1.57461600	-0.48933000
H	1.51434400	2.29944600	-0.02646300
H	2.19556700	1.78025100	-1.57073500
C	1.71936200	0.14310400	-0.24838600
H	2.44239200	-0.55898800	-0.66870400
H	1.62178900	-0.08518900	0.81617800
N	0.38010700	-0.15391800	-0.88345500
H	0.36566900	0.32751200	-1.78802400
C	0.19930900	-1.64961400	-1.20121000
H	-0.81074100	-1.74605500	-1.60268800
H	0.91596500	-1.86023600	-2.00040800
C	0.41016200	-2.57755800	-0.03091900
C	1.67883800	-3.12599900	0.21731300
C	-0.66455500	-2.95324000	0.79138800
C	1.87792000	-4.00054000	1.28494400
H	2.51377400	-2.88746500	-0.43717600
C	-0.46288700	-3.82645600	1.86094800
H	-1.66727500	-2.59190300	0.58186800
C	0.80802700	-4.34574400	2.11378300
H	2.86348300	-4.42099400	1.46078400

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### TS4



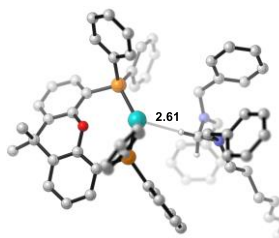
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N	2.01587000	-0.75664700	-0.17323500
C	-4.31159000	-2.06261900	0.22515000
C	-4.95332100	-3.27611000	0.52429800
C	-5.96565100	-3.34160200	1.47779700
C	-6.37015600	-2.18611900	2.14541700
C	-5.77667900	-0.95046500	1.87118700
C	-4.74489500	-0.91421600	0.92097500
C	-6.23690900	0.37739600	2.48436200
C	-4.99710400	1.26167800	2.66460000
C	-4.00027400	1.20393100	1.67890000
C	-2.87223200	2.05076200	1.68804000
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C	-3.72925600	3.02881800	3.74848600
C	-4.83366300	2.17840500	3.70694600
C	-7.18980500	1.07822500	1.47128400
C	-6.99671000	0.17048000	3.80603500
C	-3.81451000	-1.86891500	-2.64949600
C	-5.12905600	-2.31651600	-2.85149100
C	-5.72794300	-2.20658900	-4.10790400
C	-5.02131000	-1.65539300	-5.17885800
C	-3.71259300	-1.20675700	-4.98903100
C	-3.11686700	-1.30552300	-3.73087900
C	-2.29189000	-3.73059900	-1.00549600
C	-1.69987500	-4.21350800	0.17658100
C	-1.12141700	-5.48111800	0.21871200
C	-1.10845000	-6.28499600	-0.92582000
C	-1.68610600	-5.81363400	-2.10432600
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C	0.39623100	2.12066700	2.32759200
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C	-2.79708600	3.88995300	-3.10534500
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C	1.65928100	-1.89174900	2.07057000
C	0.41724700	-1.67571200	2.68577100
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C	1.48241300	-1.68984300	4.85840100
C	2.72297000	-1.89711000	4.25066400



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H	7.71575900	2.20951700	-0.68037000
C	6.13602000	1.23603500	0.42828800
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### CP6

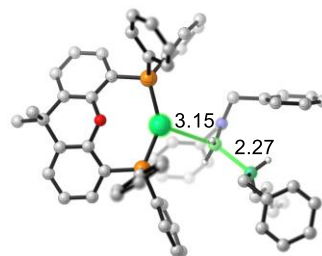


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C	5.93927100	-1.74755300	2.21860200
C	4.71455800	-2.63477700	1.96778500
C	3.72351400	-2.14694700	1.10321900
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C	4.55157800	-3.92048900	2.49146700
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C	3.43363700	2.61604700	-1.24197300
C	4.62143800	3.35779700	-1.13699200
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C	3.04291400	-4.47473300	-3.54253800
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C	2.07866200	-2.48039100	-4.50856700
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H	-2.68735500	-0.12743700	1.15645100
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C	-8.88076800	-1.28107200	3.32960000
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H	-6.69116500	-2.14382100	-0.54291100
C	-5.34093200	-0.61182800	0.18569400
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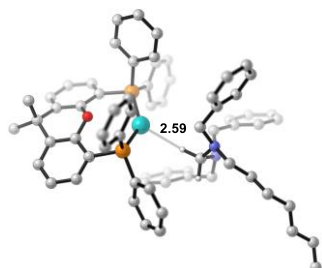


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C	5.50397200	-0.83540200	-1.83664000	H	5.02554200	-1.52471600	6.08658000
C	4.44246500	-0.79023000	-0.92029500	H	2.90887600	-0.30722100	5.61650900
C	6.04206100	0.49471700	-2.37658000	H	1.87590700	-0.44284100	3.36010400
C	4.84490100	1.43402600	-2.56561900	H	1.46094200	-3.49244000	-1.25550900
C	3.81648400	1.38486800	-1.61298200	H	0.32150400	-5.67769400	-1.34668000
C	2.72368000	2.27621400	-1.62731700	H	0.00050500	-7.01199700	0.73415000
C	2.68285400	3.22714900	-2.66040800	H	0.87049700	-6.14207900	2.89650400
C	3.67664500	3.27690600	-3.63476200	H	2.03865900	-3.97166200	2.98729900
C	4.74803900	2.38594200	-3.58473500	H	-0.35661100	1.38134500	-2.49458100
C	6.98237600	1.11310000	-1.30021300	H	-2.29531500	2.39261900	-3.63432600
C	6.84406600	0.30998500	-3.67624100	H	-3.10924400	4.65160900	-2.95590100
C	3.37784500	-1.76478900	2.56410500	H	-1.93604800	5.88570700	-1.14267400
C	4.57602900	-2.44379900	2.83887000	H	0.02216400	4.88704100	-0.01947200
C	5.16380700	-2.35675600	4.10129000	H	3.07520700	4.70732800	-0.37566800
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### CP7

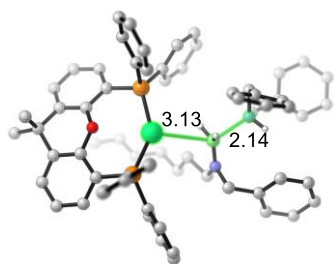


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C	6.30852700	1.80055000	1.61904400
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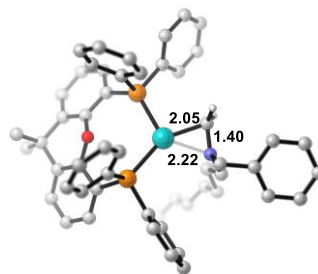
## TS6



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C	-0.59200200	4.14051500	3.19598200
H	-1.46942600	2.23932100	2.70513300
C	-0.20973400	5.40256200	2.72633900
H	-0.14627600	6.71261300	1.01548600
H	-0.44535400	3.88168600	4.24189800
H	0.24210900	6.12394200	3.40147000
Pd	-0.93633200	0.25934500	-0.54279200
C	2.09127500	0.45654400	0.23559400
H	2.04640000	0.79266100	-0.79095600
H	1.64436000	-0.49856900	0.46991100
N	3.95465500	-0.51347100	-0.17745600
C	3.88222200	-1.22716600	-1.48066300

H	2.98277600	-1.85330000	-1.46221900
H	4.74499000	-1.89933900	-1.57473700
C	4.36087200	-1.37278100	0.96605900
H	4.26426100	-0.75649000	1.86636700
H	3.62905900	-2.18486600	1.03605000
C	3.85087300	-0.26401500	-2.64668300
C	2.66791700	-0.01829200	-3.35580100
C	5.02480500	0.39922300	-3.03762700
C	2.65481600	0.88129900	-4.42525500
H	1.75529700	-0.54167900	-3.08034900
C	5.01140600	1.30310100	-4.10082600
H	5.95867000	0.19173100	-2.51800800
C	3.82365300	1.54815200	-4.79562300
H	1.73272900	1.05153300	-4.97413100
H	5.92907800	1.80299600	-4.39788600
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C	5.76703100	-1.93001700	0.86645600
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C	8.17105100	-1.60063300	0.98972300
H	6.72192900	-0.05818400	1.37827200
C	7.28408800	-3.77526900	0.41992900
C	8.37841700	-2.94004700	0.64877300
H	9.02015200	-0.95001600	1.17950100
H	9.38857200	-3.33103800	0.56821600
H	4.60920500	0.26671500	-0.25490700
H	5.13370500	-3.92577500	0.35608600
H	7.43954700	-4.81862900	0.16044600
C	-1.59224700	-2.98500300	5.67131000
H	-0.98999500	-3.88117500	5.52003500
C	-2.82999800	-3.10089400	6.17408600
H	-3.45991000	-2.23054900	6.34443000
H	-3.25205200	-4.06611300	6.43594400
C	-0.97238300	-1.71741100	5.30939300
H	-1.57406700	-0.82107700	5.47045000
C	0.27125400	-1.59065900	4.81579300
H	0.87366500	-2.48938600	4.66785000
C	0.92448600	-0.28789700	4.44723700
H	0.27959900	0.54837600	4.74649100
H	1.86522800	-0.17685500	5.00891400
C	1.23095200	-0.18770600	2.93729400
H	0.29142100	-0.20131300	2.37020800
H	1.80375100	-1.07245900	2.63283600
C	2.00325500	1.09212800	2.61852900
H	2.98834200	1.08036800	3.10307700
H	1.45727300	1.95173600	3.02244000
N	2.18581900	1.37517100	1.17857600
C	2.59918300	2.75781300	0.83222500
H	1.97915900	3.43551600	1.42716100
H	2.34157000	2.91484300	-0.21850200
C	4.07459700	3.02469000	1.06496100
C	4.99526700	2.87509300	0.01695600
C	4.54408300	3.42215200	2.32450300
C	6.35877100	3.09042000	0.23142900
H	4.64405400	2.61377600	-0.97937600
C	5.90678100	3.63499400	2.54176400
H	3.83945500	3.58262600	3.13699400
C	6.81781900	3.46369600	1.49710200
H	7.05865000	2.98391400	-0.59270300
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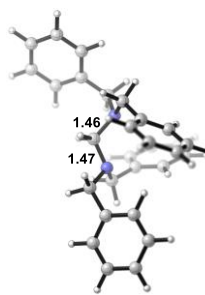


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C	4.59483800	-0.66311100	-2.99929200
C	3.45708800	-1.36202000	-2.60198100
C	2.76466300	-0.99199100	-1.43733700
H	5.94801700	0.94498100	-2.57910500
H	5.11694700	-0.95535600	-3.90525000
H	3.09792500	-2.18726800	-3.20567000
C	4.91641100	1.91182300	-0.12649000
C	5.78156400	2.94561900	-0.86863200
H	6.14083100	3.71529900	-0.17947000
H	5.22930300	3.43524700	-1.67765300
H	6.67293000	2.47470700	-1.29303200
C	5.77001400	1.26255700	1.00168600
H	6.11341000	2.02897300	1.70520100
H	6.64805600	0.76575200	0.57420500
H	5.19478400	0.51906700	1.56226800
C	3.68029400	2.55675600	0.51378400
C	3.57879500	3.90073600	0.88936600
C	2.58879800	1.73449600	0.80748900
C	2.44298500	4.38212400	1.54375600
H	4.39508900	4.58389700	0.68209100
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C	1.37214300	3.53313900	1.82239300
H	2.39363900	5.42605300	1.83841700
H	0.49291000	3.92212500	2.32419400
O	2.62420200	0.39421200	0.47662800
P	1.20655800	-1.83196100	-0.90494500
P	0.07206800	0.95703700	1.69199700
C	1.73683700	-3.09806000	0.32369500
C	3.08175800	-3.30643100	0.65756400
C	0.75182300	-3.89162400	0.93695300
C	3.43338200	-4.28669100	1.58910700
H	3.85823200	-2.71004500	0.18988500
C	1.10643000	-4.88015100	1.85386400
H	-0.29616500	-3.74106800	0.68876100
C	2.45013000	-5.07606800	2.18581200
H	4.47936900	-4.43537500	1.84158500
H	0.33574100	-5.49551800	2.31004800
H	2.72747600	-5.84190700	2.90442800
C	0.77589700	-2.81381200	-2.41132600
C	0.25143100	-2.12865000	-3.52249200
C	0.95639200	-4.20142100	-2.49626300
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C	0.61002700	-4.88926600	-3.66354200
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C	0.09285800	-4.20069600	-4.76039200
H	-0.47490300	-2.27030900	-5.54286700
H	0.75378700	-5.96491600	-3.71311300
H	-0.17132400	-4.73730200	-5.66703500
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CP8

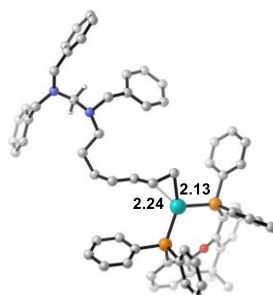
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H	-0.27331400	-1.78661200	2.60176500
C	1.22614200	-1.26211100	5.60877300
H	2.09683900	0.60700100	6.24529300
H	0.29798500	-2.98139300	4.69412900
H	1.48546200	-1.78623900	6.52427500
C	-1.36355500	2.00748100	2.20595100
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C	-3.18269200	2.54931500	3.72754900
H	-1.68644000	1.05498000	4.11859000
C	-2.97264600	3.74686800	1.64164600
H	-1.33152500	3.17110500	0.38002200
C	-3.64798500	3.52543100	2.84618300
H	-3.69537400	2.37618400	4.66964700
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C	-0.72942300	5.10278400	-4.75303900
H	-0.57028900	4.50486000	-5.65063100
C	-0.15701900	6.31169200	-4.65687300
H	-0.29576000	6.94025300	-3.77986100
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C	-1.57490100	4.51372800	-3.72346100
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C	-2.43600100	1.38367000	-2.19334100
H	-1.46093000	1.59512700	-1.73442500
H	-2.25096400	0.69114500	-3.02356500
C	-3.36781500	0.75326200	-1.15887000
H	-4.31853800	0.46557700	-1.62417800
H	-3.59291200	1.48474100	-0.37746400
N	-2.82082100	-0.44099300	-0.45558300
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H	-3.12629200	-1.72500400	1.16327300
C	-5.08377100	-1.14985800	0.43792400
C	-5.46187700	-2.34503500	-0.19153300
C	-6.07883700	-0.23218600	0.79976400
C	-6.80352800	-2.60951000	-0.46500100
H	-4.70726800	-3.08063400	-0.46093800
C	-7.42312400	-0.49658600	0.53085300
H	-5.79992000	0.69087300	1.30336400
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H	-7.08293400	-3.54094100	-0.94907000
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HNBn<sub>2</sub>



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H	-0.84962700	-2.26936300	1.53998100
C	1.26671400	-2.19785400	-0.02941300
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C	-1.66690000	-0.66724500	0.34877600
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H	-2.71385400	-1.07518500	-1.49357900
C	-1.81931100	1.63314200	1.12526600
H	-0.76592300	0.06783900	2.16123200
C	-2.58612100	1.97348000	0.00982100
H	-3.50782300	1.24669200	-1.80104500
H	-1.57202500	2.38780800	1.86746100
H	-2.94048200	2.99263000	-0.12037200
C	1.69429800	-0.73406500	-0.11140700
C	2.31195500	-0.11139400	0.97917700
C	1.52902900	0.00346000	-1.29176100
C	2.74746000	1.21395700	0.90126100
H	2.45582400	-0.67193600	1.90119900
C	1.95650300	1.32756200	-1.37521600
C	2.56830200	1.93866100	-0.27702300
H	3.22337500	1.67858500	1.76125300
H	2.90260800	2.97070700	-0.34200200
H	-0.31293200	-2.32739100	-1.34180200
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CP9



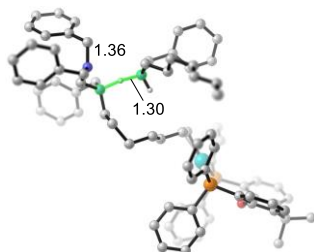
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C	-9.40895000	-2.26356300	-1.63594900	C	6.61154500	0.72018800	3.24066100
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C	-10.28312700	-3.66517500	0.13038500	H	7.52618400	1.94293500	4.79720000
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C	-9.85272700	-1.31691500	0.53955200	H	7.57227800	0.22415100	5.13477700
H	-6.59687000	1.05876600	0.95303300	C	7.94094800	0.60090100	2.44006700
H	-7.19368100	-0.58322500	0.57707300	H	8.50665200	1.53725000	2.50456200
H	-7.37476200	2.72638800	-1.40247700	H	8.55834000	-0.20720200	2.84850700
H	-9.09359500	2.69366400	-1.07050700	H	7.75254300	0.38680700	1.38373400
H	-9.22400200	2.11745900	1.85293800	C	5.76317000	1.83232000	2.61012700
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H	-7.45534000	5.55139600	3.74517200	C	5.02276900	1.52094900	1.46321300
H	-6.26612600	6.09709400	1.62945800	C	4.97794700	4.11927300	2.37643000
H	-6.54930700	4.65422200	-0.36039700	H	6.27121100	3.44505800	3.94880400
H	-9.89021200	0.81138900	-1.47415800	C	4.24827500	2.45520800	0.75990500
H	-8.52936400	0.08511200	-2.30393300	C	4.25491300	3.77574800	1.23470000
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H	-10.62996400	-2.67550200	2.01616700	P	3.35497300	-2.01774500	0.07262300
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H	-4.88031400	2.61324400	0.46522500	C	2.50819400	-4.74824500	-0.26802300
H	-4.37274400	2.48287400	-1.22400300	C	0.48456900	-4.52891500	1.64088500
C	-4.43947800	0.58450900	-0.20362400	H	1.14674300	-2.49745500	1.88743700
H	-3.65275300	0.09719900	-0.78179700	C	1.67539300	-5.83950900	0.00128900
H	-4.41878500	0.16363500	0.80504200	H	3.29984300	-4.85107900	-1.00310900
N	-5.76292900	0.18298200	-0.81701400	C	0.66636100	-5.73668000	0.95831600
H	-5.92934400	0.82159500	-1.60095800	H	-0.29009400	-4.44069200	2.39911500
C	-5.71512900	-1.22944900	-1.43051700	H	1.82735000	-6.77386500	-0.53254400
H	-6.72888500	-1.43757000	-1.77672400	H	0.03077200	-6.59075000	1.17669900
H	-5.05878300	-1.13718800	-2.30043000	C	4.47466700	1.85632100	-2.06665100
C	-5.22204700	-2.31016100	-0.50062900	C	5.74028500	2.45367100	-1.97558000
C	-3.86041300	-2.65418100	-0.47663700	C	4.10921100	1.22937200	-3.26925000
C	-6.11888600	-3.02671400	0.30821700	C	6.61975200	2.42094500	-3.06029300
C	-3.39891200	-3.66771000	0.36327500	H	6.04191600	2.94909300	-1.05803500
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H	-3.93950800	-5.14828800	1.83482200	C	2.26765500	3.41966400	-1.05837100
C	5.08765000	-0.77608200	1.91253100	C	2.57693700	4.29816600	-2.10790000
C	5.83150600	-0.59180500	3.08471400	C	1.16510100	3.71477800	-0.23839700
C	5.85254500	-1.64628400	4.00258800	C	1.80659900	5.44324600	-2.32846000
C	5.17066100	-2.83589300	3.74173500	H	3.42552500	4.09678800	-2.75322100
C	4.43996900	-2.98688800	2.56395200	C	0.41136800	4.87025900	-0.44523700
C	4.36924900	-1.94566500	1.62488500	H	0.89958300	3.03599700	0.56710500
H	6.41184300	-1.54885000	4.92676600	C	0.72714700	5.73712900	-1.49466300
H	5.20968100	-3.64928300	4.46056300	H	2.06183100	6.11170000	-3.14654500
H	3.90927800	-3.91447800	2.38003300	H	-0.42442700	5.09331800	0.21353100



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### TS7

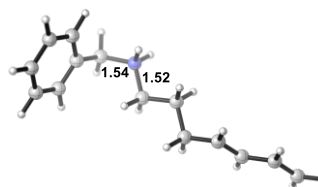


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H	6.76449200	2.55194400	-0.60477200
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H	11.26457200	3.08611600	-1.81849900
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H	9.66876400	0.37358700	-4.75148500
H	7.50687300	0.35325200	-3.56062700
H	8.03983100	1.29132800	0.91788600
H	6.82008500	0.35419400	1.75431700
H	9.46739500	-0.41852800	-0.88949500
H	11.00379100	-2.33517000	-0.65846700
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C	-0.68002300	-0.30169400	0.77178800
H	-0.55974800	0.62324100	1.33510500
C	-1.27191700	-1.42370100	1.40620900
H	-1.06637900	-2.42988200	1.04092900
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C	0.96426500	0.51489500	-0.94658200
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C	1.80440500	0.34612900	-2.18611600
H	1.66482800	1.21076000	-2.84755000
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H	2.17799900	5.19236600	3.06882500
C	3.83839700	4.12191100	2.07170200
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H	4.50175200	4.31727700	1.21840700
C	3.15844700	2.74731700	1.89857300
H	2.50691900	2.54751900	2.75588400
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C	2.78414600	0.07956000	3.99526900
C	3.47749200	0.67721400	5.05601800
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C	0.68897500	0.67062400	5.06884100
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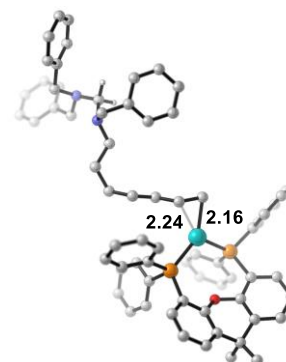
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1'



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C	4.79469500	-0.33102500	-0.19817900
H	4.87392100	0.12504400	-1.18671600
C	3.58283200	-0.67609700	0.26855100
H	3.50258700	-1.14037100	1.25249900
C	2.29398400	-0.47347400	-0.47905900
H	1.76877200	-1.43387000	-0.59309700
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C	1.35246600	0.51718300	0.24524200
H	1.17056800	0.16106700	1.26900400
H	1.85336000	1.49115500	0.32553500
C	0.02413500	0.66301000	-0.49165200
H	0.15684800	1.04864300	-1.50667600
H	-0.52574000	-0.27917000	-0.54385100
N	-0.89179300	1.64661200	0.21417700
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C	-2.29340700	1.82306800	-0.39909000
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H	-2.85485000	-0.19805500	-2.15952100
C	-4.54506500	-0.71904400	1.29888900
H	-3.68014500	1.17119900	1.85013700
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CP10

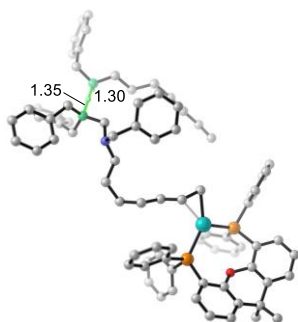


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C	9.94976200	-1.94904800	5.12470300

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C	11.16716500	1.75459000	-1.13806000	C	-7.68294500	0.54021600	-0.49614100
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H	4.55165400	-2.37508000	0.06505400	H	-6.22710900	-3.99767100	-3.81241300
H	3.95571800	-1.83375100	-1.49598100	H	-8.17899400	-2.74987400	-2.96964700
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C	6.41641000	2.58212300	-2.82773200	H	-4.65717600	-3.72959600	0.53050500
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H	-6.16619200	0.91029600	5.36728800
H	-4.21208300	-0.34061200	6.26314600
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### TS8



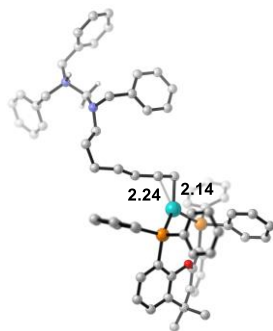
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H	6.06791500	-2.70714500	1.15157500
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H	6.35586100	0.26300200	3.20500200
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### CP11

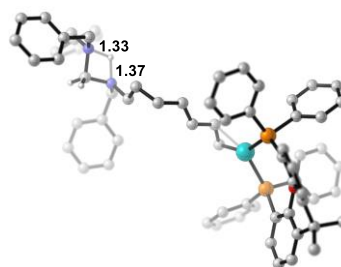


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H	-3.17008300	1.11925500	1.61682900
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C	4.67677700	-3.91162100	0.30628200
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H	4.01706400	-4.48369000	0.94830800
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C	5.38431300	-1.36857800	3.01416300
C	3.31360400	-0.28899400	3.62773300
C	5.96313100	-0.92638700	4.20707400
H	5.97402200	-1.96285700	2.32353400
C	3.88673400	0.13784900	4.82521800
H	2.28232300	-0.03069800	3.40017400
C	5.21736200	-0.17594900	5.11608000
H	6.99819800	-1.17539300	4.42543300
H	3.29694700	0.72029300	5.52858100
H	5.66811500	0.16251900	6.04507400
C	2.15403600	-2.98932900	1.70242000
C	2.22574000	-3.56003800	2.98217800
C	1.25090500	-3.53219600	0.77343000
C	1.42061300	-4.65113800	3.32097600
H	2.91863500	-3.16128500	3.71606000
C	0.46753700	-4.63842500	1.10350100
H	1.16843700	-3.08729100	-0.21462900
C	0.54652500	-5.19900200	2.38098700
H	1.49049900	-5.08104300	4.31684500
H	-0.20655300	-5.06153400	0.36291100
H	-0.06703200	-6.05769600	2.64084600
Pd	2.04350200	0.33211500	0.23180100

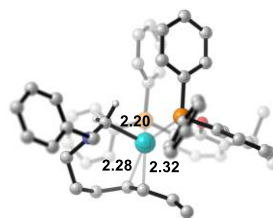
**TS9**



N	-7.63141900	-0.96059400	0.55866100
C	-7.09264200	-0.11380500	-0.56564500
C	-7.57024800	-2.45371300	0.32113600
C	-8.49132200	-2.97836900	-0.75883400
C	-9.81029700	-3.35644900	-0.46294500
C	-10.65503000	-3.83642900	-1.46412600
C	-10.19036400	-3.95321900	-2.77602100
C	-8.87394400	-3.60182800	-3.07993700
C	-8.03046400	-3.12290500	-2.07654800
C	-8.97219900	-0.56023500	1.11547400
C	-9.03746000	0.83155500	1.69282400
C	-8.44895500	1.11204800	2.93585900
C	-8.52858900	2.39186300	3.48402400
C	-9.20715700	3.40544900	2.80023700
C	-9.81189100	3.13239100	1.57223000
C	-9.72886200	1.84995900	1.02285300
H	-6.85727000	-0.70646100	-1.44694700
H	-7.77112100	0.69508100	-0.82782800
H	-6.53177300	-2.68922100	0.08669100
H	-7.79931300	-2.91012500	1.28827000
H	-10.17483200	-3.29580400	0.55959900
H	-11.67098800	-4.13036800	-1.21736500
H	-10.84626700	-4.33231100	-3.55409900

H	-8.49912900	-3.71350700	-4.09311600	C	5.22790200	-4.46739800	-1.85920500
H	-6.99593600	-2.88849500	-2.31863600	H	6.91775100	-4.00664800	-3.09721000
H	-9.72135800	-0.69132600	0.32854900	C	4.30588600	-2.64743700	-0.53138200
H	-9.18658700	-1.29584900	1.89628900	C	4.28922800	-3.98890700	-0.94719300
H	-7.93489800	0.32335100	3.48140000	H	5.19445500	-5.50687700	-2.17267100
H	-8.07364100	2.59629400	4.44876800	H	3.52662400	-4.65933800	-0.56784800
H	-9.27487200	4.40005600	3.23082500	O	5.38360900	-0.53513800	-0.59241500
H	-10.35700600	3.91129200	1.04725200	P	3.88202400	1.91732600	-0.07422500
H	-10.22267700	1.63522900	0.07739900	P	3.00392500	-1.91050100	0.57770600
C	-0.02756300	0.42002900	0.98792700	C	4.96236700	2.22838000	1.39550500
H	-0.10579900	0.03982100	2.00686400	C	6.22944700	2.82573700	1.29309900
C	0.53814700	1.70001300	0.78201600	C	4.49274800	1.85276500	2.66267300
H	0.29288600	2.26523100	-0.11687000	C	7.00223800	3.04712500	2.43387000
H	0.80681200	2.31860100	1.63654300	H	6.61639400	3.11512300	0.32039600
C	-0.93351700	-0.18822200	0.01911200	C	5.26573000	2.07585800	3.80370400
H	-0.91001200	0.24395700	-0.98499900	H	3.52538400	1.36586700	2.74731200
C	-1.79309900	-1.19894400	0.25899600	C	6.52159400	2.67395900	3.69155500
H	-1.81708300	-1.64998200	1.25296800	H	7.98197000	3.50797100	2.33945700
C	-2.74342400	-1.77602700	-0.75308900	H	4.89121100	1.76823700	4.77618300
H	-2.59981800	-2.86205600	-0.83553100	H	7.12737700	2.84267600	4.57782500
H	-2.53556700	-1.35766900	-1.74768000	C	3.23196000	3.60046900	-0.50131700
C	-4.23530900	-1.52939000	-0.40327400	C	2.34731500	3.70526100	-1.59030900
H	-4.86025200	-2.07738400	-1.12073500	C	3.53381000	4.75847400	-0.28733300
H	-4.43745400	-1.93773800	0.59662300	C	1.80087500	4.93580100	-1.95176800
C	-4.54832700	-0.03499600	-0.42227400	H	2.08926600	2.81495000	-2.15962300
H	-3.78968100	0.46816500	0.18242700	C	2.97134100	5.98949600	-0.12374900
H	-4.46588300	0.36416200	-1.43985200	H	4.21280000	4.70610000	1.07340300
N	-5.86951000	0.37817300	0.14759600	C	2.10920200	6.08383300	-1.21556300
H	-6.51546700	-0.42353000	1.04739800	H	1.13158400	4.99885800	-2.80620000
C	-5.88138700	1.85558300	0.47653800	H	3.21671900	6.87585900	0.45540200
H	-6.82081700	2.05671800	0.99244300	H	1.67956900	7.04287300	-1.49223100
H	-5.07176200	1.99350100	1.19825900	C	3.72584500	-2.12486500	2.26976300
C	-5.71336900	2.78291400	-0.70845300	C	4.92307400	-2.81035700	2.51885400
C	-4.43824200	3.16889500	-1.14997700	C	3.03344000	-1.56148500	3.35572500
C	-6.83847400	3.29576500	-1.37188400	C	5.41663700	-2.92756400	3.82100400
C	-4.29271500	4.02052700	-2.24540600	H	5.47481900	-3.25595700	1.69719800
H	-3.55328200	2.81694400	-0.62570800	C	3.51855000	-1.69217900	4.65677700
C	-6.69464000	4.14560400	-2.46970300	H	2.11075100	-1.01615400	3.17288500
H	-7.83477200	3.05785600	-1.00626500	C	4.71602100	-2.37291600	4.89245200
C	-5.42037100	4.50449600	-2.91239300	H	6.34930800	-3.45738000	3.99544800
H	-3.29879300	4.31417600	-2.57027400	H	2.96626200	-1.25636800	5.48554800
H	-7.57593400	4.53851400	-2.96868800	H	5.10045100	-2.46805500	5.90432700
H	-5.30654700	5.17098200	-3.76238900	C	1.73622900	-3.26512800	0.50232600
C	5.75252700	0.41536100	-1.52322700	C	1.55423700	-4.22269600	1.51086200
C	6.70300700	0.09605400	-2.49886100	C	0.93238400	-3.33919600	-0.64772500
C	7.02921800	1.09335600	-3.42392300	C	0.59920100	-5.23387500	1.36853100
C	6.43921900	2.35620600	-3.35136700	H	2.16663000	-4.19021800	2.40622500
C	5.50836100	2.64648300	-2.35350200	C	-0.00081600	-4.36417600	-0.80142100
C	5.13613500	1.66987900	-1.41803200	H	1.04988100	-2.59552300	-1.43191600
H	7.75568000	0.89300800	-4.20413400	C	-0.17375300	-5.31389400	0.20957800
H	6.71167500	3.12084900	-4.07321100	H	0.47463600	-5.96907600	2.15942600
H	5.06087200	3.63331500	-2.30829500	H	-0.59265100	-4.42184300	-1.71170000
C	7.35795000	-1.28951800	-2.43020400	H	-0.90130800	-6.11285000	0.09201100
C	7.98269600	-1.69829800	-3.77509300	Pd	2.12731700	0.33443000	0.37644300
H	8.46922600	-2.67506600	-3.69614300				
H	7.23513000	-1.74710600	-4.57401900				
H	8.76038900	-0.98838600	-4.07225300				
C	8.47978300	-1.24867300	-1.35216600				
H	8.94888900	-2.23453600	-1.25581500				
H	9.25075700	-0.52278200	-1.63447000				
H	8.08225500	-0.96147600	-0.37405000				
C	6.27955700	-2.28118900	-1.97340100				
C	6.20501000	-3.61681600	-2.37836700				
C	5.32954600	-1.83653500	-1.04359900				

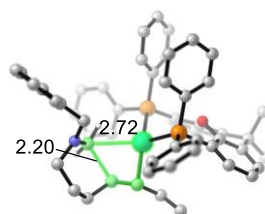
### CP12



C	3.39229700	0.19015100	-0.49751800
C	4.61360100	-0.22313700	-1.04044000
C	5.44638800	0.77375100	-1.56263800
C	5.08158000	2.11930400	-1.51322600
C	3.86301400	2.49976000	-0.95220200
C	2.98083200	1.53344100	-0.44811400
H	6.40177100	0.50508000	-1.99935600
H	5.75416600	2.87567900	-1.90632700
H	3.59595800	3.54966700	-0.91221300
C	5.00141100	-1.70427900	-0.94174000
C	5.99869700	-2.10661600	-2.04435900
H	6.28891900	-3.15605100	-1.94311300
H	5.58113300	-1.95746000	-3.04562500
H	6.92206900	-1.52621900	-1.96441200
C	5.67027400	-1.93672200	0.44471400
H	5.93662900	-2.99251400	0.56615900
H	6.58205600	-1.33547900	0.53183700
H	4.99934900	-1.65658500	1.26337100
C	3.71738900	-2.54317200	-1.00126600
C	3.65757200	-3.85004000	-1.49869600
C	2.54228500	-2.01875400	-0.45035600
C	2.48178300	-4.59664600	-1.42512600
H	4.53939300	-4.30058900	-1.94025100
C	1.34045600	-2.74022000	-0.35453900
C	1.33420600	-4.05079300	-0.85304000
H	2.46183800	-5.61149700	-1.81073100
H	0.42720200	-4.64180400	-0.80376400
O	2.52509900	-0.73166300	0.05174400
P	1.32240100	1.90039900	0.27963600
P	-0.17729900	-1.91138700	0.30592600
C	1.66119200	1.88667800	2.09624400
C	2.90794300	2.27598800	2.61324200
C	0.63449800	1.54696000	2.98791500
C	3.11686600	2.32606600	3.99127400
H	3.71646400	2.54312300	1.93997500
C	0.84140500	1.60747400	4.36769900
H	-0.32900100	1.22133600	2.60956600
C	2.08288500	1.99680500	4.87128100
H	4.08670200	2.62698800	4.37760800
H	0.03677400	1.33661900	5.04441500
H	2.24680700	2.04017300	5.94432000
C	1.05885700	3.70176200	-0.05416900
C	1.11803400	4.19582800	-1.37122100
C	0.69294900	4.58672900	0.97357600
C	0.84114400	5.53495700	-1.64641200
H	1.40164400	3.53706000	-2.18668200
C	0.39993700	5.92431600	0.69266000
H	0.64994900	4.24029200	2.00073300
C	0.47612700	6.40401100	-0.61459500
H	0.91171600	5.89923500	-2.66769300
H	0.12441200	6.59244800	1.50389800
H	0.25856900	7.44623700	-0.82936900
C	0.00659000	-1.97713700	2.14521400
C	1.21119200	-2.28981700	2.78839300
C	-1.12210000	-1.68475500	2.93279700
C	1.28531500	-2.31132000	4.18360000
H	2.09300500	-2.53409900	2.20581500
C	-1.04918300	-1.71480300	4.32490200
H	-2.07803700	-1.47323700	2.45793300
C	0.15864300	-2.02685800	4.95509700
H	2.22603500	-2.56226500	4.66557700
H	-1.93672900	-1.50666000	4.91653600
H	0.21687200	-2.05668100	6.03938300
C	-1.49096800	-3.19078100	0.04202800

C	-1.65567100	-4.28425500	0.91065100
C	-2.33722600	-3.08444500	-1.07208800
C	-2.64279400	-5.24018800	0.66869800
H	-1.01289300	-4.38998100	1.77864700
C	-3.32302800	-4.04351700	-1.31558600
H	-2.21519000	-2.25053000	-1.75428900
C	-3.47950900	-5.12187000	-0.44378000
H	-2.75756000	-6.07844300	1.35015700
H	-3.96861800	-3.94768100	-2.18451400
H	-4.24855900	-5.86634400	-0.62897600
Pd	-0.32483500	0.37098100	-0.81717500
C	-2.06369800	1.24241500	0.20890400
H	-2.02872100	0.54357900	1.04107600
H	-1.66509500	2.23499500	0.40139000
C	-0.04550900	-0.99820000	-3.53370300
H	1.00830800	-0.71767000	-3.50535200
C	-0.38734000	-2.17287700	-4.08534300
H	-1.42363400	-2.49328400	-4.16410800
H	0.36104400	-2.84759100	-4.48790200
C	-0.98865900	-0.00492000	-3.00848000
H	-2.04124200	-0.27924400	-3.05520700
C	-0.64178200	1.33736400	-2.85442700
H	0.38735100	1.59388800	-3.11093700
C	-1.58437500	2.51964400	-3.01657600
H	-1.44463800	2.86492800	-4.05290400
H	-1.24284200	3.35562500	-2.39303700
C	-3.09234200	2.31475200	-2.80195900
C	-3.57399000	2.38454000	-1.34553400
H	-3.17678700	3.28829300	-0.87040700
H	-4.66553200	2.45651300	-1.32167100
N	-3.20937800	1.24085000	-0.49855400
C	-4.08572400	0.05842000	-0.54718400
H	-4.13990800	-0.30080300	-1.58214100
H	-3.59844400	-0.73023200	0.03248400
C	-5.48514500	0.33719800	-0.02958300
C	-5.68678800	0.74705600	1.29620500
C	-6.59546800	0.16913900	-0.86447800
C	-6.97420200	0.98175800	1.77588900
H	-4.83360400	0.88340600	1.95749300
C	-7.88717600	0.40046600	-0.38495300
H	-6.45213500	-0.15032000	-1.89448100
C	-8.07795700	0.80793500	0.93536800
H	-7.11865500	1.29674000	2.80542800
H	-8.74012700	0.26370700	-1.04335600
H	-9.08101100	0.98922400	1.31037300
H	-3.43951000	1.38876900	-3.27669100
H	-3.61531400	3.12543400	-3.32426000

### TS10



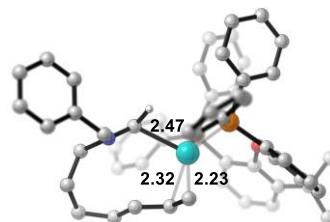
C	-3.22437100	-1.17944500	-0.09540100
C	-4.57930200	-1.22911600	-0.44113100
C	-5.06058800	-2.43842300	-0.95499500
C	-4.22297900	-3.54658400	-1.09102200
C	-2.87702200	-3.46316000	-0.73644300
C	-2.34355700	-2.26128800	-0.24676600
H	-6.10221800	-2.52810300	-1.24308000



H	-4.62232400	-4.48052500	-1.47490800
H	-2.23643700	-4.32984200	-0.85487100
C	-5.44526200	0.00913600	-0.16857700
C	-6.70326500	0.03579300	-1.05407600
H	-7.31881600	0.91080300	-0.82646000
H	-6.45281000	0.05558800	-2.11995600
H	-7.33042300	-0.83933100	-0.86198000
C	-5.88752800	-0.02263700	1.32344800
H	-6.47887600	0.86802600	1.56315200
H	-6.50079700	-0.90952800	1.51778200
H	-5.02450200	-0.05268900	1.99612000
C	-4.56564300	1.24832200	-0.38638100
C	-5.02458100	2.47997100	-0.86696200
C	-3.21652400	1.17164500	-0.02671100
C	-4.16683500	3.57609400	-0.96674500
H	-6.06100100	2.59342100	-1.16524300
C	-2.32534900	2.25248300	-0.10205900
C	-2.82890100	3.46742500	-0.58764200
H	-4.54388500	4.52262200	-1.34234000
H	-2.17509200	4.32609400	-0.68476700
O	-2.69282200	-0.02092400	0.43335600
P	-0.55943600	-2.01387600	0.17235500
P	-0.54773600	1.93731400	0.27363100
C	-0.48830400	-2.30093800	1.99009100
C	-1.41745700	-3.11708100	2.65548000
C	0.56560200	-1.73307500	2.71983000
C	-1.28620600	-3.36281900	4.02235900
H	-2.24225500	-3.56200200	2.10718100
C	0.70114200	-1.98809400	4.08558600
H	1.27365000	-1.07636500	2.22230100
C	-0.22460700	-2.80364600	4.73814200
H	-2.01166400	-3.99426200	4.52767800
H	1.52046400	-1.53917000	4.63912900
H	-0.12339900	-2.99916000	5.80198000
C	0.23566000	-3.53711600	-0.52143200
C	0.19819000	-3.74548200	-1.91345300
C	0.95449200	-4.44301900	0.27252000
C	0.84335400	-4.83868000	-2.49068200
H	-0.35750400	-3.05788300	-2.54669600
C	1.61220000	-5.53126000	-0.30980800
H	0.99677900	-4.30942800	1.34833500
C	1.55654100	-5.73482100	-1.68833000
H	0.78666900	-4.99371800	-3.56478300
H	2.15974900	-6.22521900	0.32186500
H	2.06144600	-6.58568800	-2.13652900
C	-0.44913800	1.78263600	2.11684500
C	-1.56848000	1.62392600	2.94411200
C	0.82379000	1.86827000	2.70838900
C	-1.41728800	1.55104100	4.33125800
H	-2.56372300	1.57351200	2.51773800
C	0.97131200	1.80100700	4.09251400
H	1.70388800	2.01944400	2.08817800
C	-0.15122100	1.63971500	4.90922600
H	-2.29613500	1.43466300	4.95926200
H	1.96101500	1.88483200	4.53341500
H	-0.03908100	1.59277900	5.98866600
C	0.27379600	3.58500500	0.07577300
C	-0.13586700	4.69250500	0.84173900
C	1.37264100	3.73231900	-0.78037100
C	0.51722100	5.91804800	0.72219200
H	-0.96045000	4.59358000	1.54169900
C	2.03266500	4.95927600	-0.89563700
H	1.72120600	2.87584200	-1.34610000
C	1.60120600	6.05562000	-0.15033300

H	0.18553300	6.76467600	1.31655200
H	2.88343600	5.05555100	-1.56484800
H	2.11061600	7.01086900	-0.23909600
Pd	0.29180600	0.08079600	-0.98835300
C	2.56213500	-1.18322800	-1.79003700
H	2.04435700	-1.61019900	-0.94245100
H	2.69563300	-1.88745200	-2.60523100
C	-0.97542300	0.94911800	-3.33973300
H	-1.44889800	-0.02794100	-3.44124600
C	-1.67744900	2.05049000	-3.65710000
H	-1.24226200	3.04490400	-3.59197900
H	-2.70660400	1.98928500	-3.99599600
C	0.43266000	0.95719800	-2.91438700
H	0.89818100	1.94063600	-2.95881900
C	1.27469800	-0.16815900	-3.26187600
H	0.71887200	-1.03783600	-3.61463900
C	2.47812900	0.12900400	-4.17859500
H	2.08941600	0.66661500	-5.05329300
H	2.87298100	-0.82072800	-4.56577500
C	3.64151600	0.92780600	-3.56834000
C	4.46209900	0.08772200	-2.58792300
H	4.90163900	-0.77023000	-3.11358400
H	5.28665400	0.65844700	-2.15438800
N	3.63526200	-0.41792300	-1.48553500
C	3.73669800	0.27561700	-0.19488800
H	3.53812600	1.34758400	-0.33247900
H	2.93152500	-0.11233500	0.43853800
C	5.08860900	0.08710600	0.46756600
C	5.59712500	-1.19875200	0.70105900
C	5.83451100	1.19748800	0.87868400
C	6.82606600	-1.36753900	1.33667600
H	5.03115900	-2.06917900	0.37727700
C	7.06501700	1.03021500	1.51926300
H	5.45123800	2.20004500	0.69975500
C	7.56273200	-0.25256000	1.74838200
H	7.21071100	-2.36830100	1.51214000
H	7.63382500	1.90102900	1.83253800
H	8.52053900	-0.38552900	2.24308200
H	3.27129700	1.83494100	-3.07303100
H	4.30684900	1.26104300	-4.37322000

### CP13

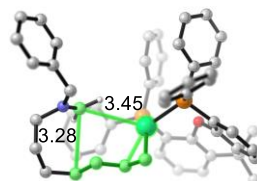


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C	-4.36073600	-1.25546100	-1.40945800
C	-4.69473500	-2.54757700	-1.83338000
C	-3.91079300	-3.64711700	-1.48046100
C	-2.76600300	-3.47876700	-0.70123900
C	-2.38274500	-2.19999400	-0.27455200
H	-5.58083000	-2.70612600	-2.43803500
H	-4.19699000	-4.64103200	-1.81111600
H	-2.16427800	-4.34008900	-0.43175500
C	-5.21075100	-0.00349400	-1.66500200
C	-6.11351100	-0.16457400	-2.90050300
H	-6.73503300	0.72376000	-3.04491400
H	-5.53124300	-0.33210900	-3.81273400
H	-6.80273300	-1.00391500	-2.77074400

C	-6.11067000	0.23711300	-0.41793000
H	-6.70861900	1.14552600	-0.55103900
H	-6.79160300	-0.60885900	-0.27229500
H	-5.51136400	0.35191000	0.49082800
C	-4.25334500	1.18825700	-1.80666000
C	-4.48353500	2.29762400	-2.62787600
C	-3.09601900	1.20720600	-1.01915000
C	-3.59948900	3.37705200	-2.64127500
H	-5.36231900	2.32901600	-3.26245200
C	-2.18154200	2.27430100	-1.00503500
C	-2.46138200	3.36928800	-1.83602900
H	-3.79974700	4.23017000	-3.28252500
H	-1.78037200	4.21212600	-1.86432900
O	-2.80673600	0.13057600	-0.19989200
P	-0.83380300	-1.84303500	0.66304100
P	-0.61700900	2.10611800	-0.02681000
C	-1.44089000	-1.46730800	2.36378100
C	-2.68803300	-1.91350900	2.82950300
C	-0.59851800	-0.77084500	3.24183700
C	-3.07642300	-1.67326700	4.14856900
H	-3.35411300	-2.45429400	2.16411000
C	-0.98365000	-0.53876600	4.56238800
H	0.35930500	-0.39690900	2.89036600
C	-2.22357100	-0.99006900	5.01801500
H	-4.04421500	-2.02345800	4.49683200
H	-0.32222200	0.00551600	5.22962300
H	-2.52623100	-0.80635200	6.04505300
C	-0.05494400	-3.50842100	0.88099000
C	0.76423700	-3.99509100	-0.15243600
C	-0.23131000	-4.29766000	2.02923100
C	1.37197000	-5.24796100	-0.05127500
H	0.92281100	-3.38927700	-1.03954900
C	0.38784200	-5.54536000	2.13311000
H	-0.85360600	-3.94366600	2.84412400
C	1.18697500	-6.02563700	1.09422300
H	1.98919200	-5.61678000	-0.86649500
H	0.24054100	-6.14351900	3.02798600
H	1.66323900	-6.99846900	1.17696400
C	-1.10676800	2.51410100	1.71156700
C	-2.43627900	2.56941900	2.14913200
C	-0.08034600	2.78012300	2.63530300
C	-2.73236100	2.88911600	3.47702500
H	-3.24793800	2.37936100	1.45507800
C	-0.37731600	3.10936500	3.95636000
H	0.95914400	2.76183500	2.31455000
C	-1.70758000	3.16348900	4.38219800
H	-3.76935100	2.93389000	3.79810100
H	0.42810400	3.33174600	4.65139300
H	-1.94162900	3.42380400	5.41058500
C	0.34392200	3.62919100	-0.45921100
C	-0.03627200	4.90671800	-0.00974100
C	1.50636100	3.51046400	-1.23439200
C	0.72078500	6.03006100	-0.34218700
H	-0.92212000	5.02251800	0.60752200
C	2.26641300	4.63494000	-1.56634100
H	1.81327500	2.52846800	-1.57970200
C	1.87339200	5.89730100	-1.12163300
H	0.41253700	7.01009900	0.01111400
H	3.16338500	4.52435000	-2.16978300
H	2.46258300	6.77369200	-1.37615400
Pd	0.26592200	-0.18232000	-0.76499600
C	2.44525400	-0.67210100	0.29906900
H	2.14713600	0.24675700	0.79298400
H	2.10696000	-1.62229800	0.69019600

C	0.74478800	-0.99961100	-2.88772600
H	-0.05715900	-1.71232600	-3.07007800
C	0.48165700	0.37037700	-2.90955600
H	1.29645500	1.07098700	-3.07694300
H	-0.50545800	0.74456300	-3.16874800
C	2.11493000	-1.48635100	-2.92197700
H	2.85742700	-0.70473300	-2.77604400
C	2.54085700	-2.75265900	-3.05126300
H	1.81940800	-3.54636800	-3.24552300
C	3.97793500	-3.17096200	-2.87414600
H	4.46322000	-3.33880800	-3.84754900
H	3.99682600	-4.15168500	-2.37689600
C	4.84570600	-2.19629800	-2.05408000
C	4.34865900	-1.93554700	-0.60927800
H	3.70809900	-2.75441000	-0.27391900
H	5.21334400	-1.89282700	0.06128900
N	3.59973200	-0.67565900	-0.35407800
C	4.28098100	0.60388900	-0.66125700
H	4.42517300	0.67186200	-1.74418400
H	3.58718800	1.40120400	-0.38045700
C	5.61217400	0.75356700	0.04991400
C	5.66652000	0.82612300	1.44942300
C	6.80113000	0.83956900	-0.68322100
C	6.88908500	0.97695800	2.10178700
H	4.75003700	0.76801900	2.03303900
C	8.02645600	0.99630600	-0.03118400
H	6.77127000	0.79233100	-1.76941500
C	8.07205100	1.06237900	1.36155500
H	6.91982500	1.03416800	3.18599100
H	8.94167500	1.06601900	-0.61171500
H	9.02394400	1.18319100	1.87025500
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H	5.85083700	-2.62539200	-1.97524000

### TS11

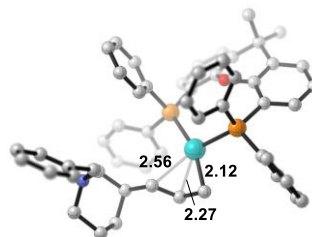


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C	-3.66429400	-4.25474200	-0.49055300
C	-2.41364800	-3.83461400	-0.03783500
C	-2.14560000	-2.47089200	0.14980700
H	-5.62878600	-3.67545000	-1.12204700
H	-3.85677000	-5.31352400	-0.63662000
H	-1.64081800	-4.57023600	0.15558400
C	-5.52229100	-0.86745200	-0.74064500
C	-6.62148800	-1.30368300	-1.72467600
H	-7.38332000	-0.52511400	-1.82473600
H	-6.21662600	-1.52200400	-2.71854500
H	-7.13836900	-2.19524000	-1.35800500
C	-6.17754000	-0.58031800	0.64174400
H	-6.91701700	0.22326300	0.55213000
H	-6.68334100	-1.47774100	1.01527000
H	-5.43104000	-0.27816000	1.38303000
C	-4.80502600	0.40657000	-1.21095300
C	-5.34683600	1.35047800	-2.09027800
C	-3.53925100	0.68179700	-0.68232100
C	-4.65055300	2.51843400	-2.40371700

H	-6.32089900	1.18124600	-2.53596000
C	-2.81407600	1.85241100	-0.95819700
C	-3.40008700	2.77192200	-1.84027800
H	-5.08723900	3.23848700	-3.08941000
H	-2.87202700	3.68150500	-2.10177500
O	-2.94013900	-0.23624300	0.16184700
P	-0.49364200	-1.77454500	0.61454100
P	-1.09889400	2.01348100	-0.27287700
C	-0.67692300	-1.45801900	2.42597400
C	-1.48924200	-2.26061000	3.24405600
C	0.05766500	-0.41882600	3.01213500
C	-1.55374200	-2.03122100	4.61841700
H	-2.07245600	-3.06587700	2.80715400
C	-0.00222400	-0.19271300	4.38912300
H	0.65711900	0.23381600	2.38359600
C	-0.80658700	-1.00000700	5.19405100
H	-2.18755900	-2.65768800	5.24005100
H	0.56112700	0.62628300	4.82609900
H	-0.85961300	-0.82204500	6.26454200
C	0.61339100	-3.26750800	0.61209600
C	0.84430000	-3.94350200	-0.60095200
C	1.33921300	-3.67024000	1.74538500
C	1.75529400	-4.99809100	-0.67371400
H	0.30316000	-3.64176700	-1.49260900
C	2.26752300	-4.71441800	1.66709200
H	1.17631200	-3.17721600	2.69785000
C	2.47717800	-5.38402500	0.46102900
H	1.90009000	-5.52081200	-1.61557500
H	2.81372700	-5.01229200	2.55816200
H	3.18694500	-6.20466000	0.40543900
C	-1.35955300	2.49191200	1.50236300
C	-2.57393900	2.33532400	2.18239700
C	-0.26620700	3.04059400	2.19605300
C	-2.69231500	2.71823600	3.52143600
H	-3.43898800	1.92910300	1.67030400
C	-0.38762900	3.43099900	3.52837100
H	0.68054400	3.19123500	1.68189400
C	-1.60408200	3.26848200	4.19768500
H	-3.64415800	2.59483100	4.03081800
H	0.46335700	3.87205700	4.04120800
H	-1.70315700	3.57598900	5.23494400
C	-0.50241000	3.64380800	-0.92284800
C	-1.14074000	4.85313000	-0.59100200
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C	-0.65276000	6.06857500	-1.06848800
H	-2.01705300	4.84455300	0.05062800
C	1.14386900	4.91053100	-2.19294100
H	1.16109800	2.76602100	-1.96040600
C	0.49002400	6.09993300	-1.87348600
H	-1.16034900	6.99298500	-0.80723900
H	2.03740600	4.92919600	-2.81146000
H	0.87002400	7.04851600	-2.24237300
Pd	-0.00953100	-0.03600300	-1.00328700
C	3.14635800	-1.19659100	-0.22627200
H	2.34620800	-0.57291900	0.17079900
H	3.01037100	-2.27088300	-0.27575800
C	0.66932500	-0.91415900	-2.98834900
H	0.02385200	-1.77126100	-3.17179200
C	0.14488900	0.38290800	-3.12886200
H	0.81517900	1.20563000	-3.36785600
H	-0.87936500	0.52410100	-3.46701800
C	2.11062000	-1.15464000	-3.07754700
H	2.72203100	-0.25281200	-3.00414900
C	2.71443600	-2.34195400	-3.27048100

H	2.08671400	-3.22460700	-3.38943000
C	4.19697000	-2.60531600	-3.40475900
H	4.43806800	-2.76123500	-4.46762500
H	4.43171500	-3.56753800	-2.92472600
C	5.17750700	-1.54995500	-2.85819200
C	5.29203800	-1.47565900	-1.32232200
H	5.25123100	-2.47612100	-0.88344900
H	6.23668400	-1.01467600	-1.02496400
N	4.22660500	-0.66439500	-0.67167100
C	4.44144100	0.81288700	-0.61221400
H	4.66365400	1.13957500	-1.63223200
H	3.48500200	1.25298900	-0.31766100
C	5.56408700	1.18741200	0.32987300
C	5.40760400	1.03218600	1.71465900
C	6.76525700	1.70346800	-0.17222000
C	6.44033500	1.38349600	2.58204600
H	4.47584800	0.64148200	2.11890800
C	7.79862000	2.05856100	0.69745900
H	6.89048800	1.84116700	-1.24389600
C	7.63777100	1.89608900	2.07391700
H	6.31047600	1.26343700	3.65348200
H	8.72413700	2.46320200	0.29905500
H	8.44030200	2.17239800	2.75130000
H	4.96522400	-0.55778300	-3.27465900
H	6.18231600	-1.80797900	-3.21326700

### CP14

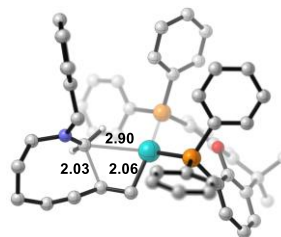


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C	-4.41790800	-2.49933900	0.69569500
C	-4.57980700	-3.85045400	0.37483800
C	-3.50465300	-4.61226200	-0.08723300
C	-2.24612700	-4.03534600	-0.24877600
C	-2.04452200	-2.67747900	0.04636200
H	-5.54990700	-4.32175800	0.48801700
H	-3.65030600	-5.66152700	-0.32531800
H	-1.42393100	-4.63747700	-0.61831400
C	-5.51271700	-1.59209700	1.27246100
C	-6.92357400	-2.11981900	0.96221800
H	-7.68518000	-1.47158500	1.40554300
H	-7.10859000	-2.18540000	-0.11514900
H	-7.07078900	-3.11152800	1.39990100
C	-5.33314300	-1.52193500	2.81705500
H	-6.07951400	-0.84929300	3.25392800
H	-5.46247100	-2.51628100	3.25818300
H	-4.33895600	-1.15445000	3.08919200
C	-5.28409200	-0.19099900	0.69061000
C	-6.29454900	0.72353700	0.37935300
C	-3.96303400	0.22873800	0.49626100
C	-5.98674700	2.00355500	-0.08628400
H	-7.33488800	0.44549700	0.50777000
C	-3.61656600	1.48694400	-0.00879800
C	-4.66136100	2.38670500	-0.27907300
H	-6.78607100	2.70476900	-0.30546300
H	-4.44017500	3.37965200	-0.65131900
O	-2.92217800	-0.61914700	0.80640300

P	-0.41127500	-1.83033200	-0.13420100
P	-1.84222500	1.90591600	-0.28956400
C	0.32705400	-1.97086200	1.54514000
C	0.11289200	-3.09379100	2.36257200
C	1.12380200	-0.92153900	2.02710000
C	0.70348200	-3.16966100	3.62401200
H	-0.52040600	-3.90643600	2.01933100
C	1.71245500	-0.99843300	3.29104400
H	1.26471600	-0.03228500	1.41983500
C	1.50633400	-2.12461600	4.08879800
H	0.53189400	-4.04326500	4.24641800
H	2.32156900	-0.17551700	3.65384700
H	1.96130900	-2.18512800	5.07326200
C	0.47656900	-3.05557300	-1.19251400
C	0.12937800	-3.09830100	-2.55543900
C	1.45392000	-3.93799900	-0.71374900
C	0.73900000	-4.01056700	-3.41596200
H	-0.62970800	-2.42152900	-2.94237400
C	2.07050700	-4.84625800	-1.58103600
H	1.73628200	-3.92536900	0.33401400
C	1.71459300	-4.88666600	-2.92943200
H	0.45383700	-4.03843400	-4.46395300
H	2.82548400	-5.52591400	-1.19589800
H	2.19154900	-5.59688300	-3.59861800
C	-1.21941500	2.43769600	1.36265300
C	-2.07214100	2.59965500	2.46397000
C	0.15123400	2.70828700	1.51808200
C	-1.56225900	3.02216700	3.69382300
H	-3.13427800	2.40127400	2.36616700
C	0.65566900	3.14202800	2.74371500
H	0.82598700	2.58579300	0.67475100
C	-0.20143500	3.29557800	3.83660500
H	-2.23370500	3.14101700	4.53932400
H	1.71567400	3.35745800	2.84604100
H	0.19049500	3.62752600	4.79362000
C	-1.99211500	3.47065000	-1.26033400
C	-1.63047800	4.72039600	-0.74050700
C	-2.48874000	3.39637900	-2.57460400
C	-1.75723000	5.87316700	-1.52280000
H	-1.25624900	4.80368500	0.27428600
C	-2.62428200	4.54831900	-3.34704500
H	-2.78170800	2.43514100	-2.99149600
C	-2.25359800	5.79106400	-2.82293800
H	-1.47231900	6.83545200	-1.10711700
H	-3.01630700	4.47690000	-4.35764800
H	-2.35406000	6.68821800	-3.42675200
Pd	-0.19047700	0.38886600	-1.18246700
C	3.94007500	-1.40389800	-0.98033200
H	3.27451000	-1.53461200	-0.12073400
H	4.34302700	-2.39793600	-1.22140900
C	1.31262100	0.75899600	-2.84568400
H	1.08858500	0.20688200	-3.75783700
C	0.52324100	1.89921100	-2.49490300
H	0.97135500	2.67631000	-1.87648300
H	-0.20049100	2.27405800	-3.21129500
C	2.24783800	0.24942700	-1.95788000
H	2.51337100	0.88559100	-1.11459300
C	3.13800400	-0.93543200	-2.22783100
H	2.51252200	-1.76872100	-2.56876700
C	4.14487600	-0.61822400	-3.37751800
H	3.61505600	-0.20061000	-4.24179200
H	4.57542200	-1.57527600	-3.70427500
C	5.27832000	0.30990200	-2.91955600
C	5.97958000	-0.28027700	-1.68352100

H	6.46571600	-1.22520400	-1.96861500
H	6.76761700	0.38487700	-1.31843000
N	5.05850800	-0.55896000	-0.57969200
C	4.78693400	0.56912200	0.30700300
H	4.47351100	1.48899800	-0.22389800
H	3.93916700	0.27586700	0.94199700
C	5.96897800	0.92437200	1.19760000
C	6.71012000	-0.07927400	1.83582100
C	6.30560200	2.26253500	1.42933500
C	7.75895400	0.25154600	2.69323400
H	6.46453900	-1.11910400	1.64022000
C	7.35352500	2.59762000	2.29055600
H	5.74685800	3.05133000	0.92848700
C	8.08231500	1.59161200	2.92579600
H	8.32747600	-0.53655100	3.17996500
H	7.60530900	3.64173500	2.45599100
H	8.90150200	1.84803700	3.59184300
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### TS12

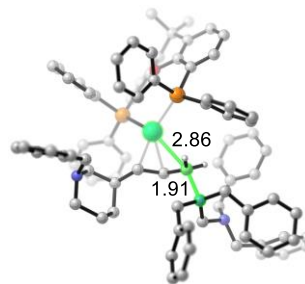


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C	-3.44772500	-4.15770600	-1.57651200
C	-2.22249100	-3.80635900	-1.01515100
C	-2.00769500	-2.50789400	-0.52382600
H	-5.40929000	-3.50606200	-2.14436300
H	-3.59951500	-5.16400100	-1.95482800
H	-1.41957100	-4.53476100	-0.98091300
C	-5.41247500	-0.84295100	-1.18728600
C	-6.42890300	-1.07165400	-2.31963600
H	-7.20884000	-0.30495000	-2.29908000
H	-5.95278400	-1.05633100	-3.30566800
H	-6.93864100	-2.03139600	-2.19645900
C	-6.16314700	-0.88666400	0.17561900
H	-6.93210600	-0.10695000	0.21107800
H	-6.64950000	-1.85939700	0.30784800
H	-5.47806900	-0.73137800	1.01507100
C	-4.71927200	0.52188200	-1.30896100
C	-5.23597700	1.63646300	-1.98087300
C	-3.50441400	0.69768300	-0.64254300
C	-4.56850900	2.86304700	-1.96255300
H	-6.16986600	1.55506000	-2.52597200
C	-2.82599100	1.92405500	-0.56517800
C	-3.37591000	3.01451700	-1.25366100
H	-4.98595800	3.71031000	-2.49787300
H	-2.87287200	3.97498100	-1.24441100
O	-2.89683800	-0.36962000	-0.01557900
P	-0.33935600	-1.92933900	0.03009500
P	-1.22090600	1.91991500	0.32797600
C	-0.19173200	-2.40841800	1.79959600
C	-1.22379400	-3.04738400	2.49981100
C	1.00568400	-2.10622700	2.47213400
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H	-2.15463900	-3.28966900	1.99701400
C	1.17339600	-2.45730500	3.81094700
H	1.82091600	-1.61137900	1.94936100
C	0.13750600	-3.09149900	4.50283300
H	-1.86820800	-3.87298000	4.37934100
H	2.11185800	-2.23231200	4.31019200
H	0.26463200	-3.36022100	5.54770900
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C	0.85162300	-3.00159300	-2.26205000
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C	2.44817000	-4.81630700	-2.34816800
H	1.72011200	-3.75417500	-4.08160700
H	2.96410600	-5.69264700	-0.44781700
H	3.09453200	-5.47531700	-2.92062300
C	-1.62907600	1.48660400	2.07073300
C	-2.92574600	1.61881200	2.58937300
C	-0.58552900	1.09921000	2.92289800
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H	-4.17636600	1.47758300	4.33338300
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C	0.12964500	6.32282800	0.98846300
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H	3.10771700	2.65582200	-2.57782900
C	3.80419700	1.48328700	-4.16532600
H	3.59594700	0.65793300	-4.84703400
C	5.23098200	1.96459800	-4.05156300
H	5.34852900	3.01818100	-4.33727700
H	5.86336600	1.39163600	-4.73911900
C	5.73836000	1.76760500	-2.59505300
C	5.29614100	0.43776400	-1.92483900
H	5.29012200	-0.36981100	-2.66438000
H	6.04817600	0.16878700	-1.17243000
N	4.00060400	0.40129500	-1.21623000
C	3.95326100	1.02630700	0.10143900
H	4.36859000	2.04198400	0.04430600
H	2.89379300	1.15008500	0.36272500

C	4.66651300	0.25963300	1.21023000
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C	5.81248800	0.28569000	3.35386100
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C	5.87950000	-1.10932800	3.34551300
H	5.40555200	-2.90396200	2.24754800
H	6.23648600	0.84728600	4.18161600
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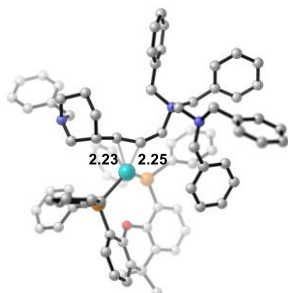


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H	-6.57156500	-4.64320300	-2.28821700
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H	-6.25753700	-3.13980000	-1.39921700
C	-3.87104600	-4.45852600	-1.73724700
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C	-2.42009800	-4.80931700	-3.65561000
H	-3.83261400	-6.25153600	-2.93364000
C	-2.24979300	-2.72512900	-2.41639400
C	-1.84292100	-3.55436900	-3.47384000
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H	-1.05859400	-3.22468600	-4.14538900
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P	-1.42746300	-1.11537700	-2.00642600
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H	-6.08315600	-0.55280700	2.44275300
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C	-7.00857300	1.88582800	0.25966400
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H	-5.68466500	2.87270700	-1.13009400	C	-2.14977500	7.49193800	-2.23933300
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H	-1.26804500	-1.37012500	3.51261300	H	1.18794500	4.40295600	1.16233100
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C	-2.39191000	0.57451500	6.06801100	H	4.94419000	1.34670200	1.25819600
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C	-2.17129900	1.50121300	-2.69609900	H	2.47207400	2.45480500	-1.15659100
C	-4.20781200	0.78522600	-4.45421600	H	3.36524500	0.96877100	1.95445200
H	-3.70186000	-1.25152100	-3.98491900	N	4.59714800	-0.68514400	1.43087800
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C	1.08155800	-2.16509900	-2.68969600	C	6.79378100	-2.60331200	3.41433800
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H	1.62356500	0.00854500	-5.85186500	H	8.34932400	-4.24537600	0.27280700
H	2.97069800	-3.07023500	-3.16054200	H	7.56988300	-4.29313200	4.50273400
H	3.34061600	-1.66613400	-5.19209300	H	8.55800700	-5.36087600	2.48529100
Pd	-1.15225100	-0.15227500	0.29294700	C	3.03250500	-2.69650900	1.32054200
C	-1.74910400	3.19487700	2.21443300	C	3.72598600	-3.33794200	0.28583300
H	-2.53807800	2.62824900	1.71304800	C	1.76138900	-3.17196300	1.67215800
H	-2.10683100	3.40555300	3.23179900	C	3.16424400	-4.43547400	-0.37112500
C	0.86378500	0.56691300	1.02007300	H	4.71547000	-2.98675500	0.01450000
H	1.07087400	0.04606100	1.95384900	C	1.19575600	-4.26657800	1.01455800
C	1.66180700	0.18522600	-0.11913700	C	1.89859900	-4.90495900	-0.00998900
H	1.38290000	0.59299100	-1.08545700	H	3.72507800	-4.93684800	-1.15604400
H	1.96593600	-0.85469600	-0.16209300	H	1.46698600	-5.76330700	-0.51708600
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H	0.41195300	3.44899900	3.97827000	C	5.64869900	4.79237400	-1.78901100
C	0.81599600	4.56645300	2.18321100	H	4.17641300	3.42422900	-2.55321600
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H	-0.84091800	5.56621400	3.14690900	H	6.28147100	5.34880700	1.50752600
H	-0.45873000	6.23158900	1.55915700	H	5.95642500	5.12336300	-2.77659200
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H	-0.66791400	4.28239500	-0.40177000	C	5.99090400	-0.92804200	-2.28322200
H	-2.30903400	3.66843000	-0.22446000	C	6.53116200	1.08556600	-1.08463100
C	-2.18241700	5.79020100	-0.50103300	C	7.33297100	-1.10103200	-2.61974100
C	-3.27836800	6.43729800	0.08524900	H	5.25773200	-1.65161100	-2.63137100
C	-1.62144300	6.33361500	-1.66295700	C	7.88076100	0.90196300	-1.40331200
C	-3.80487600	7.59626800	-0.48470500	H	6.25254600	1.95639700	-0.50665600
H	-3.70149700	6.02839700	0.99809400	C	8.28867300	-0.18514600	-2.17469200

H	7.63138300	-1.95450500	-3.22238000
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### CP15

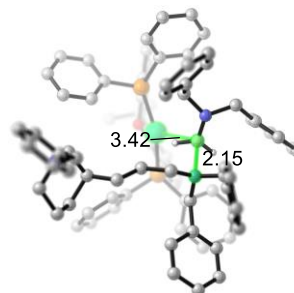


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C	-4.50245800	-4.29263800	0.58312000
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C	-4.59704100	-4.15887900	3.00734800
C	-4.11016100	-2.85208100	2.97449500
C	-3.78128300	-2.24055400	1.75544900
H	-5.19778700	-5.87572200	1.87264100
H	-4.83849600	-4.61995300	3.96065100
H	-3.98216900	-2.30745900	3.90295700
C	-4.80382200	-4.93952700	-0.77528900
C	-4.90655300	-6.47116700	-0.67468100
H	-5.15613300	-6.90831600	-1.64585700
H	-3.97224400	-6.92113100	-0.32225100
H	-5.70975900	-6.76108900	0.00894100
C	-6.16363200	-4.38200800	-1.28872200
H	-6.39612400	-4.80147900	-2.27406200
H	-6.96966400	-4.65104700	-0.59695200
H	-6.14000900	-3.29155200	-1.37744100
C	-3.70217400	-4.50268400	-1.74831000
C	-3.22912900	-5.27790000	-2.81132300
C	-3.16469100	-3.21707600	-1.60157100
C	-2.27054500	-4.77611700	-3.69305000
H	-3.61666500	-6.27885200	-2.96731900
C	-2.15474400	-2.70169300	-2.42855900
C	-1.73670500	-3.50325100	-3.50306500
H	-1.93289500	-5.38413600	-4.52732400
H	-0.97617400	-3.13725600	-4.18319800
O	-3.63193700	-2.39089600	-0.60252400
P	-3.18506500	-0.48658100	1.58657000
P	-1.37364500	-1.07206700	-1.99829800
C	-4.75065800	0.35048500	1.06310600
C	-6.00264900	0.01931500	1.60970000
C	-4.68774200	1.33337100	0.06642000
C	-7.15699300	0.67419500	1.18092000
H	-6.07746500	-0.75501300	2.36782100
C	-5.84415100	1.98740600	-0.36548300
H	-3.73215900	1.56765900	-0.39155300
C	-7.07950400	1.66160100	0.19417300
H	-8.11836500	0.41005700	1.61318600
H	-5.77591000	2.74012400	-1.14574900
H	-7.98113500	2.16666700	-0.14138500
C	-2.99417200	-0.02383200	3.37239200
C	-1.90869400	-0.57976600	4.07529600
C	-3.83015200	0.88003100	4.04256700
C	-1.67940600	-0.25815500	5.41244600
H	-1.24400700	-1.27688000	3.56887200

C	-3.58999200	1.21570400	5.37924300
H	-4.67400600	1.32544000	3.52634700
C	-2.51974500	0.64661700	6.06892600
H	-0.84533700	-0.71093000	5.94247500
H	-4.24918800	1.91915300	5.88078000
H	-2.34068800	0.90272900	7.10941400
C	-2.42356100	0.15823100	-2.90272800
C	-3.43403800	-0.21026400	-3.80194900
C	-2.19314800	1.52660900	-2.67474200
C	-4.19428500	0.76442700	-4.45364300
H	-3.62998200	-1.25971800	-3.99717600
C	-2.94290300	2.50127900	-3.33516100
H	-1.42509400	1.82756500	-1.96615200
C	-3.95023900	2.11949900	-4.22574500
H	-4.97665400	0.46076400	-5.14384200
H	-2.74997300	3.55435900	-3.14628800
H	-4.54085300	2.87452600	-4.73708300
C	0.14342800	-1.15351500	-3.07299000
C	0.35560000	-0.33090600	-4.18994900
C	1.13990100	-2.08554000	-2.72862400
C	1.52896700	-0.43940100	-4.94486500
H	-0.40192000	0.38630700	-4.48848500
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H	1.00272500	-2.73160200	-1.86494800
C	2.49791400	-1.38558400	-4.60995700
H	1.66962200	0.20215000	-5.81090800
H	3.03236500	-2.96590100	-3.23275600
H	3.39707400	-1.48522400	-5.21198800
Pd	-1.12527000	-0.12346000	0.30519600
C	-1.72482800	3.15055000	2.19474900
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H	-2.08298000	3.32504500	3.21875900
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H	1.12212600	0.07106000	1.84959400
C	1.85414700	0.29120100	-0.19693400
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H	2.08931600	-0.77106900	-0.24135600
C	0.01315800	1.67052500	0.99896600
H	-0.06365300	2.30737200	0.11580100
C	-0.40981700	2.32963300	2.30487200
H	-0.58269200	1.53239200	3.03663200
C	0.68669100	3.26128300	2.89897700
H	1.65625400	2.74348700	2.91268000
H	0.42896300	3.44681800	3.95192900
C	0.78653600	4.61803900	2.18306100
C	-0.59383200	5.29914200	2.14703300
H	-0.90106200	5.53300400	3.17706600
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N	-1.62691800	4.45779600	1.54473000
C	-1.67862200	4.49316700	0.08804000
H	-0.69664400	4.32533100	-0.39811000
H	-2.31670200	3.65869800	-0.22941600
C	-2.25536100	5.78884800	-0.46496700
C	-3.36077400	6.40020400	0.14166000
C	-1.72114900	6.36255200	-1.62498200
C	-3.92185600	7.55365700	-0.40637300
H	-3.76408700	5.96750600	1.05245800
C	-2.28413700	7.51497200	-2.17962000
H	-0.85161900	5.90705300	-2.09647800
C	-3.38765800	8.11342700	-1.57059800
H	-4.77794300	8.01846600	0.07575600
H	-1.85462100	7.94894800	-3.07877900
H	-3.82521100	9.01280500	-1.99517800
H	1.15658800	4.49295300	1.15582600

H	1.50894300	5.26556800	2.69668700
C	4.05500300	0.65324900	1.17024600
H	4.90532600	1.33215900	1.18424800
N	3.32162000	0.98432200	-0.14226700
C	4.02562900	0.50820100	-1.42049300
H	3.55047100	-0.43922700	-1.66883500
C	3.03214900	2.49373200	-0.16825300
H	2.48578500	2.68714900	0.75340600
H	2.32930800	2.62199500	-0.99431100
H	3.34549800	0.97346900	1.94560300
N	4.52378700	-0.69314700	1.35017500
C	5.88989400	-0.66324200	1.96949300
H	6.51367300	-0.05424000	1.30945500
H	5.84640600	-0.15419600	2.94724400
C	3.58610500	-1.60237200	2.04830200
H	2.78198300	-1.02356400	2.52046200
H	4.12966800	-2.07609600	2.87286000
C	6.55081400	-2.01063100	2.16382500
C	7.14923100	-2.68118400	1.08719200
C	6.62939400	-2.58584500	3.43947300
C	7.79005600	-3.90485900	1.27993000
H	7.12505800	-2.23240200	0.09843500
C	7.26938800	-3.81149400	3.63583700
H	6.19736900	-2.06408600	4.29103300
C	7.84854100	-4.47542800	2.55414700
H	8.25386300	-4.41006600	0.43702700
H	7.32140200	-4.24069800	4.63238600
H	8.35168100	-5.42652500	2.70349500
C	2.97752700	-2.71631500	1.20947700
C	3.69571400	-3.34815500	0.18612100
C	1.70400800	-3.20291500	1.53635000
C	3.15741900	-4.45023800	-0.48247900
H	4.68464900	-2.98488500	-0.07007400
C	1.16233500	-4.30255000	0.86732100
C	1.89059700	-4.93300600	-0.14415300
H	3.73619000	-4.94336200	-1.25955300
H	1.47613100	-5.79384100	-0.66108800
H	3.71144100	1.22272100	-2.18723700
C	4.17476000	3.46414000	-0.31893600
C	4.85078200	3.96494200	0.80557000
C	4.51714500	3.96020400	-1.58628400
C	5.87637400	4.90012600	0.66108800
H	4.56393600	3.63592900	1.80138700
C	5.53849800	4.89879400	-1.73254200
H	3.97589200	3.61826300	-2.46529900
C	6.22662100	5.36325400	-0.60954900
H	6.38996200	5.27803700	1.54024700
H	5.79107400	5.27221000	-2.72045600
H	7.01988300	6.09648000	-0.72175800
C	5.52908700	0.29410400	-1.49688100
C	5.94005100	-0.86873600	-2.17028000
C	6.51652300	1.20494100	-1.09301800
C	7.28653200	-1.11299100	-2.44101600
H	5.19276900	-1.58466400	-2.50140700
C	7.86774700	0.94879400	-1.34185800
H	6.24952800	2.12388200	-0.58905400
C	8.25975100	-0.20462100	-2.02139900
H	7.57283500	-2.01473700	-2.97512300
H	8.61340700	1.66687000	-1.01258300
H	9.31017000	-0.39192800	-2.22378800
H	1.13083600	-2.72494000	2.32809200
H	0.17562000	-4.66699600	1.13921000

### TS14

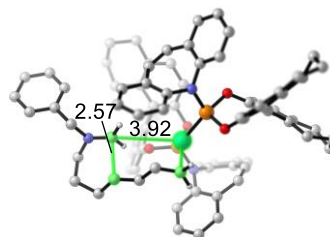


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C	-6.73862100	2.32850200	-2.20328300
C	-5.34637400	2.30607500	-2.17987400
C	-4.64303600	1.17745800	-1.72678700
H	-8.54541100	1.24000000	-1.82401800
H	-7.26061600	3.21573900	-2.54935200
H	-4.79503600	3.18161400	-2.50601600
C	-7.52226400	-1.24608200	-0.96829500
C	-9.00288600	-1.01657700	-0.62096700
H	-9.49438500	-1.96298000	-0.37743400
H	-9.12517700	-0.33493700	0.22760100
H	-9.54131100	-0.60248800	-1.47837200
C	-7.44690100	-2.21767000	-2.18288900
H	-7.92110000	-3.17318900	-1.93244900
H	-7.96846800	-1.78623100	-3.04463100
H	-6.41111900	-2.41633800	-2.47390000
C	-6.74553500	-1.86835600	0.19708600
C	-7.33717500	-2.58194900	1.24277600
C	-5.34604000	-1.76632400	0.17840400
C	-6.55754900	-3.19319700	2.22407700
H	-8.41639200	-2.67310300	1.29354300
C	-4.52752000	-2.37002200	1.15362500
C	-5.17013800	-3.09184800	2.17381700
H	-7.03232700	-3.74968500	3.02677600
H	-4.57546900	-3.56364300	2.94897100
O	-4.74366800	-1.05192700	-0.84111200
P	-2.78491900	1.15515200	-1.68593300
P	-2.67654900	-2.21725000	1.10768100
C	-2.32762100	0.59048500	-3.38625700
C	-3.20936200	0.63350500	-4.47720700
C	-1.02931100	0.09296600	-3.58736500
C	-2.79866300	0.19519000	-5.73842200
H	-4.22080500	1.00450600	-4.34465700
C	-0.61651700	-0.33353800	-4.84959700
H	-0.34638500	0.02923000	-2.74335100
C	-1.50242900	-0.28574300	-5.92855300
H	-3.49486200	0.22969200	-6.57196000
H	0.39199500	-0.71376800	-4.98866500
H	-1.18613100	-0.62744500	-6.91019500
C	-2.37896300	2.96396500	-1.70435000
C	-2.38815500	3.64163200	-0.47238200
C	-2.04795200	3.67979000	-2.86467500
C	-2.10066500	5.00523900	-0.40556600
H	-2.62723600	3.09491200	0.43712900
C	-1.74721900	5.04338200	-2.79532700
H	-2.02956600	3.17638200	-3.82637200
C	-1.77968600	5.71044400	-1.56982900
H	-2.12325300	5.51296100	0.55514300
H	-1.49358300	5.58364200	-3.70330500
H	-1.55695600	6.77296400	-1.52130500



C	-2.13116200	-3.77876300	0.28016500	C	1.54869900	2.78054600	-0.63807000
C	-2.81008400	-5.00025200	0.41847100	H	0.66964000	3.31549100	-0.26416800
C	-0.97916500	-3.73360700	-0.52087700	H	1.17822200	1.95354200	-1.25132000
C	-2.33937400	-6.14848800	-0.21988600	H	0.33039500	0.59198200	0.73697100
H	-3.71397000	-5.05660600	1.01703700	N	0.71544200	0.79529300	2.75572500
C	-0.50523400	-4.88411500	-1.15417600	C	0.48307700	1.56523800	4.01309600
H	-0.46925800	-2.78312500	-0.65920800	H	-0.04392700	0.86802700	4.67480900
C	-1.18469600	-6.09399100	-1.00433700	H	1.44928400	1.77720400	4.48014000
H	-2.87726600	-7.08573500	-0.10671200	C	1.02874400	-0.64848500	2.95255500
H	0.38678800	-4.83286800	-1.77309500	H	0.97427900	-1.11853300	1.96872400
H	-0.82214600	-6.98898900	-1.50225700	H	0.21236900	-1.06051100	3.55440900
C	-2.23585400	-2.48351700	2.89004400	C	-0.33216800	2.83007100	3.87400000
C	-1.43164400	-3.54262200	3.33467300	C	-1.70301500	2.75952100	3.57872600
C	-2.64761500	-1.51361300	3.82348800	C	0.24764100	4.08238700	4.11155200
C	-1.04599100	-3.62887400	4.67726200	C	-2.47407500	3.91999500	3.51728000
H	-1.10882000	-4.30834500	2.63638500	H	-2.16638600	1.79161800	3.40171000
C	-2.27419400	-1.60711100	5.16382300	C	-0.52383900	5.24587900	4.05259800
H	-3.27816700	-0.68987500	3.49625600	H	1.30353400	4.14917400	4.36255500
C	-1.46503800	-2.66536000	5.59494900	C	-1.88514100	5.16636700	3.75520000
H	-0.42467400	-4.45842900	5.00380300	H	-3.53621400	3.85136800	3.29961400
H	-2.62073000	-0.86087000	5.87446500	H	-0.06294800	6.20945800	4.24976200
H	-1.17448400	-2.74124400	6.63910700	H	-2.48925100	6.06870300	3.72245600
Pd	-2.10622900	-0.28000200	-0.00796700	C	2.36407200	-0.94590300	3.61074700
C	3.57438400	-3.07824200	-2.08130400	C	2.52551300	-0.84379300	5.00092900
H	3.41511400	-3.22422300	-1.00672900	C	3.44912100	-1.39183600	2.84245700
H	2.99853600	-3.85799100	-2.60393700	C	3.75178400	-1.13402700	5.60043200
C	2.66563200	-0.01277900	-0.68231700	H	1.68266200	-0.55877900	5.62498400
H	1.67521400	-0.42543300	-0.48692400	C	4.67538300	-1.69076400	3.44029500
C	3.17535700	1.07045800	0.23127300	C	4.83226800	-1.55212300	4.82042300
H	4.08951700	1.50754100	-0.18765400	H	3.85846100	-1.04897800	6.67813100
H	3.45842400	0.64245600	1.20009000	H	5.78410800	-1.78669100	5.28810600
C	3.40022300	-0.55150200	-1.66588100	H	2.52292000	2.64366700	2.54218800
H	4.39317900	-0.13920200	-1.85285300	C	2.36445500	3.73370800	-1.49058400
C	2.96843700	-1.70725500	-2.53011700	C	2.08894000	5.10790300	-1.44629600
H	1.87749800	-1.80637800	-2.42900000	C	3.35841400	3.27638200	-2.36863300
C	3.31075200	-1.48615400	-4.02525400	C	2.80793900	6.00884700	-2.23470100
H	2.98752600	-0.48824600	-4.34806000	H	1.29219000	5.47292700	-0.80260900
H	2.73156800	-2.21071400	-4.61589200	C	4.08342800	4.17498100	-3.15162000
C	4.80602500	-1.69981500	-4.31760000	H	3.55221900	2.21137600	-2.45427200
C	5.26579100	-3.07806700	-3.80863700	C	3.81499100	5.54430000	-3.08253200
H	4.74717400	-3.86128300	-4.38095800	H	2.57761200	7.06978800	-2.19084200
H	6.33806800	-3.22115600	-3.97175800	H	4.85206500	3.80527800	-3.82465600
N	4.97850800	-3.29724200	-2.38674900	H	4.37683700	6.24194500	-3.69706000
C	5.94957200	-2.71516200	-1.46225500	C	4.23271700	3.42896200	1.56978300
H	6.13306800	-1.63746400	-1.62991600	C	5.09842400	2.68241700	2.38517000
H	5.51210200	-2.79090900	-0.45670000	C	4.76429900	4.49802200	0.83502100
C	7.28764700	-3.43755100	-1.47980800	C	6.46055200	2.97764500	2.44778200
C	7.34315700	-4.83808900	-1.48048200	H	4.70307500	1.86455400	2.98433600
C	8.48580000	-2.71538400	-1.45239800	C	6.12582800	4.79840500	0.90033100
C	8.57068000	-5.49882200	-1.44835400	H	4.11511900	5.10318200	0.21191300
H	6.41474900	-5.40039500	-1.52142200	C	6.97883800	4.03783000	1.70200100
C	9.71744200	-3.37426100	-1.41622100	H	7.11222300	2.38744800	3.08602900
H	8.45664500	-1.62732400	-1.46084500	H	6.51796300	5.63325300	0.32630100
C	9.76236400	-4.76874500	-1.41371000	H	8.03764000	4.27560800	1.75296100
H	8.59934300	-6.58531700	-1.45111600	H	3.32952000	-1.53046700	1.77046300
H	10.63885100	-2.79822800	-1.39845300	H	5.50212800	-2.04249500	2.82951200
H	10.71840500	-5.28456100	-1.39037900				
H	5.40581900	-0.90892500	-3.84683300	<b>3</b>			
H	4.99084100	-1.62320300	-5.39619100	C	-3.31381400	-1.18392100	-1.83361400
C	0.50731100	1.29014800	1.54785500	H	-3.21000300	-0.32172500	-2.50170500
H	0.01111000	2.24920200	1.48693400	H	-3.65343300	-2.03133800	-2.44911900
N	2.20198200	2.14848200	0.54810500	C	-0.01304200	0.06516800	-1.20398200
C	2.74535900	3.10172300	1.57387400	H	0.42659600	-0.41797500	-2.07836000
H	2.14855600	4.01492700	1.50021100				

C	0.74539700	1.25508000	-0.68285100
H	0.20344300	1.70260100	0.17308400
H	0.77474600	2.02277800	-1.46789500
C	-1.15417900	-0.40700200	-0.68920000
H	-1.56370000	0.08446100	0.19439000
C	-1.92320200	-1.57771500	-1.24749400
H	-1.33502800	-1.98347500	-2.08297300
C	-2.12609200	-2.70981000	-0.20775800
H	-1.17677200	-2.93604800	0.29233800
H	-2.42280800	-3.62099500	-0.74838600
C	-3.22126100	-2.37138200	0.81697300
C	-4.53003900	-1.99720100	0.09811200
H	-4.89935600	-2.87841200	-0.44825000
H	-5.30956300	-1.71729100	0.81403400
N	-4.37222000	-0.90505700	-0.86678100
C	-4.40332900	0.43419100	-0.28557400
H	-3.71558000	0.56589300	0.57005200
H	-4.05082200	1.12889900	-1.05972700
C	-5.79862500	0.85312500	0.15614900
C	-6.92049800	0.54918000	-0.62674400
C	-5.97973800	1.59022900	1.33191500
C	-8.19112600	0.97877200	-0.24445100
H	-6.78242800	-0.03952800	-1.52883700
C	-7.25023200	2.02622800	1.71586500
H	-5.11796900	1.82500300	1.95391600
C	-8.36058500	1.72134600	0.92752300
H	-9.05202000	0.73412300	-0.86179200
H	-7.37192000	2.59636200	2.63339600
H	-9.35118700	2.05501900	1.22540600
H	-2.89897800	-1.54244200	1.46156400
H	-3.39544000	-3.22841000	1.48039900
N	2.14507000	0.93081700	-0.35236500
C	2.95761500	2.14900800	-0.23887400
H	2.66478200	2.80411800	-1.06990600
C	2.23402100	0.07576300	0.84232300
H	1.29834600	-0.49288400	0.89411300
H	2.27641400	0.68816900	1.76219000
H	2.72043600	2.70364600	0.69053900
C	3.37712700	-0.92401400	0.84708800
C	3.58962700	-1.76848600	-0.25110700
C	4.18042900	-1.08513500	1.98028800
C	4.58298300	-2.74559800	-0.21665600
H	2.97425600	-1.64305500	-1.13765400
C	5.17554600	-2.06512000	2.02091900
H	4.02925600	-0.43463400	2.83927000
C	5.38003200	-2.89897900	0.92170000
H	4.73601900	-3.39108000	-1.07818800
H	5.79308500	-2.17117200	2.90928800
H	6.15491300	-3.66072700	0.94865500
C	4.45819500	1.93589300	-0.31311800
C	5.03046200	1.25603600	-1.39684600
C	5.30305500	2.48037800	0.65911500
C	6.41320300	1.12038600	-1.50068200
H	4.37885600	0.82092700	-2.14928300
C	6.69075600	2.35066400	0.55718600
H	4.87133600	3.01194700	1.50475400
C	7.24952200	1.66937600	-0.52368000
H	6.84159200	0.58573400	-2.34469000
H	7.33157500	2.77874900	1.32386700
H	8.32815600	1.56367300	-0.60561700

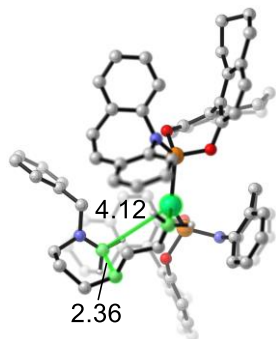


C	3.14629000	-1.83349200	1.69673000
H	2.30326000	-2.43975100	1.37629400
H	3.07416700	-0.75304400	1.62740100
C	0.13990400	-1.22969100	3.59259600
H	0.06407900	-2.30820900	3.45890100
C	-1.01371400	-0.48357900	3.54368500
H	-1.01242400	0.56814500	3.82300800
H	-1.98248700	-0.96724900	3.49184200
C	1.44341400	-0.70068800	3.92304900
H	1.52270000	0.38423000	3.98252300
C	2.55017200	-1.45367700	4.17039600
H	2.44278800	-2.53862900	4.22421500
C	3.87439300	-0.86518800	4.61241900
H	3.92142100	-0.87735000	5.71203900
H	3.91283100	0.19372300	4.32359000
C	5.15190300	-1.57898600	4.11292800
C	5.35729800	-1.60803000	2.59000400
H	5.32490900	-0.60098400	2.16379500
H	6.31426000	-2.06288100	2.32397500
N	4.28527600	-2.40369400	1.94552500
C	4.45666600	-3.87774000	1.90228000
H	4.67127100	-4.22072200	2.91988600
H	3.49063700	-4.29489600	1.60581500
C	5.56447900	-4.29564400	0.95920100
C	5.43330800	-4.09502300	-0.42252300
C	6.72357100	-4.90301000	1.45611500
C	6.44775100	-4.49554000	-1.29049800
H	4.53514900	-3.62889600	-0.82231000
C	7.73916800	-5.30673700	0.58614300
H	6.82975200	-5.07337700	2.52517400
C	7.60267400	-5.10182000	-0.78697700
H	6.33537800	-4.34137500	-2.35971800
H	8.63180200	-5.78182200	0.98205000
H	8.39041400	-5.41685100	-1.46494000
H	5.18190700	-2.60408700	4.50537000
H	6.02386900	-1.07010400	4.54003100
C	3.93356900	1.88663300	-1.15080700
C	3.75286100	1.84490500	0.23923000
C	4.58413200	2.55949700	1.10226600
C	5.56621400	3.38275900	0.56545000
C	5.69361600	3.55374100	-0.82062200
C	4.86345900	2.81635500	-1.68846900
C	3.10158700	0.99724600	-2.01929300
C	1.70327900	1.09522000	-1.94049600
C	0.86860400	0.37911100	-2.79323300
C	1.44316500	-0.45976300	-3.74045600
C	2.82911400	-0.65222300	-3.80145900
C	3.66631600	0.04988700	-2.91064400
H	4.43989800	2.47811600	2.17541800
H	6.21924100	3.94308200	1.23091700
H	-0.20675100	0.48198700	-2.70300000
H	0.80139100	-0.99690700	-4.43479200
C	3.38942000	-1.58396800	-4.86699700
H	3.41051200	-1.03989700	-5.82354600
H	2.70135700	-2.42471000	-5.02090100

TS11-Si

C	5.14573100	-0.31108600	-2.83000100	H	-3.44106800	3.69815300	-2.56507100
H	5.74947000	0.54847000	-2.53504600	C	-5.76987800	4.39024300	-1.40362500
H	5.26361000	-1.03816000	-2.00933500	H	-6.31698800	4.40716300	-2.35879800
C	5.69851700	-0.94237800	-4.11298300	H	-5.03204200	5.19977400	-1.47187600
H	5.75000000	-0.18609000	-4.90897000	C	-6.77299800	2.23204100	0.38068600
H	6.72478300	-1.28829100	-3.94001100	H	-7.38708200	1.33718200	0.49161200
C	4.80164200	-2.09719500	-4.56653400	H	-6.36412900	2.42355300	1.38570900
H	4.75923800	-2.85616600	-3.77056500	C	-7.63672400	3.43126200	-0.02660700
H	5.21437600	-2.59276600	-5.45298300	H	-8.19522400	3.19602400	-0.94418200
C	4.91332500	3.06648000	-3.19154700	H	-8.38080100	3.62813300	0.75424000
H	5.46543100	2.26071300	-3.69405000	C	-6.75969400	4.66287700	-0.26596000
H	3.89564100	3.02328100	-3.59497000	H	-6.21210500	4.90204500	0.65683300
C	6.70093800	4.57554300	-1.32923700	H	-7.37086900	5.54039600	-0.50720200
H	7.65104200	4.44245000	-0.79560900	C	-7.48999000	-0.41228500	-1.61862100
H	6.34453600	5.57918300	-1.05310900	H	-7.97082600	0.54424400	-1.37420400
C	6.92412700	4.52901800	-2.84433900	H	-6.72408800	-0.17520000	-2.36539500
C	5.57805600	4.39878400	-3.56015600	C	-8.75484200	-2.65914000	-0.10440600
H	5.70257600	4.45435800	-4.64768600	H	-9.36691800	-2.81854700	0.79278300
H	4.92595200	5.23554800	-3.27253700	H	-8.58308100	-3.66063200	-0.52715300
H	7.55825300	3.67008600	-3.10597800	C	-9.51565800	-1.81285800	-1.13001700
H	7.46123200	5.42779400	-3.16784100	C	-8.55396200	-1.33829900	-2.22129900
O	1.13545400	1.96083400	-1.01261600	H	-9.09015100	-0.80733600	-3.01641400
O	2.73320500	1.07201700	0.78873100	H	-8.07237600	-2.20835100	-2.69037900
P	1.06962900	1.48253000	0.58303200	H	-9.96446300	-0.93851700	-0.63795100
N	0.86175800	3.06440400	1.20111200	H	-10.34175800	-2.39565200	-1.55333400
C	0.74339200	4.26520800	0.41101900	O	-2.96978000	-0.57127300	-1.12916300
C	-0.54265000	4.77811100	0.13004900	O	-3.55362400	-0.85786100	1.36047100
C	1.88281300	4.90169200	-0.08609600	P	-2.26608800	-1.07433800	0.29549200
C	-0.63693000	5.90502900	-0.70943400	N	-2.20041600	-2.72768600	-0.18194500
C	1.76328800	6.02810700	-0.89816200	C	-2.78487600	-3.28389700	-1.37890200
H	2.85886000	4.49793000	0.15606500	C	-1.95816800	-3.55221200	-2.49285500
C	0.49770000	6.52675600	-1.21877800	C	-4.15691400	-3.53345500	-1.45065300
H	-1.62230900	6.30101200	-0.94235700	C	-2.56319100	-3.99711800	-3.68374100
H	2.65631900	6.50930500	-1.28707500	C	-4.73063500	-3.99715000	-2.63386600
H	0.39780000	7.39931100	-1.85796700	H	-4.77338200	-3.34620500	-0.58026700
C	0.45659500	3.19352200	2.57543800	C	-3.93383400	-4.21765000	-3.75987000
C	1.41814100	3.11196100	3.58904900	H	-1.93418700	-4.18984700	-4.54941500
C	-0.90460800	3.38670200	2.90011200	H	-5.80146900	-4.17464200	-2.67699400
C	1.04544300	3.17013700	4.93218300	H	-4.37760600	-4.56690400	-4.68763600
H	2.46051300	3.00937800	3.30471900	C	-1.32862300	-3.60733600	0.53951800
C	-1.26186100	3.41649700	4.26301700	C	-1.69401100	-4.05270600	1.81573100
C	-0.30474400	3.30973700	5.26815900	C	-0.10178600	-4.02185400	-0.03109700
H	1.80083800	3.10739500	5.71046100	C	-0.85149300	-4.88233800	2.55600000
H	-2.30833700	3.55079100	4.52519600	H	-2.65422500	-3.74228200	2.21510800
H	-0.60752400	3.35085100	6.31051900	C	0.73499100	-4.85901900	0.73594000
C	-1.76941700	4.21302000	0.68819000	C	0.37118300	-5.28690700	2.01107500
H	-2.66859200	4.39279100	0.10447300	H	-1.15371900	-5.22239700	3.54237800
C	-1.93119400	3.60171000	1.88366800	H	1.66040500	-5.21711200	0.28789800
H	-2.94598100	3.34172500	2.17832800	H	1.02228500	-5.95627200	2.56723500
C	-5.55521400	-0.49892000	0.04655600	C	-0.50309800	-3.44539900	-2.44912300
C	-4.86277100	-1.20294700	1.03922500	H	-0.01915900	-3.29550400	-3.41231600
C	-5.45538300	-2.25275000	1.73999600	C	0.30509000	-3.65483600	-1.38576500
C	-6.73542100	-2.65822000	1.38676200	H	1.37807600	-3.66183400	-1.57209000
C	-7.41107200	-2.07268600	0.30545500	Pd	-0.38607400	-0.16624300	1.33293200
C	-6.81623100	-0.99679300	-0.38192200				
C	-4.93825000	0.71994900	-0.56305800				
C	-3.68065200	0.62441700	-1.17961800				
C	-3.13586300	1.68383000	-1.89926100				
C	-3.84625200	2.87476600	-1.98107900				
C	-5.05159100	3.05265700	-1.28944400				
C	-5.58527600	1.98299900	-0.54270900				
H	-4.90867200	-2.73499400	2.54442300				
H	-7.20980300	-3.47175000	1.93105700				
H	-2.17267500	1.56521400	-2.38273400				

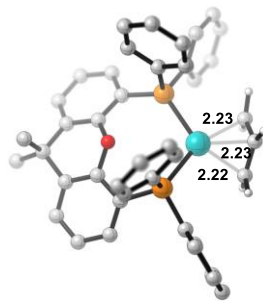
**TS11-Re**



Pd	0.18511500	0.54282400	1.51521500
C	-3.05988200	2.87304500	0.49424500
H	-2.55111800	1.92842900	0.35597800
H	-4.10988700	2.85312300	0.76318400
C	-0.91428500	1.58363900	3.26979400
H	-1.57086500	0.81200200	3.65902500
C	0.47056500	1.50026100	3.47015200
H	1.07605400	2.39678600	3.40565400
H	0.88129100	0.69631000	4.07623100
C	-1.52132700	2.83846000	2.88786400
H	-0.81749000	3.64248800	2.66316700
C	-2.86304100	3.10893100	2.83908100
H	-3.53737500	2.30036000	3.12039900
C	-3.49063600	4.50077800	2.84203300
H	-3.42715400	4.90463100	3.86202400
H	-4.56696600	4.39974100	2.64326500
C	-2.91389900	5.55236300	1.87023900
C	-3.19442100	5.25480900	0.38864800
H	-4.27220400	5.17250700	0.21017000
H	-2.80504200	6.03761300	-0.26520900
N	-2.56698200	3.97752400	-0.00735800
C	-1.18346000	4.02685900	-0.54045400
H	-0.55531100	4.54972700	0.18918000
H	-0.82287700	2.99586700	-0.59135700
C	-1.11797700	4.71390300	-1.88731600
C	-1.62316500	4.07784200	-3.03008200
C	-0.54981800	5.98840200	-2.00956000
C	-1.55982400	4.70986100	-4.27135800
H	-2.05974500	3.08509200	-2.94883600
C	-0.48586300	6.62133100	-3.25344900
H	-0.14736000	6.48727200	-1.13024000
C	-0.99274000	5.98256900	-4.38550400
H	-1.94726200	4.20773900	-5.15344300
H	-0.04039000	7.60847100	-3.33581700
H	-0.94274200	6.47099900	-5.35431700
H	-1.83533800	5.67720000	2.02751600
H	-3.36859000	6.52359800	2.09659200
C	-4.84455100	-0.96373100	-0.03753000
C	-4.27912400	-0.71738200	1.22002200
C	-4.94681200	-1.04966100	2.39812700
C	-6.16716900	-1.70788400	2.31376100
C	-6.70067200	-2.09818900	1.07589200
C	-6.03124000	-1.74074000	-0.11088500
C	-4.15311600	-0.43456900	-1.25357900
C	-2.81885200	-0.80259000	-1.49688600
C	-2.16322700	-0.43840500	-2.67000900
C	-2.83733900	0.33828300	-3.60492500
C	-4.13419300	0.81095200	-3.36063300
C	-4.78813000	0.45070800	-2.16423800
H	-4.49948600	-0.80395100	3.35631100
H	-6.69903400	-1.96936800	3.22578700
H	-1.14988100	-0.78527900	-2.83056500

H	-2.34413200	0.60079800	-4.53852700
C	-4.81362200	1.65992300	-4.42643500
H	-5.18914800	0.98810900	-5.21315100
H	-4.06936000	2.30075700	-4.91620300
C	-6.11387000	1.11577500	-1.80671100
H	-6.74167300	0.45564000	-1.20711000
H	-5.88692400	1.97008800	-1.14628300
C	-6.89028000	1.64373100	-3.01834300
H	-7.28068100	0.80066300	-3.60567800
H	-7.75866900	2.21849200	-2.67544600
C	-5.98069700	2.50206700	-3.90061800
H	-5.59546900	3.34710200	-3.31153400
H	-6.53842100	2.93135400	-4.74075700
C	-6.53366700	-2.24609000	-1.45858300
H	-7.05610200	-1.44415500	-1.99778700
H	-5.67337300	-2.51093000	-2.08336300
C	-7.96842200	-2.94027900	1.07309700
H	-8.69763200	-2.49700900	1.76360200
H	-7.72787400	-3.92884900	1.49186400
C	-8.58856200	-3.12773500	-0.31560900
C	-7.49091100	-3.43865500	-1.33507800
H	-7.91865300	-3.66520200	-2.31845600
H	-6.93514300	-4.33221400	-1.01744700
H	-9.11670700	-2.21277700	-0.61931500
H	-9.33723800	-3.92721600	-0.28229200
O	-2.13511100	-1.59046900	-0.58133500
O	-3.02842200	-0.11428400	1.31026900
P	-1.59630500	-0.92604400	0.85462500
N	-1.53219500	-2.40515100	1.69523900
C	-1.93957200	-3.68924500	1.17415300
C	-0.96144900	-4.53957900	0.61392000
C	-3.27865100	-4.08238500	1.21410100
C	-1.38788500	-5.75308400	0.04122100
C	-3.67277400	-5.29958700	0.66044900
H	-4.00816400	-3.42377900	1.66928000
C	-2.72520400	-6.13352700	0.06131200
H	-0.64464600	-6.40922200	-0.40505600
H	-4.71885100	-5.59137100	0.69072000
H	-3.02727100	-7.07909000	-0.37986300
C	-0.71373300	-2.45913700	2.87955300
C	-1.23003700	-2.00919900	4.09955600
C	0.60637200	-2.95366700	2.79851100
C	-0.43311800	-1.99242400	5.24347100
H	-2.26331800	-1.67735800	4.13661700
C	1.40046500	-2.90480200	3.96062100
C	0.89298300	-2.43178300	5.16695800
H	-0.84181200	-1.64039200	6.18639500
H	2.42421200	-3.26587800	3.90770000
H	1.52296600	-2.42080400	6.05200100
C	0.46722800	-4.23469600	0.63674200
H	1.05109300	-4.71097800	-0.14801100
C	1.15064600	-3.54764900	1.57970600
H	2.23335500	-3.51284900	1.49021100
C	4.56477900	-1.68309000	-0.56572900
C	4.36231900	-1.26132700	0.75446600
C	5.40137900	-1.24372500	1.68429300
C	6.68282500	-1.57627100	1.26677500
C	6.95683000	-1.86484600	-0.07875400
C	5.89919000	-1.90257000	-1.00798800
C	3.39553300	-1.84588700	-1.48496000
C	2.54021200	-0.75884300	-1.72126500
C	1.56235300	-0.80048900	-2.71165100
C	1.38969300	-1.97099900	-3.43840000
C	2.13428200	-3.12242200	-3.14973300

C	3.12564900	-3.07177700	-2.15068700
H	5.19201200	-0.97199300	2.71388300
H	7.49902600	-1.57259900	1.98556400
H	0.96816500	0.08765000	-2.89921300
H	0.64394400	-2.00822000	-4.22959800
C	1.87632500	-4.37717100	-3.97224400
H	2.36849200	-4.25414700	-4.94932100
H	0.80378100	-4.45824700	-4.18790000
C	3.81218300	-4.36146300	-1.71335000
H	4.82733300	-4.17376300	-1.36165200
H	3.27138600	-4.73539100	-0.82934000
C	3.80551900	-5.46100300	-2.78167800
H	4.47713600	-5.18465100	-3.60727200
H	4.19833400	-6.39043700	-2.35278100
C	2.38902400	-5.66727900	-3.32366700
H	1.72478800	-5.96010400	-2.49769100
H	2.36190500	-6.48550600	-4.05266100
C	6.19122200	-2.10416600	-2.49143500
H	5.93959000	-3.12853500	-2.79595200
H	5.53332300	-1.45215600	-3.07681100
C	8.40704500	-2.08854400	-0.48350200
H	8.88161500	-2.76562300	0.23845600
H	8.94499800	-1.13302500	-0.39123500
C	8.57926100	-2.61833200	-1.91047200
C	7.65838400	-1.84878900	-2.85933600
H	7.82806600	-2.14461700	-3.90108000
H	7.88084400	-0.77384900	-2.79559300
H	8.32664900	-3.68739600	-1.94876100
H	9.62823900	-2.53070500	-2.21554400
O	2.69585900	0.42860400	-1.01965700
O	3.09861100	-0.85666600	1.17827800
P	2.36201700	0.53617500	0.60879100
N	3.42669100	1.87596400	0.82173700
C	4.30621000	2.40820800	-0.19435300
C	3.93427600	3.58926800	-0.87428800
C	5.50467000	1.76674500	-0.51373800
C	4.74383400	4.03351700	-1.93742700
C	6.30637900	2.24208500	-1.55052800
H	5.79770900	0.88635300	0.04408900
C	5.91604200	3.36863500	-2.27886600
H	4.45228000	4.93145700	-2.47667800
H	7.23006500	1.72508300	-1.79477000
H	6.52966800	3.73389100	-3.09725300
C	3.38144200	2.65174100	2.02589300
C	3.88698600	2.12009700	3.21739900
C	2.81726500	3.94970900	2.01246500
C	3.80778400	2.83716000	4.41053600
H	4.33877400	1.13452400	3.19446700
C	2.73746000	4.65055500	3.23244800
C	3.22429500	4.10746500	4.41792600
H	4.19780400	2.40707400	5.32844000
H	2.30304000	5.64771700	3.23484100
H	3.15876500	4.67481800	5.34179200
C	2.80574200	4.42130700	-0.46707000
H	2.40219900	5.07155300	-1.24160600
C	2.33756700	4.59320000	0.79164300
H	1.60743300	5.38771700	0.94650000

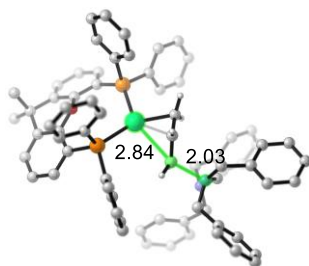


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O	-0.04487200	1.76209100	0.22330700
C	-2.24765500	1.38533100	-0.53948600
C	-3.44773900	1.89902400	-1.05651400
C	-3.56097300	3.25719900	-1.34928000
C	-2.48878200	4.12351800	-1.12576900
C	-1.28487900	3.65586900	-0.58929100
C	-1.20455700	2.28812700	-0.30850400
C	-0.07565300	4.53230000	-0.23694100
C	1.18021700	3.69461900	-0.51366900
C	1.12495900	2.32186100	-0.24588100
C	2.20396100	1.45168500	-0.43521400
C	3.41663000	2.00839800	-0.87514800
C	3.50837500	3.37292300	-1.14049800
C	2.39834700	4.20383800	-0.97334800
C	-0.12882400	4.85710600	1.28447500
C	-0.07207200	5.85245200	-1.02581400
C	-2.29632900	-0.46861300	1.69484100
C	-3.12830000	0.45904800	2.34258800
C	-3.36995000	0.34960500	3.71228400
C	-2.78700700	-0.68405400	4.44925900
C	-1.95693200	-1.60893700	3.81372100
C	-1.71006000	-1.49943400	2.44456700
C	-3.49046200	-1.16805000	-0.88213700
C	-3.58151900	-1.20638600	-2.28548100
C	-4.67461200	-1.80615300	-2.90859100
C	-5.68700400	-2.38836400	-2.13924600
C	-5.60174700	-2.35967300	-0.74764900
C	-4.51152800	-1.74950000	-0.11851100
C	3.49248700	-1.03809700	-0.95291200
C	3.51815100	-1.04046100	-2.35911600
C	4.61810400	-1.55054600	-3.04643200
C	5.70401400	-2.07609800	-2.33894900
C	5.68513100	-2.08027300	-0.94454700
C	4.58726800	-1.56005200	-0.25106400
C	2.34093200	-0.54632500	1.68908200
C	2.90690800	0.48112900	2.45828500
C	3.18022100	0.27747300	3.81254100
C	2.90063900	-0.95220300	4.41056600
C	2.33960700	-1.98219700	3.65164800
C	2.05427500	-1.77762300	2.30210000
H	-4.28642800	1.23814000	-1.24159100
H	-4.49050500	3.64372900	-1.75581600
H	-2.60204900	5.17467600	-1.36725900
H	4.28228500	1.37363200	-1.02443900
H	4.44843900	3.79168200	-1.48626500
H	2.49278700	5.26024700	-1.19941500
H	-1.03545500	5.42603100	1.51780700
H	0.74075800	5.45748300	1.57350700
H	-0.13195900	3.94547800	1.88990900
H	-0.03498800	5.68303600	-2.10706400

CP16

H	0.78479200	6.47065300	-0.74261700
H	-0.96509200	6.44174800	-0.79811400
H	-3.58730000	1.26655900	1.78074600
H	-4.01383000	1.07336600	4.20366100
H	-2.97642600	-0.76530600	5.51570500
H	-1.49473000	-2.40990700	4.38347800
H	-1.04965700	-2.21053700	1.95630100
H	-2.80011400	-0.75650200	-2.89439400
H	-4.73623900	-1.82056400	-3.99308100
H	-6.53646200	-2.86003800	-2.62447000
H	-6.38603500	-2.80715100	-0.14380300
H	-4.46472800	-1.72688300	0.96522800
H	2.67969300	-0.63231400	-2.91961300
H	4.62817600	-1.53932300	-4.13265600
H	6.55922100	-2.47804500	-2.87426400
H	6.52719200	-2.48280200	-0.38878400
H	4.59216500	-1.56012000	0.83398500
H	3.13784900	1.43937600	2.00458700
H	3.61584900	1.08183500	4.39823500
H	3.11811500	-1.10789600	5.46325000
H	2.12105900	-2.94217900	4.11103800
H	1.60845800	-2.57963200	1.71937200
C	1.24776800	-3.34426300	-1.41889100
H	1.31836000	-3.04269200	-2.46212700
H	2.19155700	-3.57963600	-0.93864200
C	0.04362000	-3.85811300	-0.90624200
H	0.05520200	-4.40779800	0.03373400
C	-1.17964900	-3.37295600	-1.40309700
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H	-2.10949200	-3.62938300	-0.90717400

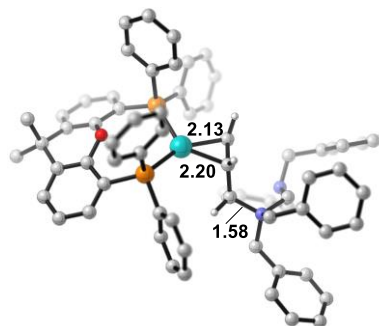
### TS15



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P	-2.79318900	1.85176100	0.72635300
P	-2.10013100	-2.08206600	0.26566600
O	-4.33837800	-0.35091100	-0.53093100
C	-4.04296600	1.99918200	-0.62921600
C	-4.39623800	3.22827700	-1.20929000
C	-5.32382200	3.28105900	-2.24799200
C	-5.92263100	2.11216000	-2.72113200
C	-5.61684600	0.86941500	-2.15812700
C	-4.67691400	0.85011200	-1.12042100
C	-6.27858300	-0.45795100	-2.55120700
C	-5.21049000	-1.55117300	-2.42183100
C	-4.28668000	-1.44114500	-1.37526800
C	-3.28632600	-2.38866600	-1.12167800
C	-3.24960200	-3.52257600	-1.94885600
C	-4.15651400	-3.66457400	-2.99768000
C	-5.12013300	-2.68311900	-3.23731000
C	-7.41792400	-0.76071600	-1.53467400
C	-6.88102900	-0.40453600	-3.96523500
C	-3.81472400	1.87811000	2.26416100
C	-5.16700300	2.25157600	2.26788200
C	-5.89027800	2.27735400	3.46247800

C	-5.27211400	1.94016700	4.66741200
C	-3.92498300	1.57123400	4.67517800
C	-3.20454100	1.53287900	3.48160800
C	-2.00898000	3.52653600	0.67978400
C	-1.07858700	3.79255900	-0.34085800
C	-0.44563400	5.03200300	-0.42315800
C	-0.72355900	6.02320000	0.52325400
C	-1.64090800	5.76823200	1.54230800
C	-2.28433400	4.52875400	1.62009000
C	-0.76704700	-3.31388000	-0.11634700
C	-0.04618600	-3.18039200	-1.31795200
C	1.00881300	-4.04170200	-1.61806200
C	1.37717200	-5.04270000	-0.71258300
C	0.67789700	-5.17601000	0.48716900
C	-0.39071700	-4.32194800	0.78261100
C	-2.96699000	-2.81570700	1.72171500
C	-3.83067900	-3.91696600	1.60410000
C	-4.44549100	-4.45573000	2.73444100
C	-4.20757100	-3.90293600	3.99551300
C	-3.35372000	-2.80662200	4.12278400
C	-2.73980600	-2.26464900	2.99172900
H	-3.93553500	4.14358600	-0.85532700
H	-5.58203100	4.23783300	-2.69188600
H	-6.64040500	2.17799700	-3.53148200
H	-2.49971500	-4.28805800	-1.78304900
H	-4.11225100	-4.54385800	-3.63348300
H	-5.81020600	-2.81350900	-4.06396100
H	-8.18202600	0.02332700	-1.57880500
H	-7.89113100	-1.72031700	-1.77078200
H	-7.03718800	-0.81087500	-0.51010400
H	-6.12249700	-0.18981900	-4.72546100
H	-7.36418300	-1.35326900	-4.21628300
H	-7.65833500	0.36284100	-4.02562600
H	-5.65937700	2.52495300	1.34021100
H	-6.93788900	2.56487600	3.44898800
H	-5.83671500	1.96309700	5.59519100
H	-3.43682100	1.30740000	5.60949500
H	-2.16023800	1.23287800	3.49211500
H	-0.85320400	3.02580000	-1.07908400
H	0.26980600	5.22123100	-1.21864100
H	-0.22759400	6.98790700	0.46371600
H	-1.86484900	6.53467700	2.27919100
H	-3.00286900	4.34967400	2.41335300
H	-0.32127000	-2.40629400	-2.03084400
H	1.54390200	-3.93190900	-2.55764200
H	2.19700800	-5.71601500	-0.94666500
H	0.94909300	-5.95677900	1.19277800
H	-0.93578800	-4.45301500	1.71193500
H	-4.02888100	-4.35259000	0.62944900
H	-5.11344700	-5.30616900	2.62961000
H	-4.69089600	-4.32246400	4.87337600
H	-3.17292800	-2.36557300	5.09909500
H	-2.08871100	-1.40008900	3.08839300
C	1.56155100	-0.70934400	0.66859900
C	0.88471900	-0.02562300	1.72064500
H	0.80379600	-0.54223500	2.67555000
C	0.39809400	1.31219300	1.62606300
H	0.75203600	1.97198800	0.83679600
H	0.12107700	1.83776000	2.53785800
C	4.05119800	0.52494900	-0.01838600
H	5.14695500	0.53702700	0.00164100
N	3.58358500	-0.64101700	0.82262200
C	3.99406700	-1.98546400	0.29698900
H	3.80104500	-1.95380200	-0.77804600

C	3.86694800	-0.42737400	2.28563000
H	3.00968800	0.13675800	2.66610800
H	3.83823600	-1.41576900	2.75208000
H	3.72174100	1.41548800	0.51632600
N	3.52567900	0.53318500	-1.36944200
C	4.48970200	0.14893100	-2.41391500
H	5.06515600	-0.69985100	-2.03274900
H	5.22037000	0.95101200	-2.60730500
C	2.73727400	1.74397700	-1.71833400
H	2.26464200	1.53802600	-2.68325100
H	1.93085200	1.83081600	-0.98361600
C	3.84738600	-0.27074300	-3.72561700
C	2.66535500	-1.02398700	-3.75852100
C	4.47805600	0.04129400	-4.93648000
C	2.12902400	-1.45252400	-4.97370400
H	2.16206600	-1.26527900	-2.82633500
C	3.94794400	-0.39372500	-6.15334100
H	5.39607300	0.62509600	-4.92766500
C	2.76986200	-1.14112100	-6.17552800
H	1.20812700	-2.03025100	-4.98456100
H	4.45279900	-0.14294500	-7.08205300
H	2.35185600	-1.47524600	-7.12081700
C	3.49641200	3.06026200	-1.79077000
C	4.14284900	3.45308400	-2.97319000
C	3.55688500	3.91831400	-0.68232400
C	4.85305300	4.65313300	-3.03601700
H	4.07131400	2.82343500	-3.85673400
C	4.26507000	5.12026600	-0.74167100
C	4.92109000	5.48721500	-1.91803200
H	5.34435200	4.94184100	-3.96115300
H	5.47037900	6.42312300	-1.96768800
H	3.28333700	-2.70495300	0.71246000
C	5.12627900	0.31879000	2.70683900
C	5.07027300	1.70913500	2.89542800
C	6.32257500	-0.34577700	3.01212400
C	6.18416400	2.42227800	3.33827700
H	4.13823200	2.23993800	2.71180000
C	7.43681300	0.36438900	3.46219500
H	6.38409100	-1.42369700	2.91196100
C	7.37488700	1.74998400	3.61890700
H	6.11744400	3.49768600	3.47694300
H	8.35278200	-0.17018800	3.69759200
H	8.24300500	2.29999700	3.97092300
C	5.38721400	-2.50813400	0.60424700
C	6.55416700	-2.02176000	-0.00494900
C	5.50965600	-3.57486300	1.50851100
C	7.80096900	-2.56995400	0.29670700
H	6.50551300	-1.20715500	-0.71943000
C	6.75479200	-4.12902900	1.81144500
H	4.61643400	-3.98368300	1.97608600
C	7.90691100	-3.62328100	1.20773700
H	8.69094500	-2.17590300	-0.18553600
H	6.82207300	-4.95611100	2.51252500
H	8.87827700	-4.05168700	1.43717100
H	3.02630300	3.65711900	0.23136000
H	4.29644200	5.77325200	0.12634700
H	1.56862500	-0.28973900	-0.32944900
H	1.53845600	-1.79146200	0.69525800



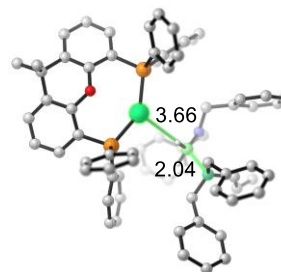
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P	2.29089900	-2.06041400	-0.01096500
O	4.52050300	-0.17361800	-0.44652200
C	4.08571700	2.15439700	-0.53988900
C	4.42511400	3.41588000	-1.05317400
C	5.46859500	3.55366100	-1.96741700
C	6.20302400	2.43891900	-2.37546100
C	5.91451400	1.16606200	-1.87313300
C	4.85210200	1.06131600	-0.96744700
C	6.71655500	-0.10385700	-2.18777000
C	5.72474000	-1.27416800	-2.20887300
C	4.65932700	-1.24794200	-1.29954500
C	3.70259700	-2.26854900	-1.19780600
C	3.87122200	-3.38948800	-2.02702100
C	4.92551600	-3.45074100	-2.93642200
C	5.83547700	-2.39684500	-3.03412800
C	7.73360100	-0.34110400	-1.03351100
C	7.49190400	0.01737700	-3.51076200
C	3.51827100	1.91606000	2.29059600
C	4.82849600	2.38250100	2.47370600
C	5.40176300	2.40346000	3.74732200
C	4.67234600	1.96872900	4.85485000
C	3.36527800	1.50655400	4.68461500
C	2.79645400	1.47325300	3.41155500
C	1.81654900	3.50844900	0.55551700
C	0.94843800	3.73599400	-0.52672900
C	0.25413900	4.93924400	-0.64668400
C	0.40599300	5.93317100	0.32502500
C	1.26003900	5.71681300	1.40641700
C	1.96528400	4.51448700	1.52040700
C	1.12710400	-3.36854800	-0.63499000
C	0.60570100	-3.24194200	-1.93677900
C	-0.30016200	-4.17677700	-2.44108400
C	-0.72565300	-5.24420100	-1.64175300
C	-0.23622200	-5.36518800	-0.34016400
C	0.68699600	-4.43925400	0.15752600
C	2.95933700	-2.80244200	1.54642000
C	3.90969200	-3.83617400	1.54659700
C	4.36937500	-4.37381400	2.74922800
C	3.88695900	-3.88763900	3.96706800
C	2.94515100	-2.85787100	3.97847700
C	2.48742400	-2.31656300	2.77537500
H	3.86373500	4.29068200	-0.74421000
H	5.71432200	4.53537000	-2.36155600
H	7.01268500	2.57134700	-3.08488400
H	3.16572400	-4.21124400	-1.97468400
H	5.03781000	-4.32220400	-3.57477600
H	6.64298000	-2.46144400	-3.75502700
H	8.43653500	0.49713200	-0.97128100
H	8.30312300	-1.25983600	-1.21333200
H	7.22759700	-0.43623700	-0.06794600

CP17

H	6.82349500	0.18190800	-4.36262900
H	8.07936400	-0.88573100	-3.70112200
H	8.20552500	0.84534200	-3.46638500
H	5.40438700	2.73235700	1.62293300
H	6.41940400	2.76331400	3.87215300
H	5.12004600	1.98784800	5.84457200
H	2.79152800	1.16548300	5.54233200
H	1.78480200	1.09832600	3.28074700
H	0.81792800	2.96217300	-1.28001400
H	-0.41082300	5.09594900	-1.49205300
H	-0.13893000	6.86912900	0.23835000
H	1.38518800	6.48532800	2.16443500
H	2.63301900	4.36550400	2.36285700
H	0.93214400	-2.41960300	-2.56952800
H	-0.65947700	-4.08178100	-3.46294000
H	-1.41513100	-5.98488600	-2.03863300
H	-0.55271400	-6.19510100	0.28617300
H	1.07928600	-4.56469300	1.16158200
H	4.29790600	-4.21835300	0.60744100
H	5.10779300	-5.17078400	2.73495900
H	4.25000100	-4.30544300	4.90199000
H	2.57592400	-2.46635300	4.92247400
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C	-1.65384000	-0.84265800	-0.41248200
C	-0.98325300	-0.37878400	0.84207000
H	-1.01512100	-1.05904800	1.69230600
C	-0.65615700	0.97848900	1.08019600
H	-0.93263400	1.74388800	0.36100500
H	-0.54231900	1.34263400	2.10022300
C	-4.06595500	-0.03104900	0.14564400
H	-5.09194800	-0.39708200	0.04665000
N	-3.18376500	-1.23081600	-0.32103200
C	-3.55221600	-1.69683400	-1.74370900
H	-3.52015600	-0.79887500	-2.36058600
C	-3.30462200	-2.42681300	0.67324300
H	-2.33531800	-2.49143400	1.16166700
H	-3.41792600	-3.31506600	0.05530000
H	-3.84185300	0.05628200	1.20356000
N	-3.80033300	1.22002300	-0.49869800
C	-4.63679500	1.56646800	-1.66308600
H	-4.80714200	0.65924500	-2.24715200
H	-5.63103400	1.91699700	-1.34483300
C	-3.67308500	2.36208100	0.45476200
H	-3.17785200	3.17180400	-0.08863200
H	-2.98928900	2.04442300	1.24421600
C	-4.01019900	2.60682300	-2.57806400
C	-2.64797000	2.57336100	-2.90526100
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C	-2.10703700	3.49971400	-3.79849300
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H	-5.87599600	3.63074300	-2.91847100
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H	-4.92206000	5.27120400	-4.50589800
H	-2.50132000	5.19443200	-5.07613600
C	-4.97195800	2.87548900	1.05936900
C	-5.60541500	4.00522800	0.52155300
C	-5.55765400	2.25021800	2.17112800
C	-6.79781900	4.48790300	1.06482000
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C	-6.75042500	2.72799900	2.71567500
C	-7.37577700	3.84736500	2.16174000
H	-7.26982500	5.36770900	0.63610200

H	-8.30061700	4.22356700	2.58985700
H	-2.71583800	-2.32773500	-2.05114700
C	-4.38744500	-2.38127100	1.72985300
C	-4.10158100	-1.83911000	2.99331200
C	-5.65053500	-2.94935600	1.50911700
C	-5.06202400	-1.84057800	4.00512500
H	-3.11559000	-1.42329400	3.18978100
C	-6.61100400	-2.95300800	2.52198700
H	-5.88199400	-3.40060200	0.54965100
C	-6.32203100	-2.39512400	3.76878700
H	-4.82221600	-1.42279700	4.97867000
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H	-7.06994300	-2.40367900	4.55636800
C	-4.83493500	-2.47837200	-1.92793300
C	-6.10139900	-1.87777200	-2.01320900
C	-4.74865400	-3.87153700	-2.09238800
C	-7.24481400	-2.64967800	-2.22285600
H	-6.21131300	-0.80249700	-1.92698400
C	-5.89024100	-4.64542800	-2.30380500
H	-3.77371000	-4.35337100	-2.06806100
C	-7.14443100	-4.03533600	-2.36303000
H	-8.21436100	-2.16445100	-2.28609600
H	-5.79806600	-5.72006400	-2.43098700
H	-8.03553500	-4.63289600	-2.53120900
H	-5.07413000	1.39199000	2.63322300
H	-7.18473100	2.23406500	3.58061600
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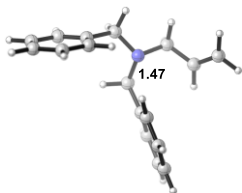
### TS16



Pd	-1.23484900	0.01508900	0.20554300
P	-2.51731600	1.90044700	0.57877900
P	-1.30401900	-2.28047500	0.03563200
O	-3.97254300	-0.80449900	0.37057400
N	1.97494100	1.94316200	-1.64777100
C	-4.26673300	1.56033700	0.05636200
C	-5.12456400	2.60870100	-0.31821100
C	-6.43174400	2.36251300	-0.72784800
C	-6.91634600	1.05536700	-0.76342700
C	-6.10805400	-0.02032400	-0.38673400
C	-4.78968300	0.25248200	0.00954900
C	-6.58534200	-1.47540300	-0.32134600
C	-5.40947900	-2.35653800	-0.75879200
C	-4.12510200	-1.98667500	-0.33247700
C	-2.98375000	-2.77405300	-0.58655300
C	-3.16927200	-3.95301500	-1.32753200
C	-4.42942000	-4.32546600	-1.78896200
C	-5.54022900	-3.53290900	-1.50192400
C	-6.93064900	-1.81471700	1.15869600
C	-7.83918300	-1.71320200	-1.17935400
C	-2.67425100	2.38138800	2.35775900
C	-3.73817700	3.14893500	2.85926400
C	-3.79222300	3.48394300	4.21264900
C	-2.78698200	3.05621200	5.08408900

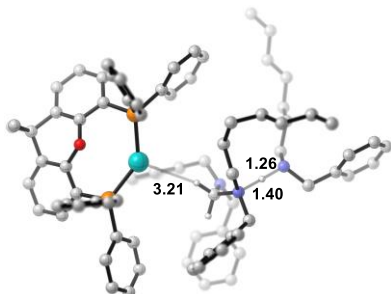


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C	-2.16152000	3.49707300	-0.29253000	H	0.17092500	-1.68619800	2.43515700
C	-2.17488200	3.50728600	-1.70039800	H	2.18666700	-0.03495000	-2.11745000
C	-1.80916200	4.65056600	-2.40979000	H	1.35108700	0.33998900	-0.51309200
C	-1.40330500	5.80263700	-1.72583800	H	3.47255300	2.57480200	-3.01370600
C	-1.37751800	5.80055200	-0.33134000	H	1.89864200	3.36086300	-3.15162500
C	-1.75745900	4.65813200	0.38167100	H	-0.11200500	1.50065000	-3.68633200
C	-0.17760000	-3.21436800	-1.10293800	H	-0.73108500	0.02972200	-5.57213400
C	0.12299600	-2.61422300	-2.33922400	H	1.02455600	-0.87975200	-7.08136000
C	0.97196800	-3.24082100	-3.25193500	H	3.41167600	-0.30316100	-6.68729600
C	1.54898200	-4.47487700	-2.93690000	H	4.03387900	1.17759300	-4.79899600
C	1.26610800	-5.07635200	-1.70949500	H	0.74223200	2.42209500	-0.04182500
C	0.40743500	-4.45294400	-0.79755100	H	0.76590900	3.60828600	-1.33478200
C	-1.16141500	-3.18270500	1.64400400	H	1.66890100	3.13818500	1.96744100
C	-1.84161600	-4.37810200	1.92549800	H	3.24660700	4.51795500	3.27966300
C	-1.67616300	-5.01394100	3.15789100	H	4.89049300	5.98186200	2.11678700
C	-0.83042800	-4.46610000	4.12466800	H	4.91335100	6.07348800	-0.36805300
C	-0.15505100	-3.27293900	3.85913300	H	3.32736000	4.71693100	-1.67724100
C	-0.32575800	-2.63374000	2.63044900	C	4.84003100	0.86147600	-0.43187700
C	2.03509400	0.65955600	-1.30003000	C	5.47750900	0.90759000	-1.79490700
C	2.39381900	2.39664700	-3.00028000	H	5.69134700	-0.03607400	-2.29185800
C	2.00908900	1.44650100	-4.11671300	C	5.91917800	2.03922200	-2.35066100
C	0.66378200	1.11229800	-4.34293600	H	5.76568500	3.00794600	-1.87954800
C	0.31349100	0.27487400	-5.40128700	H	6.47721300	2.03338600	-3.28278800
C	1.30110900	-0.23695100	-6.25044900	N	3.65255400	-0.02350500	-0.26344700
C	2.63964100	0.08831000	-6.03097500	C	3.14497100	0.02697800	1.15995600
C	2.99042900	0.92351800	-4.96625100	H	2.32151900	-0.69095700	1.20975800
C	1.40451700	2.95729500	-0.72871600	C	3.78765300	-1.40753600	-0.82399300
C	2.40920000	3.78997000	0.04980800	H	2.78298500	-1.84005700	-0.78309800
C	2.39422700	3.76296100	1.45074100	H	4.01946300	-1.27878200	-1.88578200
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C	4.21620400	5.41742900	0.14582500	C	6.15123300	-2.20503100	-0.19156300
C	3.32276000	4.64091200	-0.59330200	C	4.25072100	-3.59792400	0.31026800
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H	-7.07380600	3.18826800	-1.01985300	H	6.59117300	-1.30549500	-0.60935800
H	-7.93738800	0.87941200	-1.08298500	C	5.09884100	-4.57450100	0.83467000
H	-2.31286800	-4.57821200	-1.55755300	H	3.17901200	-3.77845200	0.28217100
H	-4.54757500	-5.23676500	-2.36776500	C	6.47740600	-4.36171300	0.86032800
H	-6.51647500	-3.84231300	-1.85821600	H	8.07297500	-3.00595800	0.34404000
H	-7.74870100	-1.17652900	1.51117000	H	4.68130400	-5.50048500	1.22033100
H	-7.24521300	-2.86098000	1.24296900	H	7.14127800	-5.11784200	1.26944500
H	-6.07032800	-1.66154400	1.81691800	C	4.10571500	-0.20317000	2.31427400
H	-7.66239600	-1.48836800	-2.23665100	C	4.16334000	-1.44105600	2.96928300
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H	-8.67048300	-1.09503300	-0.82818000	C	4.99745300	-1.62844600	4.07158500
H	-4.53292200	3.47875100	2.19713700	H	3.55369200	-2.26614200	2.61529600
H	-4.62268100	4.07558200	4.58801700	C	5.71812200	0.66973600	3.91669000
H	-2.83485400	3.31498200	6.13823800	H	4.80627900	1.84111700	2.36412200
H	-0.95179700	1.93925900	5.27426100	C	5.78423400	-0.57608000	4.54316800
H	-0.86901700	1.32557800	2.86518500	H	5.02935100	-2.59649900	4.56331600
H	-2.48401600	2.61663200	-2.24245500	H	6.30983100	1.50076700	4.29029900
H	-1.84519900	4.64578400	-3.49628500	H	6.43389000	-0.72176200	5.40150500
H	-1.11872100	6.69433700	-2.27749100	H	4.52589200	1.86814700	-0.13950500
H	-1.07097900	6.69179300	0.20955900	H	5.59576600	0.54116700	0.29657500
H	-1.74449300	4.67871000	1.46681600				
H	-0.31557400	-1.64919700	-2.58385800	4			
H	1.18471000	-2.76214200	-4.20428900				
H	2.21397700	-4.96406000	-3.64320700				
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H	-2.50951800	-4.81092700	1.18702600				
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C	-0.79398600	-2.47376800	-0.27988500
C	-2.19279900	-2.30898700	0.25690400
H	-2.85562700	-1.63630600	-0.28204600
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H	-3.68246700	-2.86194200	1.65673200
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H	-0.72357300	-0.60772200	-2.11135100
H	0.44045800	0.45334100	-1.32404300
H	1.59583200	-1.90421000	-1.58283700
C	-1.53601600	0.66837100	-0.57207800
C	-1.54466100	1.06045300	0.77283000
C	-2.54212400	1.14942900	-1.41876500
C	-2.53616000	1.91319200	1.25737800
H	-0.77510700	0.67626700	1.43447700
C	-3.53462200	2.00648900	-0.93720500
H	-2.54954800	0.84997100	-2.46515200
C	-3.53465300	2.39112500	0.40431500
H	-2.53113100	2.20489700	2.30471200
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H	-4.30777900	3.05429400	0.78352400
C	2.43425200	-0.52435800	-0.15641000
C	2.43530000	0.02308800	1.13500000
C	3.38078000	-0.06725200	-1.08006800
C	3.36147800	1.00197600	1.49146200
H	1.69860400	-0.32387400	1.85427400
C	4.31297800	0.91192900	-0.72557000
H	3.38850200	-0.48150200	-2.08614300
C	4.30502700	1.44940300	0.56152200
H	3.34988100	1.41644700	2.49632100
H	5.03994100	1.25580000	-1.45680400
H	5.02683000	2.21271800	0.83986400
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### TS17



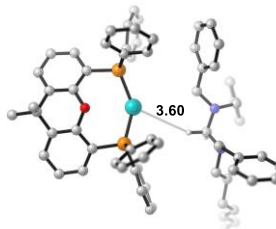
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C	0.92671500	-0.23732600	-4.82449400
C	-0.11142900	-0.43760700	-5.73810500
C	-1.41985700	-0.60203800	-5.28057100

C	-1.68551400	-0.55360900	-3.90880100
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C	3.11198300	-2.17913400	-2.64404500
C	2.49366000	-3.55427700	-2.87715000
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C	0.76326900	-4.99248400	-3.79426300
C	1.47236700	-6.12900100	-3.39220700
C	2.69154500	-5.98103400	-2.73152400
C	3.19480800	-4.70141300	-2.48120600
H	0.95127200	-1.06490800	-0.30886600
H	1.44815300	-2.70911800	-0.67241500
H	1.50439100	0.66066000	-1.66071500
H	2.64398200	0.49029500	-2.98494600
H	1.94214000	-0.09524900	-5.19022200
H	0.10158900	-0.45801200	-6.80339100
H	-2.23017500	-0.75290800	-5.98841400
H	-2.70392300	-0.65614700	-3.54349200
H	-0.88017500	-0.29476900	-1.93272900
H	3.28086300	-1.69523700	-3.61203200
H	4.11410800	-2.34268800	-2.21299300
H	0.70648500	-2.84409300	-3.85866500
H	-0.17887100	-5.09959100	-4.32540300
H	1.08046900	-7.12046100	-3.60109800
H	3.25485900	-6.85582900	-2.41884100
H	4.16073800	-4.59450000	-1.98984900
C	5.87375900	1.65369900	4.16185700
H	6.37560100	2.34522300	3.48382900
C	6.55545400	1.13820200	5.19726800
H	6.08901600	0.45722800	5.90571400
H	7.59382900	1.39517700	5.38252100
C	4.47220200	1.37001800	3.87670400
H	3.95369200	0.72289300	4.58648800
C	3.78923000	1.88019900	2.83341400
H	4.31431900	2.54910900	2.14720000
C	2.33915800	1.63269700	2.52135900
H	1.85243700	2.58807000	2.29370700
H	1.82653200	1.21630400	3.39846600
C	2.13155500	0.68859600	1.31010300
H	1.10922700	0.81430600	0.93618500
H	2.80389200	0.99234400	0.49722600
C	2.36339600	-0.77498700	1.70866400
H	3.16054100	-0.82938000	2.46165600
H	1.45690900	-1.17364600	2.17621800
N	2.79401700	-1.66853100	0.59076100
H	5.20141000	0.06418600	1.01331800
C	3.09041600	-3.06026700	1.10489900
H	3.33075000	-3.66527100	0.22579900
H	4.00081900	-2.97467900	1.70800900
C	2.02271900	-3.73956800	1.94058400
C	2.06423300	-3.64168400	3.33995900
C	0.99747400	-4.49480000	1.35252900
C	1.09345600	-4.25497000	4.13172000
H	2.87085300	-3.08783100	3.81592100
C	0.01979900	-5.10396700	2.14120900
H	0.96326100	-4.62609100	0.27446700
C	0.06330900	-4.98188700	3.53143200
H	1.14629400	-4.17199400	5.21371400
H	-0.77268500	-5.67331300	1.66587600
H	-0.69471800	-5.46147900	4.14408700
C	5.65887700	6.19562500	-2.34646300
H	6.53095300	6.47699100	-1.75596500
C	4.86728500	7.15458000	-2.85106700
H	3.99351100	6.91450700	-3.45318000
H	5.07143500	8.20824600	-2.68872900

C	5.43291700	4.76868900	-2.53240200
H	4.55957300	4.49117100	-3.12582100
C	6.21625700	3.79897400	-2.03144000
H	7.09444800	4.07637300	-1.44585200
C	5.96520900	2.32703200	-2.20157600
H	6.81435100	1.85646100	-2.72031800
H	5.08366500	2.17654000	-2.83895000
C	5.75741700	1.60589800	-0.85296000
H	6.67233300	1.67725100	-0.25153400
H	4.96163000	2.11774000	-0.29574400
C	5.37866600	0.13780400	-1.05050900
H	4.43135100	0.05205300	-1.58740400
H	6.14719100	-0.37686300	-1.63319200
N	5.20130700	-0.61252900	0.24345300
H	4.05962000	-1.13671500	0.29079800
C	6.27292900	-1.63413400	0.52980500
H	6.01813800	-2.07964200	1.49605900
H	6.17106900	-2.41158400	-0.23281100
C	7.68034800	-1.08432200	0.55461900
C	8.55845400	-1.31821000	-0.51165800
C	8.12940800	-0.34089800	1.65686000
C	9.85798400	-0.80727400	-0.48701000
H	8.23165600	-1.91624400	-1.35968800
C	9.42589600	0.17271300	1.67999400
H	7.47188800	-0.16985400	2.50738900
C	10.29190300	-0.05804800	0.60734500
H	10.53040800	-1.00107400	-1.31758900
H	9.76517400	0.74200600	2.54064000
H	11.30370100	0.33606800	0.63045300
Pd	-1.91272300	0.16576100	0.45171000
P	-3.49931600	-1.51921800	0.54027700
P	-1.90525300	2.47148300	0.57271500
O	-4.59244000	1.23575700	-0.13832400
C	-4.89257100	-1.09106500	-0.61579900
C	-5.59284300	-2.07467900	-1.33248800
C	-6.60947100	-1.73286300	-2.22202800
C	-6.96668400	-0.39694000	-2.39772000
C	-6.31391600	0.61864500	-1.69204000
C	-5.27281400	0.24996900	-0.82801600
C	-6.71497600	2.09761100	-1.74159500
C	-5.43196300	2.92745300	-1.61915400
C	-4.42028100	2.45180200	-0.77272000
C	-3.23223800	3.16822000	-0.52664800
C	-3.09114400	4.41296600	-1.16102800
C	-4.07595600	4.90278400	-2.01578000
C	-5.23362700	4.16134000	-2.24599000
C	-7.61478400	2.40151000	-0.50779300
C	-7.50396800	2.44003500	-3.01699000
C	-4.32503600	-1.56117900	2.19622800
C	-5.71753700	-1.58256300	2.36202300
C	-6.27851300	-1.62540700	3.64130400
C	-5.45677300	-1.65680100	4.76867100
C	-4.06819700	-1.63989800	4.61369600
C	-3.50732200	-1.58396700	3.33819400
C	-3.23743000	-3.32054200	0.17787600
C	-2.30102500	-3.66575200	-0.80999200
C	-2.07329000	-5.00221400	-1.14198700
C	-2.76873900	-6.01727700	-0.47872200
C	-3.69120900	-5.68706400	0.51657700
C	-3.92550000	-4.34859800	0.84165800
C	-0.45610900	3.54921200	0.13570000
C	0.16310700	3.34433900	-1.11134500
C	1.28513700	4.08482900	-1.48167100
C	1.82597900	5.03260000	-0.60619400

C	1.22546100	5.23741000	0.63636300
C	0.09057400	4.50570000	1.00435700
C	-2.39780500	3.07773600	2.25041500
C	-3.10065500	4.27658300	2.45055800
C	-3.43993800	4.69166600	3.73946800
C	-3.08109300	3.91631000	4.84461800
C	-2.38597200	2.72037700	4.65645200
C	-2.05160600	2.30153700	3.36745100
H	-5.33268100	-3.11872100	-1.19947900
H	-7.13155000	-2.51079700	-2.77156400
H	-7.76995600	-0.15064800	-3.08324600
H	-2.19304700	4.99812500	-0.99584400
H	-3.94193300	5.86485400	-2.50170100
H	-5.99140900	4.55814800	-2.91243000
H	-8.53105300	1.80168900	-0.54976800
H	-7.89334300	3.46130900	-0.49433000
H	-7.09825800	2.17228000	0.42918600
H	-6.91887000	2.25082500	-3.92340000
H	-7.80745700	3.49097900	-3.01456000
H	-8.42584400	1.85385300	-3.07103800
H	-6.36835700	-1.56631200	1.49310400
H	-7.35931700	-1.63615900	3.75402700
H	-5.89492300	-1.69006000	5.76240300
H	-3.42228400	-1.65991100	5.48771600
H	-2.42695900	-1.54988900	3.22079300
H	-1.74936000	-2.88136400	-1.32317100
H	-1.34647500	-5.24933100	-1.91058600
H	-2.59240700	-7.05848500	-0.73567800
H	-4.23613200	-6.47020700	1.03725100
H	-4.65125200	-4.10566900	1.61139600
H	-0.24785500	2.61045700	-1.80127700
H	1.73588000	3.92513800	-2.45825500
H	2.70058700	5.60937200	-0.89511600
H	1.63021100	5.97804100	1.32137900
H	-0.37385200	4.69099200	1.96762000
H	-3.39087100	4.88437100	1.59872400
H	-3.98808800	5.61944000	3.87961300
H	-3.35046900	4.23923200	5.84653200
H	-2.11745900	2.10558400	5.51145200
H	-1.53924500	1.35487100	3.21459200

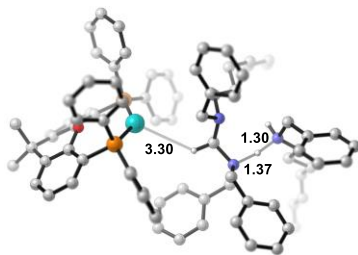
### CP18



Pd	1.39236500	-0.06193900	-0.32292700
P	3.11226200	1.46414300	-0.39045200
P	1.03873100	-2.28804800	0.10134700
O	3.98511700	-1.47425100	-0.16921100
N	-2.86975500	2.02134300	0.42601400
C	4.65933700	0.65799100	-1.04458300
C	5.61876100	1.39110200	-1.76171600
C	6.75464700	0.78064700	-2.28815800
C	6.96745300	-0.58358100	-2.09577400
C	6.05186800	-1.35413200	-1.37402300
C	4.90598300	-0.71891900	-0.87126000
C	6.24548200	-2.83756700	-1.03966500
C	4.86406500	-3.49899100	-1.10002100

C	3.77220100	-2.76809000	-0.60731600	H	1.56485300	4.05512400	-4.30839800
C	2.46826400	-3.29885600	-0.53662000	H	2.65449100	6.19089100	-3.63840200
C	2.29049000	-4.61284900	-0.99915600	H	3.97428400	6.29456400	-1.53269500
C	3.35392300	-5.35283700	-1.51148000	H	4.21040600	4.28567000	-0.11249500
C	4.63162300	-4.79776400	-1.56109600	H	-0.33449900	-2.08204000	-2.40543200
C	6.78263700	-2.94901300	0.41731600	H	-2.24113400	-3.25819100	-3.46334700
C	7.25392800	-3.51634300	-1.98147100	H	-3.44476400	-5.05051300	-2.22035100
C	3.63829100	2.08931600	1.27067400	H	-2.72157600	-5.65107400	0.08163600
C	4.95190800	2.00448700	1.75425600	H	-0.79436400	-4.50808100	1.11930000
C	5.27152800	2.48443500	3.02753700	H	2.05916300	-4.60053300	1.78264200
C	4.28715300	3.06533100	3.82745500	H	1.93082700	-5.06194100	4.20505800
C	2.97639500	3.15999300	3.35179300	H	0.81340600	-3.44690800	5.73046300
C	2.65180500	2.66722500	2.08886900	H	-0.16150300	-1.35008600	4.80790300
C	3.02866900	3.01769800	-1.40186500	H	-0.00462600	-0.87419500	2.38037000
C	2.27610900	2.97444800	-2.58723800	H	-3.56096600	0.57560500	-0.98771300
C	2.14927700	4.10643900	-3.39332800	H	-2.18301200	0.10727300	0.02087900
C	2.76004200	5.30570600	-3.01657000	H	-4.86626300	2.47437600	0.72119700
C	3.49996000	5.36378700	-1.83373100	H	-3.77203200	3.85768800	0.81423900
C	3.63566400	4.22754100	-1.03200500	H	-5.85774900	1.80308000	-1.41408200
C	-0.41122400	-3.22709600	-0.57890400	H	-6.40068300	2.38451900	-3.75630700
C	-0.84567900	-2.87875100	-1.86948700	H	-5.23031700	4.27484200	-4.87566100
C	-1.92411000	-3.53568700	-2.46138500	H	-3.52425300	5.58055700	-4.61960800
C	-2.60178400	-4.53928700	-1.76269600	H	-2.98445700	4.99144300	-1.27798600
C	-2.19403500	-4.87785500	-0.47112000	H	-0.85079300	1.70136200	0.05505500
C	-1.10413400	-4.22963700	0.11663000	H	-1.58818500	2.78275400	-1.11786900
C	1.01106000	-2.71403800	1.90470900	H	-0.12816300	4.63716400	-0.96215300
C	1.56476900	-3.88865800	2.43699600	H	0.81002200	6.53490800	0.31397300
C	1.49307900	-4.14972400	3.80759100	H	0.40302500	6.71769500	2.76535700
C	0.86539500	-3.24338200	4.66408800	H	-0.94496200	4.97021300	3.91832900
C	0.31598200	-2.06818200	4.14632700	H	-1.87345700	3.06281900	2.62658300
C	0.39573000	-1.80264400	2.77854400	C	-8.53010300	-2.56737700	-4.28836500
C	-3.14812200	0.64532400	0.03019200	H	-9.41013700	-2.05849800	-3.89300400
C	-4.00426300	2.95072600	0.24599500	C	-8.53736700	-2.99335900	-5.56048800
C	-4.35584800	3.33014200	-1.18622800	H	-7.68119500	-3.50536200	-5.99467100
C	-5.32826200	2.61701600	-1.90241000	H	-9.39601800	-2.84524600	-6.20839900
C	-5.64118700	2.94991000	-3.22205800	C	-7.41530100	-2.73246200	-3.36595500
C	-4.98709300	4.01172800	-3.84946300	H	-6.53213700	-3.24149400	-3.75607400
C	-4.02761700	4.74196900	-3.14468400	C	-7.41612000	-2.30499700	-2.09184400
C	-3.71917200	4.40534700	-1.82540900	H	-8.30413000	-1.79376400	-1.71342600
C	-1.57905600	2.52184600	-0.04494000	C	-6.27772300	-2.45099300	-1.12360900
C	-1.06477500	3.71514500	0.74602600	H	-5.46755900	-3.03210500	-1.58331100
C	-0.31042200	4.70903500	0.10768200	H	-6.61651600	-3.02538000	-0.24676800
C	0.22159700	5.78041600	0.82924700	C	-5.72906100	-1.09439600	-0.63538900
C	-0.00311900	5.88079800	2.20319400	H	-5.37656300	-0.52554800	-1.50358000
C	-0.75829400	4.89815400	2.84942900	H	-6.53766700	-0.50814800	-0.17898800
C	-1.28047900	3.82336500	2.12736200	C	-4.60905100	-1.26650000	0.39741800
H	5.46405500	2.45248300	-1.92259700	H	-5.00998300	-1.84144200	1.23900000
H	7.47603400	1.36948900	-2.84774200	H	-3.78984700	-1.87352100	-0.03282400
H	7.85886200	-1.04437500	-2.50734800	N	-4.10042700	0.00214300	0.94170300
H	1.30042800	-5.05508900	-0.97270500	C	-3.50793400	-0.18215600	2.27191600
H	3.18648300	-6.36428900	-1.87096500	H	-2.74478400	-0.98446100	2.26618400
H	5.45068900	-5.38794800	-1.95758900	H	-2.98188900	0.75048500	2.50334100
H	7.75708000	-2.45385700	0.50040200	C	-4.52261300	-0.46843000	3.36275800
H	6.90210300	-4.00196800	0.69783500	C	-5.73308300	0.23623400	3.42912300
H	6.09869500	-2.48072100	1.13106700	C	-4.24424600	-1.41432900	4.35756000
H	6.93180800	-3.47102300	-3.02737700	C	-6.63637400	0.00488000	4.46649800
H	7.39268200	-4.56651300	-1.70737400	H	-5.96153100	0.95989600	2.65239800
H	8.23720100	-3.04284800	-1.90169100	C	-5.14406600	-1.64429300	5.40113800
H	5.72976400	1.56385500	1.13866000	H	-3.31250200	-1.97516500	4.31353800
H	6.29336400	2.40535800	3.39019100	C	-6.34458200	-0.93517600	5.45874800
H	4.53797700	3.43972800	4.81660300	H	-7.57067000	0.55999000	4.50184900
H	2.20060100	3.61303100	3.96278900	H	-4.90952400	-2.38320600	6.16340700
H	1.62631300	2.73391300	1.73595400	H	-7.04892800	-1.11517900	6.26681200
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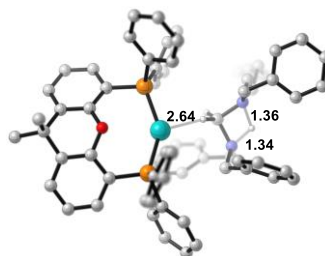
**TS18**



Pd	-2.25374400	0.00496500	0.24941500
P	-3.16347300	-2.09321200	-0.08375300
P	-2.92391800	2.20424100	0.39042600
O	-5.02462200	0.27089200	-0.68087300
N	3.04891300	-0.72225800	-0.66331200
C	-4.55596300	-1.99520800	-1.31166600
C	-4.88456100	-3.09103800	-2.12682400
C	-5.89973900	-3.00711400	-3.07625300
C	-6.62394300	-1.82434000	-3.22179700
C	-6.35244900	-0.71391000	-2.41772800
C	-5.31273100	-0.81865000	-1.48113300
C	-7.16397200	0.58618700	-2.44161600
C	-6.18902500	1.73897700	-2.17779300
C	-5.16117700	1.52428500	-1.24772400
C	-4.26523300	2.53818400	-0.85436500
C	-4.42851000	3.80180300	-1.44533900
C	-5.42573900	4.03435500	-2.38979700
C	-6.29756900	3.00850800	-2.75258400
C	-8.19646500	0.54169500	-1.27667400
C	-7.92950900	0.76701500	-3.76331400
C	-3.97417200	-2.79101100	1.42615600
C	-5.27643600	-3.31200300	1.43404400
C	-5.82931000	-3.81984200	2.61270000
C	-5.08648100	-3.82548900	3.79397500
C	-3.78602000	-3.31426800	3.79590600
C	-3.23966800	-2.79230500	2.62417300
C	-2.19217000	-3.53303500	-0.74010700
C	-1.34909900	-3.30390800	-1.84216200
C	-0.59523300	-4.34235300	-2.39035000
C	-0.64776800	-5.62217600	-1.82778900
C	-1.46489400	-5.85513700	-0.72100700
C	-2.23794200	-4.82070600	-0.18489800
C	-1.78392700	3.64064000	0.09498300
C	-0.98845300	3.61327400	-1.06593300
C	-0.09198500	4.64307600	-1.34550400
C	0.04274300	5.71528900	-0.45651300
C	-0.72675000	5.74553900	0.70706000
C	-1.63662800	4.71766200	0.98032300
C	-3.74784300	2.62331500	1.99435900
C	-4.74393700	3.60667800	2.10882500
C	-5.32703000	3.88443100	3.34626500
C	-4.92534600	3.18328400	4.48564300
C	-3.94149900	2.19842200	4.38228600
C	-3.36088500	1.91762900	3.14417800
C	1.86872500	-0.05599000	0.02141800
C	3.17263100	-0.18047200	-2.07136500
C	2.03535000	-0.44925700	-3.04100000
C	2.13725700	-1.49067600	-3.97525700
C	1.12327600	-1.71567700	-4.90844900
C	-0.00957700	-0.89967900	-4.92375500
C	-0.11582600	0.15141800	-4.00986400
C	0.90254000	0.37846800	-3.08311100
C	2.89872900	-2.21382000	-0.61724100
C	3.89743100	-3.04270000	-1.40474500

C	5.26240800	-2.74167800	-1.49577900
C	6.13488900	-3.57644500	-2.19715700
C	5.65844700	-4.73852500	-2.80502800
C	4.30290800	-5.05887100	-2.70738600
C	3.43091000	-4.21489200	-2.01876400
H	-4.32819900	-4.01629600	-2.02328700
H	-6.13025400	-3.86523300	-3.70088500
H	-7.41464100	-1.77663700	-3.96253800
H	-3.75718100	4.60879300	-1.17192700
H	-5.52773800	5.01784300	-2.83931100
H	-7.07428000	3.20811300	-3.48260400
H	-8.89085800	-0.29425900	-1.41806000
H	-8.77458500	1.47220600	-1.24728400
H	-7.70218500	0.41598100	-0.30873300
H	-7.25506100	0.80757700	-4.62541100
H	-8.52213500	1.68629200	-3.74395900
H	-8.63755500	-0.05268300	-3.91623300
H	-5.86350200	-3.32132400	0.52127800
H	-6.84213100	-4.21359000	2.60416600
H	-5.51857300	-4.22276900	4.70833500
H	-3.19916500	-3.31321300	4.71071200
H	-2.23479800	-2.37933400	2.63748800
H	-1.29408600	-2.31108500	-2.28315000
H	0.02821600	-4.14899600	-3.25943400
H	-0.06254700	-6.43277200	-2.25424100
H	-1.51480700	-6.84670100	-0.27889500
H	-2.88386200	-5.02231700	0.66368200
H	-1.09027000	2.78231400	-1.76083200
H	0.49680300	4.61529800	-2.25912700
H	0.73461600	6.52398200	-0.67652200
H	-0.63359300	6.57692100	1.40090700
H	-2.23956400	4.76537100	1.88126500
H	-5.07332700	4.15212700	1.22950100
H	-6.09910000	4.64567200	3.41884400
H	-5.38414600	3.39774200	5.44694200
H	-3.63554700	1.63948700	5.26268200
H	-2.61695600	1.12995600	3.05403200
H	1.94136200	0.99937600	-0.24759200
H	0.94574600	-0.44448700	-0.43085700
H	3.31135200	0.89915600	-1.95676000
H	4.09887100	-0.58989800	-2.47748100
H	3.01998400	-2.12285200	-3.98228600
H	1.22665500	-2.51937800	-5.63227600
H	-0.79738100	-1.07089400	-5.65165400
H	-0.98563700	0.80179900	-4.02480800
H	0.81444900	1.21762300	-2.39814500
H	2.95670300	-2.47792100	0.44360700
H	1.88802100	-2.46850500	-0.95678400
H	5.65909500	-1.85460700	-1.01446600
H	7.18875300	-3.32063500	-2.26020500
H	6.33729000	-5.38896400	-3.34877900
H	3.92091200	-5.96224400	-3.17442500
H	2.37518800	-4.46694500	-1.95532900
C	4.47806800	6.56497900	2.27125700
H	5.25291300	6.31774200	2.99768200
C	4.58931700	7.69060500	1.55042800
H	3.83508600	7.97681900	0.82046800
H	5.43077200	8.36592500	1.67002000
C	3.37128500	5.62448100	2.15919700
H	2.58661400	5.87631500	1.44400400
C	3.25931000	4.49330900	2.87640800
H	4.04381800	4.24672000	3.59523400
C	2.13194400	3.50580000	2.75688800
H	1.31932800	3.93073600	2.15599300

H	1.71525300	3.29474600	3.75287000
C	2.59169600	2.17277400	2.12688400
H	2.94729600	2.39672000	1.10965200
H	3.44356600	1.78336200	2.70281900
C	1.48261200	1.11844400	2.10761000
H	1.21685000	0.89614200	3.14385300
H	0.57637200	1.53053700	1.63111100
N	1.85132400	-0.17566000	1.47422800
H	4.53145600	1.05122100	1.07423400
C	0.88388800	-1.22509300	1.91971100
H	-0.14798600	-0.88769200	1.70593900
H	1.04781400	-2.11303800	1.30473400
C	1.02024100	-1.60419800	3.38005300
C	2.09621300	-2.38729400	3.82334500
C	0.05806900	-1.20359200	4.31710800
C	2.21587900	-2.74964800	5.16464500
H	2.84140400	-2.72961900	3.10895200
C	0.17123000	-1.56597200	5.66213700
H	-0.78924600	-0.60676200	3.98728100
C	1.25233200	-2.33744600	6.08930500
H	3.05425300	-3.36071700	5.48775800
H	-0.58520700	-1.24569200	6.37336600
H	1.34188700	-2.62244000	7.13371900
C	7.35979500	4.29810700	-4.79192300
H	6.86179200	5.20538300	-4.44948700
C	7.73571600	4.19671600	-6.07517600
H	8.23872400	3.30966200	-6.45396300
H	7.55797000	4.99635800	-6.78743100
C	7.57537200	3.25996300	-3.79334000
H	8.08081700	2.35552800	-4.13675900
C	7.20425400	3.35442100	-2.50555500
H	6.70385800	4.26259700	-2.16456700
C	7.42061900	2.28836100	-1.46823400
H	8.01220100	2.69543200	-0.63389200
H	8.00654100	1.46490500	-1.89682800
C	6.09236300	1.73732000	-0.90577000
H	5.50394400	2.56957900	-0.49175300
H	5.50970600	1.31356500	-1.73041200
C	6.32654200	0.68661600	0.17963100
H	6.85264800	-0.18493400	-0.21762100
H	6.96193700	1.11014800	0.96794000
N	5.05691200	0.21306300	0.81151800
H	4.15903800	-0.33463400	0.04430500
C	5.26370500	-0.51360300	2.12784600
H	5.61683900	0.23506500	2.84698200
H	4.26532600	-0.82907100	2.43824800
C	6.23495300	-1.67107300	2.10078300
C	5.80122900	-2.97795700	1.83975700
C	7.58861400	-1.46576600	2.40997600
C	6.69684400	-4.04788100	1.86220200
H	4.75337700	-3.16767100	1.62577600
C	8.48828800	-2.53154800	2.43108600
H	7.93939900	-0.46631100	2.65636300
C	8.04370700	-3.82609000	2.15383400
H	6.34029700	-5.05323200	1.65843800
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H	8.74075600	-4.65871900	2.17797200



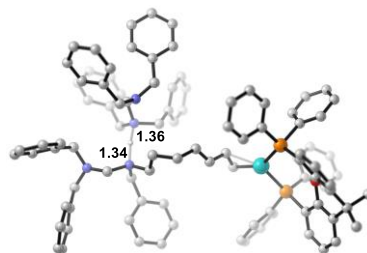
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O	3.64841200	-1.27189600	0.44530500
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C	4.22958100	0.25046300	-1.32003200
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C	6.15804800	-0.27759800	-2.71448900
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C	5.76652200	-3.02342800	-0.02743400
C	4.38671800	-3.55235200	0.38088600
C	3.38086200	-2.61235700	0.65126000
C	2.10892300	-2.97917000	1.13621700
C	1.86251600	-4.34964900	1.32353200
C	2.83461600	-5.30365700	1.03455000
C	4.08694000	-4.90451600	0.56827900
C	6.51096800	-2.55724700	1.25860200
C	6.61799600	-4.10211900	-0.71833700
C	3.64039600	2.67649200	0.15332400
C	4.70809200	3.46241100	-0.31191800
C	5.31024300	4.40388100	0.52200100
C	4.86081200	4.56865000	1.83550700
C	3.80723500	3.78777400	2.31138400
C	3.19986500	2.84809300	1.47446000
C	2.44621100	2.21746400	-2.48306800
C	2.20800400	1.43439000	-3.62871800
C	1.78683300	2.02242200	-4.82133400
C	1.57856800	3.40383200	-4.89041300
C	1.80007600	4.18843100	-3.75853200
C	2.23041100	3.60180700	-2.56425300
C	-0.75158500	-2.69865300	1.38887200
C	-1.15753100	-3.11662700	0.10707500
C	-2.35460700	-3.80873200	-0.07277100
C	-3.17983200	-4.08257400	1.02435100
C	-2.79399400	-3.66213800	2.29804000
C	-1.58685400	-2.97723300	2.48086400
C	1.00168800	-1.42490600	3.33825300
C	1.46970400	-2.40545500	4.22745300
C	1.57697900	-2.13041700	5.59194500
C	1.21711300	-0.87502900	6.08749900
C	0.75464100	0.10948400	5.21211000
C	0.65415400	-0.16273600	3.84667500
C	-2.45957800	0.27366700	-0.46525400
C	-3.29082500	0.75544400	-2.81338500
C	-2.63940800	-0.47754700	-3.41059400
C	-1.29344000	-0.49580200	-3.81048500
C	-0.73669000	-1.64843200	-4.36497100
C	-1.51568600	-2.79504600	-4.54405000
C	-2.85880000	-2.78177000	-4.16759100
C	-3.41354700	-1.63113400	-3.60133900
C	-1.50151600	2.22810400	-1.79253000
C	-1.58644500	3.52051100	-1.01004900
C	-0.65075000	3.80538500	-0.00715300

TS19

C	-0.69440600	5.02232800	0.67941500
C	-1.67267900	5.96697500	0.36730000
C	-2.60794400	5.69388000	-0.63617800
C	-2.56288500	4.47946000	-1.32152000
H	4.94322900	1.46979300	-2.94947200
H	6.81593600	-0.01773100	-3.53853900
H	7.19763100	-2.09876500	-2.27313700
H	0.89138600	-4.67202500	1.68494100
H	2.61962400	-6.35840500	1.17834300
H	4.83699400	-5.65897500	0.35900300
H	7.49287400	-2.14608000	0.99900200
H	6.65714700	-3.40406800	1.93847400
H	5.94752800	-1.78487700	1.79068700
H	6.14517800	-4.47460500	-1.63341500
H	6.78856800	-4.94868000	-0.04697300
H	7.60619500	-3.70969300	-0.97471000
H	5.07338000	3.34250800	-1.32746800
H	6.13400900	5.00591900	0.14848300
H	5.33535500	5.29940900	2.48456400
H	3.46120100	3.90327800	3.33508000
H	2.38910300	2.22454100	1.84444800
H	2.37077600	0.36030800	-3.59027700
H	1.62880600	1.40319600	-5.70067000
H	1.25515200	3.86230100	-5.82071900
H	1.64810500	5.26356800	-3.80149100
H	2.40511500	4.23085400	-1.69733700
H	-0.52706700	-2.90337100	-0.75325500
H	-2.64163600	-4.13382200	-1.06919000
H	-4.10884800	-4.62940200	0.88680600
H	-3.42158800	-3.88077300	3.15815900
H	-1.29150100	-2.67552000	3.48092500
H	1.76040300	-3.38329600	3.85605300
H	1.94590100	-2.89712800	6.26768200
H	1.30543200	-0.66308400	7.14940300
H	0.48507500	1.09232300	5.58971700
H	0.32308000	0.61112900	3.15815500
H	-2.68742800	-0.73666100	-0.79887200
H	-1.44166400	0.30798000	-0.05916100
H	-4.33596700	0.53361700	-2.58529000
H	-3.29399100	1.58984900	-3.52083200
H	-0.67050100	0.38666600	-3.70219300
H	0.30632600	-1.64694000	-4.66873100
H	-1.07973900	-3.68738100	-4.98387300
H	-3.47877700	-3.66111200	-4.31758100
H	-4.46445800	-1.63004000	-3.32102100
H	-0.57332500	1.69631200	-1.55860100
H	-1.49224200	2.45216300	-2.86159500
H	0.12074700	3.07364400	0.22550200
H	0.04302700	5.23206600	1.44909200
H	-1.70334600	6.91575400	0.89522900
H	-3.36188200	6.43249700	-0.89390200
H	-3.28054500	4.28408000	-2.11598100
C	-8.56079300	-3.49693300	-2.57090700
H	-9.10327500	-2.68693200	-3.05879000
C	-8.72263700	-4.75472300	-3.00712400
H	-8.20395000	-5.59081500	-2.54293400
H	-9.38231800	-4.99157100	-3.83596500
C	-7.69438000	-3.12187200	-1.46162700
H	-7.15808700	-3.93574500	-0.96994400
C	-7.53160600	-1.86564000	-1.01253900
H	-8.07738400	-1.05639700	-1.50137500
C	-6.63638100	-1.46832900	0.12789000
H	-6.22243400	-2.36451200	0.60740100
H	-7.22078400	-0.93856200	0.89506000

C	-5.47892200	-0.55466400	-0.33116000
H	-4.89564300	-1.09833400	-1.08200000
H	-5.89340400	0.33879600	-0.81849800
C	-4.59702000	-0.13432100	0.84206700
H	-5.20644300	0.37933500	1.58857600
H	-4.15381000	-1.01625300	1.32429900
N	-3.49096300	0.80819900	0.49105500
H	-3.54544400	1.62518400	-0.59172700
C	-2.87256100	1.40577300	1.72912400
H	-2.45011800	0.58590600	2.32249200
H	-2.04538900	2.03363100	1.38861100
C	-3.84213300	2.21530100	2.55857500
C	-4.34078400	3.43774900	2.08538300
C	-4.23167100	1.76944400	3.82857800
C	-5.21977700	4.19032900	2.86360000
H	-4.03142600	3.80934500	1.11197300
C	-5.10724100	2.52540200	4.61094500
H	-3.84275100	0.82819600	4.21085000
C	-5.60553300	3.73592300	4.12765500
H	-5.59721400	5.13718300	2.48768800
H	-5.39732200	2.16882500	5.59510000
H	-6.28659300	4.32598800	4.73417200

### TS20



N	-6.13342500	2.55696100	-0.04616600
C	-4.86256900	2.41256700	-0.68547800
C	-7.15811500	1.52299700	-0.27572800
C	-8.07858500	1.70080400	-1.47475900
C	-9.33104600	2.31072600	-1.32065900
C	-10.17316600	2.50742000	-2.41645800
C	-9.77709800	2.08549900	-3.68662800
C	-8.54013800	1.45826500	-3.85286800
C	-7.70124500	1.26506100	-2.75439500
C	-6.62292800	3.89541200	0.31612200
C	-6.54468300	5.01792800	-0.71681900
C	-6.63378900	4.80676400	-2.09841300
C	-6.60687400	5.88556700	-2.98549400
C	-6.49892800	7.19217000	-2.50742500
C	-6.41299800	7.41544900	-1.13179100
C	-6.42908700	6.33583200	-0.24802400
H	-4.92523500	1.74100300	-1.54470600
H	-4.50214000	3.37929600	-1.05203000
H	-6.63217800	0.56650700	-0.35767300
H	-7.77304700	1.46078400	0.63108100
H	-9.65619400	2.62929400	-0.33246900
H	-11.13942500	2.98367400	-2.27653500
H	-10.43261500	2.23318100	-4.54001300
H	-8.23370900	1.10863300	-4.83480700
H	-6.75014000	0.75785100	-2.89789800
H	-7.67020500	3.76498300	0.61146600
H	-6.11257100	4.24546200	1.22449900
H	-6.73644800	3.79966500	-2.48806200
H	-6.67657400	5.70130500	-4.05410800
H	-6.48072900	8.02890200	-3.19989100
H	-6.32949300	8.42777900	-0.74606300

H	-6.35880000	6.51964400	0.82262000	C	4.71921500	4.12229000	4.15202600
C	1.62958400	-0.15445700	0.56867200	C	5.24860500	2.99540400	3.51407700
H	1.41607600	-1.20344000	0.77400500	C	3.31569500	-2.31221300	-2.46909500
C	2.25367400	0.63064700	1.56599300	C	2.43976000	-1.48193200	-3.18897500
H	2.12090100	1.71189600	1.56851000	C	1.45809200	-2.02729100	-4.01676500
H	2.45340200	0.20223300	2.54711000	C	1.31319000	-3.41359600	-4.11520900
C	0.82936400	0.46398100	-0.48587000	C	2.16153800	-4.24804100	-3.38610000
H	1.00370900	1.53199900	-0.64001600	C	3.16102300	-3.70276100	-2.57531100
C	-0.10977100	-0.14113300	-1.24038200	C	5.42235400	-2.94149700	-0.59138800
H	-0.28696600	-1.21033000	-1.10800500	C	6.50251000	-3.64852800	-1.14018900
C	-0.98206200	0.55817600	-2.24851900	C	7.05371900	-4.73987900	-0.46475700
H	-1.02104200	-0.01807100	-3.18301600	C	6.52887400	-5.14553000	0.76333800
H	-0.55351900	1.53678800	-2.50532500	C	5.45092200	-4.45163900	1.31719600
C	-2.44009800	0.75628500	-1.75191500	C	4.90684900	-3.35494100	0.64797100
H	-3.06188100	1.09093700	-2.59181100	H	7.14046800	3.93134100	1.33119000
H	-2.83424800	-0.20732300	-1.41195000	H	8.89826800	4.90058000	-0.10427200
C	-2.47377400	1.77074900	-0.60863500	H	9.79253700	3.63179400	-2.01831300
H	-1.67188600	1.52637800	0.09166600	H	4.92555400	-2.08244400	-4.39782500
H	-2.25957300	2.77546400	-0.99121500	H	6.58263500	-1.34284000	-6.06881100
N	-3.74761400	1.83183800	0.18994900	H	8.47399300	0.09259300	-5.40840100
C	-3.53343100	2.67019500	1.44096500	H	10.98774100	0.56885800	-1.75069000
H	-4.52988700	2.94613700	1.78818600	H	10.52520600	-0.67268300	-2.93779900
H	-3.11224900	1.99833400	2.19153100	H	9.69620100	-0.58711700	-1.37106200
C	-2.61890300	3.87686000	1.33437100	H	9.11162000	2.50959300	-4.37770200
C	-1.31142100	3.78885900	1.83654600	H	10.19430100	1.13355000	-4.67599400
C	-3.04006300	5.09528900	0.78149700	H	10.65074000	2.35490600	-3.50499300
C	-0.44228100	4.87902200	1.78017000	H	8.43616100	1.40573400	2.37057500
H	-0.96623600	2.85883500	2.28324900	H	9.55372500	0.09099800	4.13552600
C	-2.17169000	6.18626500	0.71807100	H	8.32814200	-1.72677300	5.30906300
H	-4.04945800	5.20995400	0.40058100	H	5.97238700	-2.22808900	4.68687300
C	-0.87153400	6.08168600	1.21581100	H	4.86008100	-0.92573400	2.89172900
H	0.56494300	4.78606100	2.17699800	H	4.05138700	3.54937400	0.37964800
H	-2.51835600	7.12048200	0.28544600	H	3.16298600	5.56770800	1.49534400
H	-0.20040900	6.93475500	1.17061900	H	3.57067600	5.93390200	3.92789300
H	-4.00678600	0.57950600	0.64815600	H	4.90645000	4.27547600	5.21163800
Pd	3.82632500	0.06761000	0.22873200	H	5.84602700	2.29170500	4.08480700
P	5.64572900	1.29461300	1.22056000	H	2.53127400	-0.40295900	-3.10151400
P	4.62088700	-1.49729800	-1.43137500	H	0.80531900	-1.36823300	-4.58373800
O	7.08351800	0.10137900	-1.07681600	H	0.54757600	-3.83983100	-4.75842200
C	7.01906700	2.07188200	0.24280600	H	2.05914700	-5.32784900	-3.45819200
C	7.52974300	3.35449000	0.49953200	H	3.82785500	-4.36573800	-2.03380700
C	8.51937900	3.90437300	-0.31381900	H	6.91688700	-3.34964500	-2.09792700
C	9.02552600	3.18311400	-1.39637100	H	7.89391700	-5.27334500	-0.90133300
C	8.56355600	1.89386100	-1.67683200	H	6.95966300	-5.99444300	1.28733300
C	7.56825100	1.37161600	-0.84079200	H	5.03977900	-4.75770400	2.27572800
C	9.10615300	0.99104000	-2.79188400	H	4.07985500	-2.80406300	1.08918700
C	7.92325200	0.17219800	-3.32506700	C	-4.76963800	-1.74557000	0.66066200
C	6.96238300	-0.26138000	-2.40325800	H	-5.82107700	-1.47288700	0.55967400
C	5.86207200	-1.06102600	-2.74457700	N	-4.21396000	-2.10025600	-0.60933100
C	5.75297800	-1.45475600	-4.08728100	C	-4.95693300	-1.70654700	-1.82284100
C	6.68806300	-1.03458500	-5.03255300	H	-5.34882900	-0.70012900	-1.64470200
C	7.75919500	-0.22320800	-4.65614400	C	-3.35207500	-3.28423700	-0.72452200
C	10.14332900	0.01073300	-2.17083000	H	-2.36331200	-3.06402400	-0.29805000
C	9.79679600	1.79880100	-3.90354100	H	-3.16907400	-3.42114900	-1.79657900
C	6.56093500	0.34082000	2.51585200	H	-4.72612700	-2.58326200	1.36037700
C	7.89044600	0.61343700	2.87354400	N	-4.11169400	-0.55315000	1.36577300
C	8.52238700	-0.12905600	3.87292000	C	-4.97099800	-0.08300600	2.53929800
C	7.83410200	-1.14943400	4.53225600	H	-4.28494300	0.34218600	3.27434000
C	6.51137000	-1.42947300	4.18386100	H	-5.57342700	0.73951300	2.14020800
C	5.88212900	-0.69415600	3.17858700	C	-2.66564000	-0.83393200	1.72655000
C	5.02150200	2.77597600	2.14855000	H	-2.18379000	0.13894800	1.84139100
C	4.24747100	3.71047100	1.43745400	H	-2.22791000	-1.28125600	0.83288600
C	3.73738400	4.84422200	2.06895100	C	-5.90737000	-1.06574200	3.22631700
C	3.96877700	5.05212300	3.43292200	C	-5.49653300	-1.84799300	4.31552400



C	-7.25122800	-1.13508000	2.82614600
C	-6.39833500	-2.69391000	4.96324000
H	-4.47379700	-1.79045500	4.67007600
C	-8.15362700	-1.98166300	3.46974300
H	-7.60144300	-0.50727700	2.00975100
C	-7.72620500	-2.76925300	4.54000200
H	-6.06099500	-3.28952600	5.80670900
H	-9.18930700	-2.01677300	3.14362600
H	-8.42583500	-3.42646400	5.04843700
C	-2.36460600	-1.65096900	2.96526600
C	-1.93285900	-0.99275200	4.12775800
C	-2.44786100	-3.05108700	2.98419700
C	-1.62088800	-1.70638500	5.28644000
H	-1.82447600	0.08984200	4.12452800
C	-2.14075700	-3.76729400	4.14157100
C	-1.73132700	-3.09821900	5.29726400
H	-1.28524600	-1.17673300	6.17345400
H	-1.48692000	-3.65811800	6.19548000
H	-4.22691700	-1.60774200	-2.63479100
C	-3.81922900	-4.61497000	-0.13463100
C	-2.83589900	-5.56272100	0.19193900
C	-5.16321000	-4.95442400	0.05996000
C	-3.18419800	-6.81893600	0.68814200
H	-1.78523500	-5.31544800	0.04965600
C	-5.51358800	-6.20828300	0.56782900
H	-5.94474500	-4.24660100	-0.19317500
C	-4.52869300	-7.14507900	0.88104400
H	-2.40675600	-7.53941200	0.92739400
H	-6.56255800	-6.45182900	0.71260500
H	-4.80454300	-8.12004700	1.27277200
C	-6.08515700	-2.61627100	-2.28484600
C	-7.39028800	-2.46626000	-1.79224200
C	-5.83842300	-3.62957100	-3.22159200
C	-8.41306400	-3.32407000	-2.20069100
H	-7.61925000	-1.66320000	-1.09554600
C	-6.85744100	-4.48937600	-3.63334700
H	-4.84030600	-3.74508000	-3.63847800
C	-8.14692000	-4.34209600	-3.11880900
H	-9.41879800	-3.18932200	-1.81236600
H	-6.64577000	-5.26956000	-4.35903300
H	-8.94246700	-5.00787700	-3.44092800
H	-2.74959600	-3.59783600	2.09736400
H	-2.21528100	-4.85092900	4.13391700