

## SUPPORTING INFORMATION

for

### Deprotonation-Controlled Copper-Free Pd-Catalyzed Sonogashira Coupling versus Kumada–Tamao–Corriu Reaction: A DFT Investigation toward Anticancer Carborane Alkynes

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#### Title

**Figure S1.** Optimized structures of reactants, transition states, and intermediates for the standard Sonogashira reaction (showing the common structures) involved in the synthesis of 3-quinolyethynyl carborane. All structures were calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

**Figure S2.** Optimized structures of reactants, transition states, and intermediates for the copper-free carbopalladation mechanism of the Sonogashira reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

**Figure S3.** Optimized structures of reactants, transition states, and intermediates for the cationic mechanism of the Sonogashira reaction for the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

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† Electronic Supplementary Information (ESI) available: See DOI:

**Figure S4.** Optimized structures of reactants, transition states, and intermediates for the anionic mechanism of the Sonogashira reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

**Figure S5.** Optimized structures of reactants, transition states, and intermediates for the ionic mechanism of the Sonogashira reaction for the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

**Figure S6.** Optimized structures of reactants, transition states, and intermediates for the Kumada reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

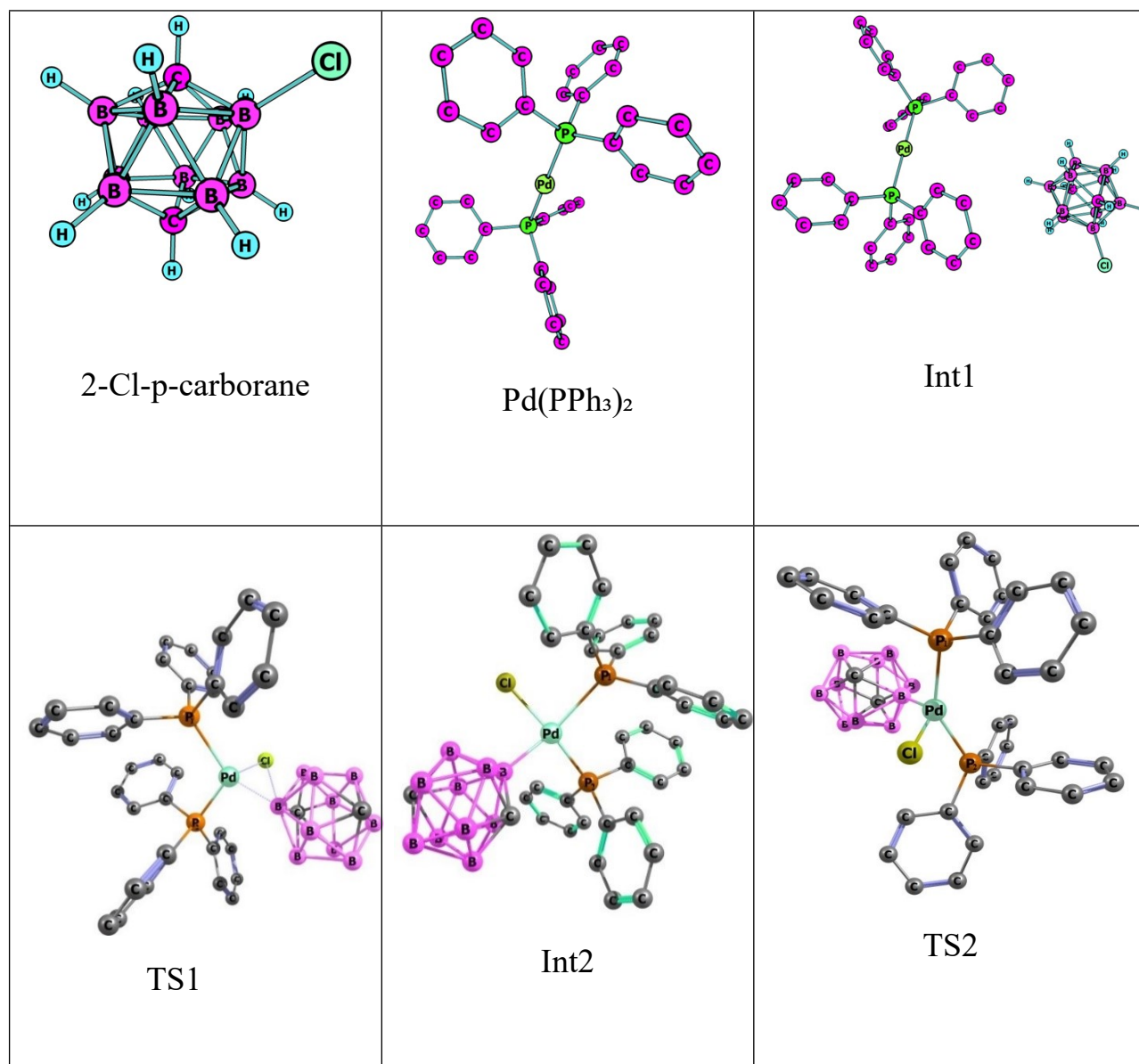
**Figure S7.** Optimized geometries of the transition states for 3-quinolyethynyl carborane synthesis, along with key bond lengths and Wiberg bond indices. All calculations were performed at the B3LYP-D3/BSL level of theory in 1,4-dioxane solvent. Bond lengths are reported in Angstroms (Å).

**Figure S8.** Some of the intrinsic reaction coordinate (IRC) analyses for the transition states involved in the formation of 3-quinolyethynyl carborane via Sonogashira and Kumada coupling reactions. All calculations were performed at the B3LYP-D3/BSL level of theory in 1,4-dioxane solvent.

**Table S1.** The resulting energies are Included the Monomeric MgCl<sub>2</sub> (Int3-K) vs Dimeric MgCl<sub>2</sub> (Int3-K) comparison for the Kumada reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

**Table S2.** The resulting energies are Included the Int3-K, Int4-K, TS-RE1 and Int5 comparison for the Kumada reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL and CAM-B3LYP/BSL level of theory with 1,4-dioxane as the solvent.

Figure S1. Optimized structures of reactants, transition states, and intermediates for the standard Sonogashira reaction (showing the common structures) involved in the synthesis of 3-quinolyneethynyl carborane. All structures were calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.



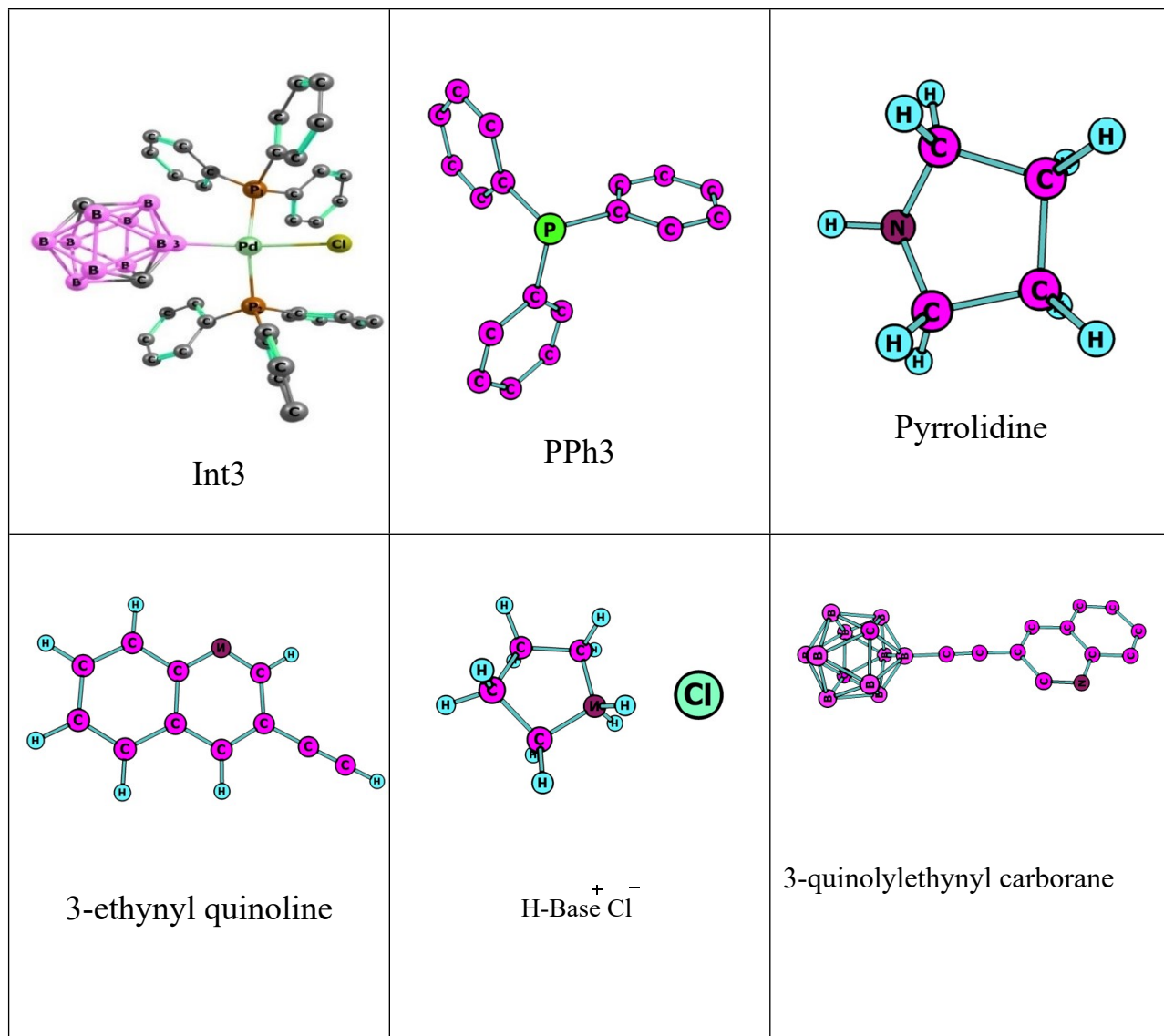


Figure S2. Optimized structures of reactants, transition states, and intermediates for the copper-free carbopalladation mechanism of the Sonogashira reaction in the synthesis of 3-quinolyylethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

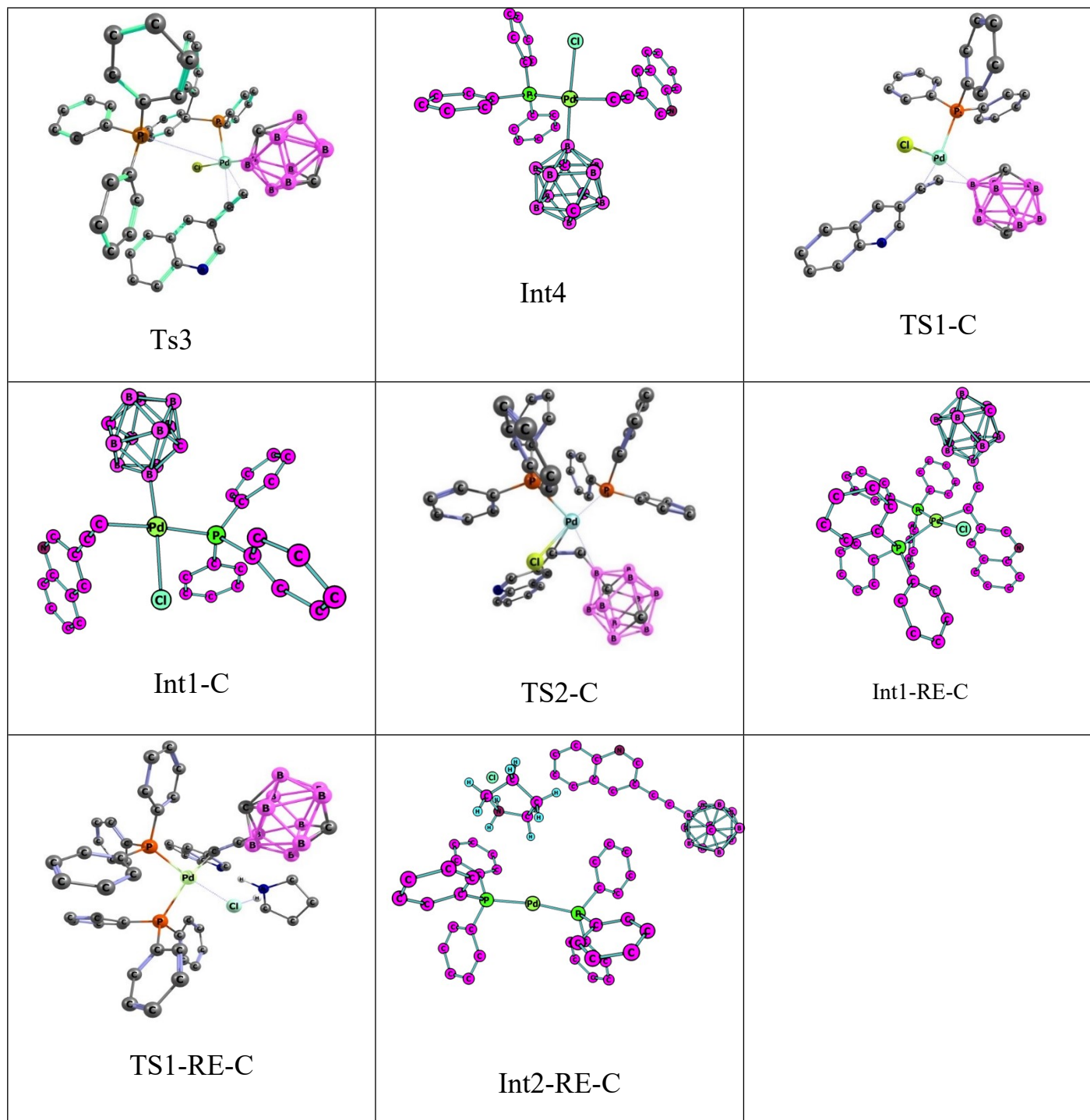


Figure S3. Optimized structures of reactants, transition states, and intermediates for the cationic mechanism of the Sonogashira reaction for the synthesis of 3-quinolyneethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

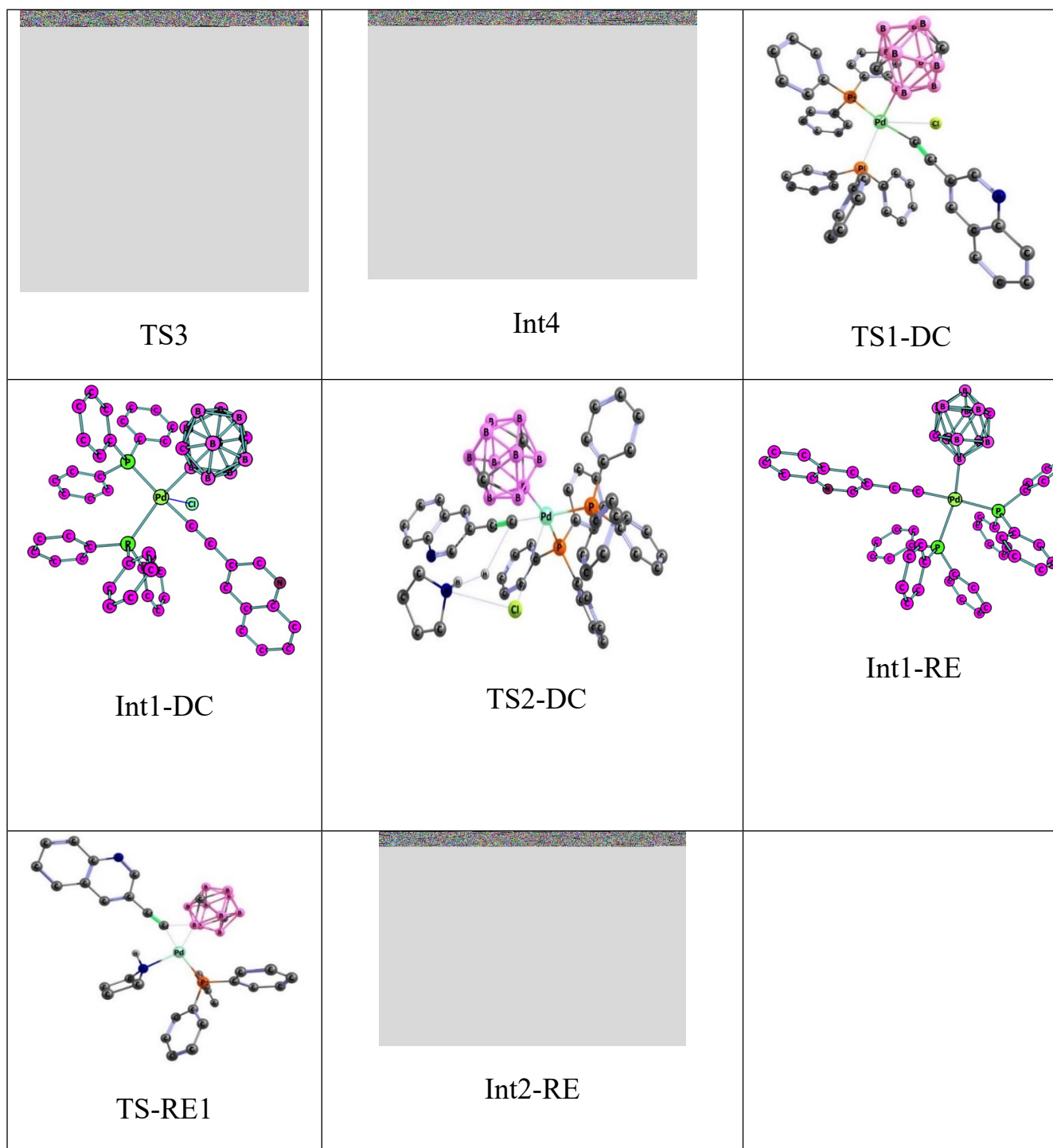


Figure S4. Optimized structures of reactants, transition states, and intermediates for the anionic mechanism of the Sonogashira reaction in the synthesis of 3-quinolyylethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

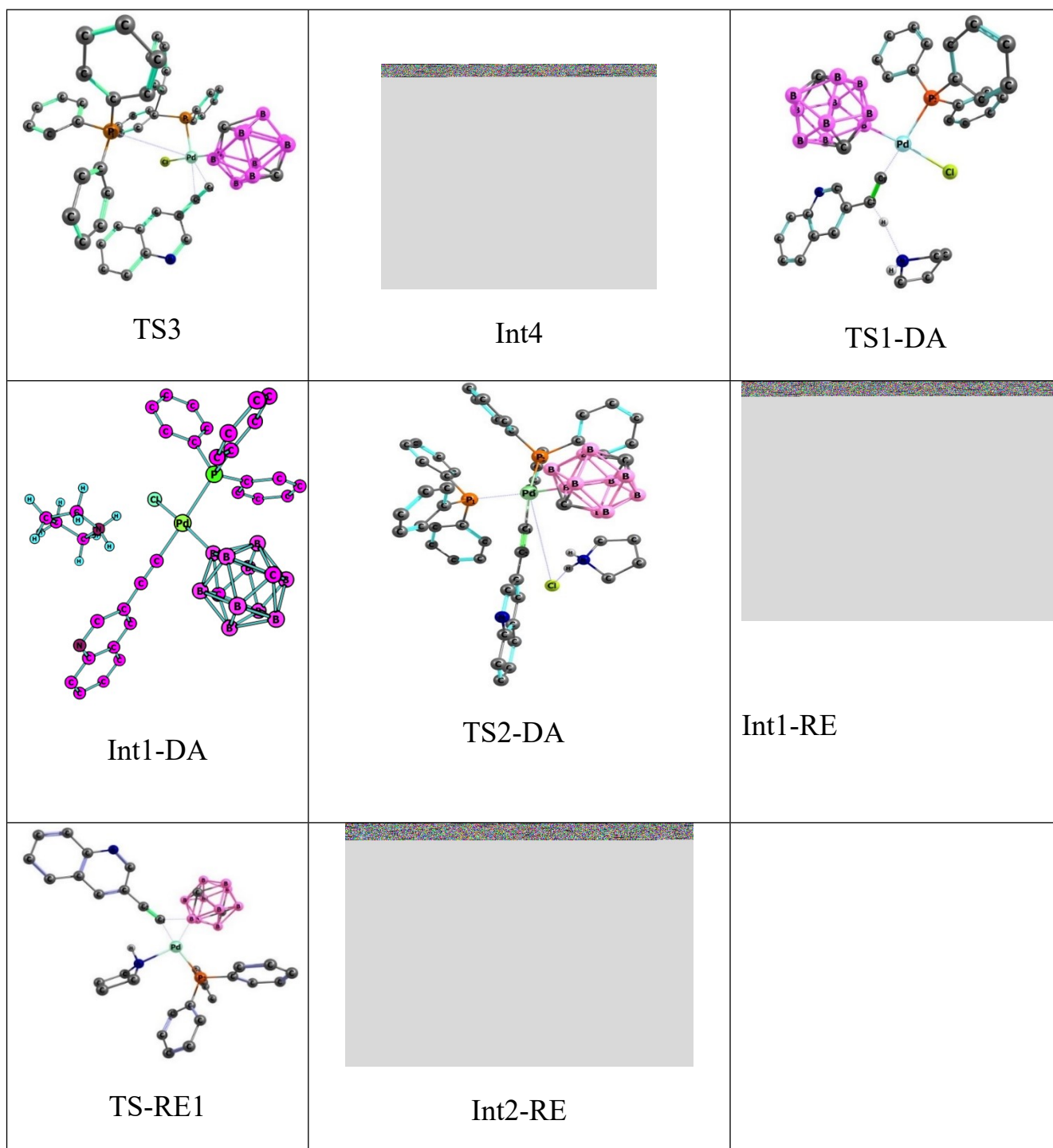


Figure S5. Optimized structures of reactants, transition states, and intermediates for the ionic mechanism of the Sonogashira reaction for the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

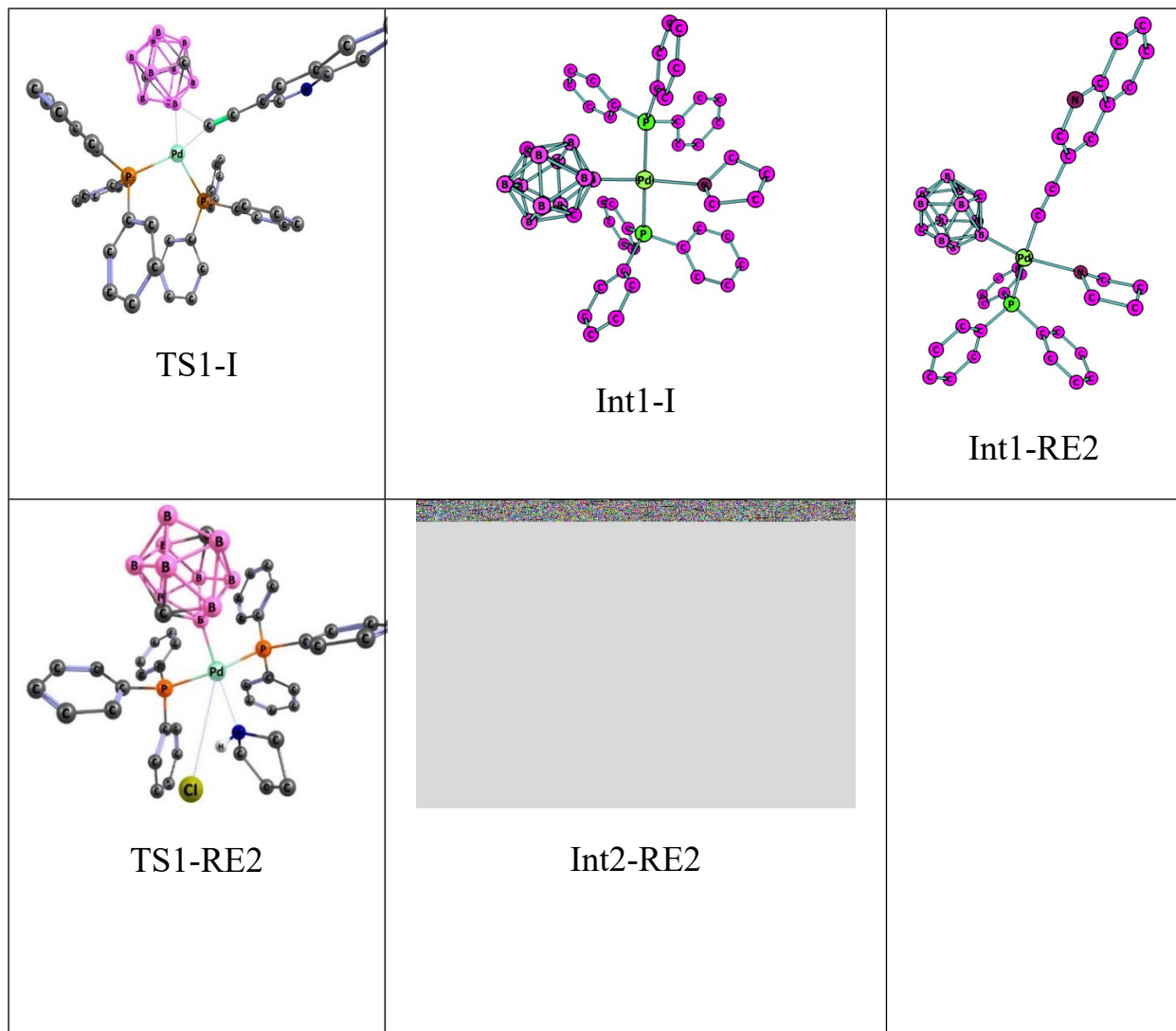
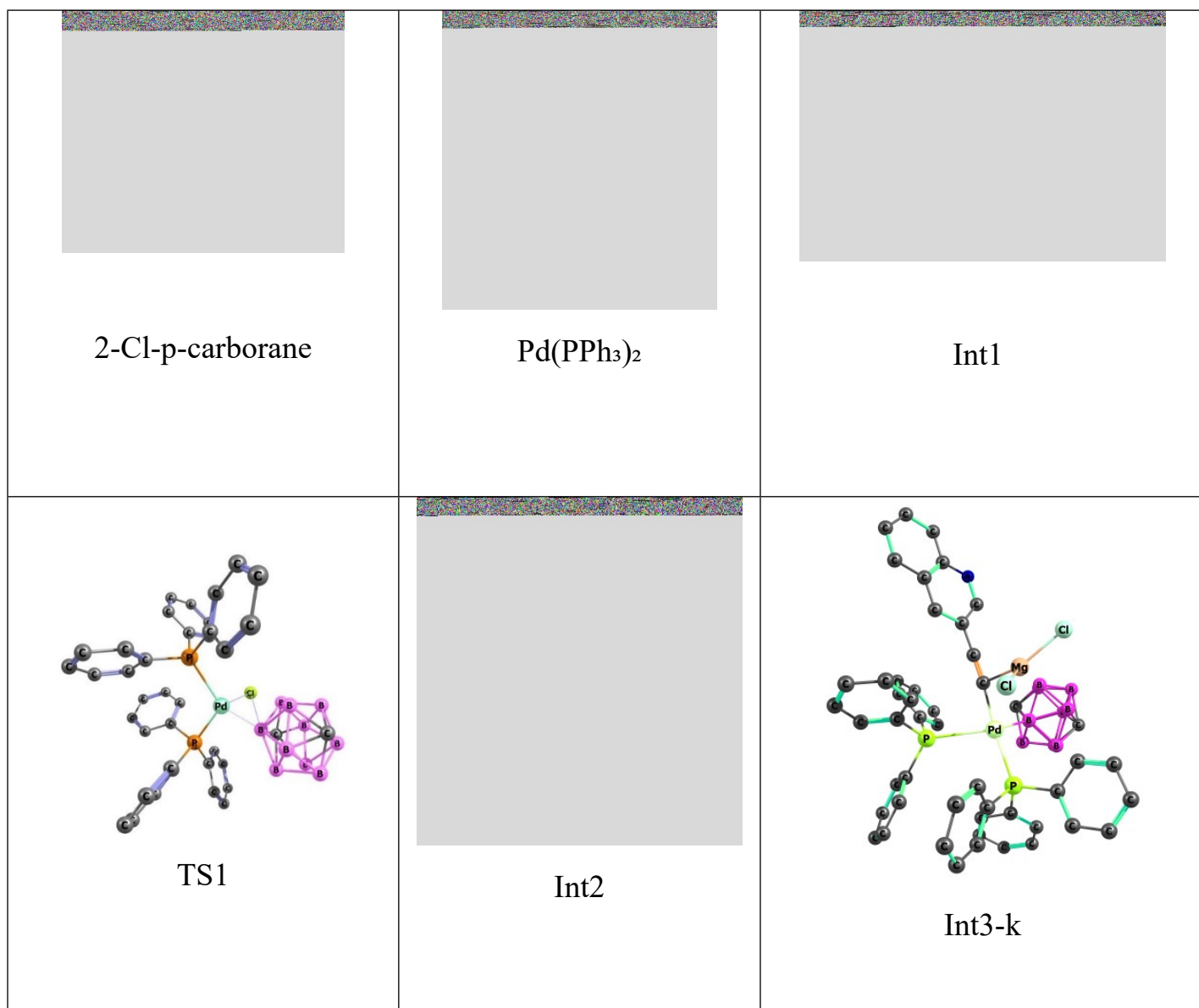
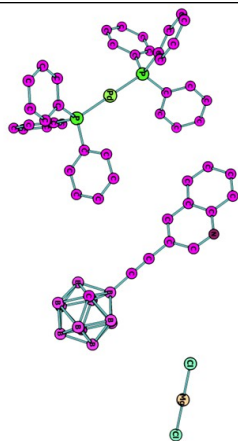
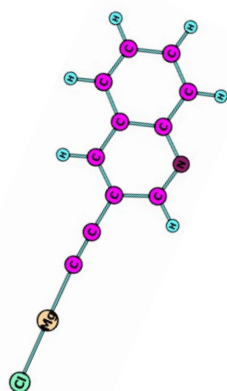


Figure S6. Optimized structures of reactants, transition states, and intermediates for the Kumada reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

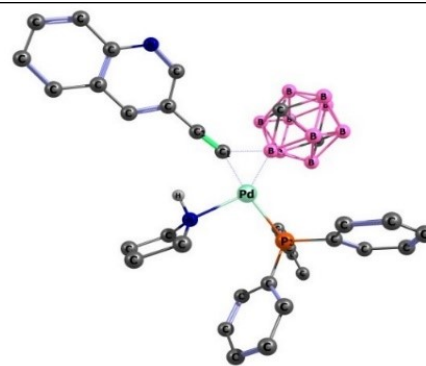




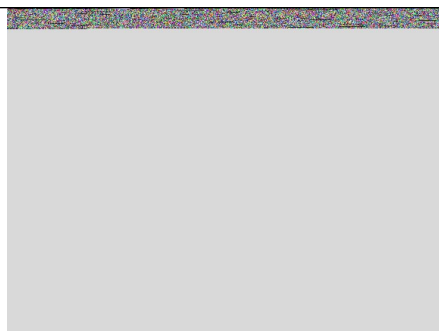
Int5



3-quinolyethynyl magnesium  
bromide



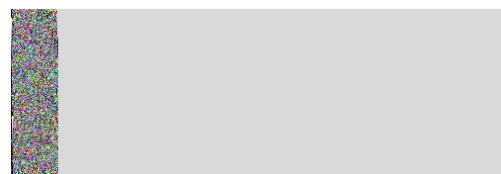
TS-RE1



Int4-K



MgCl<sub>2</sub>



3-quinolyethynyl carborane

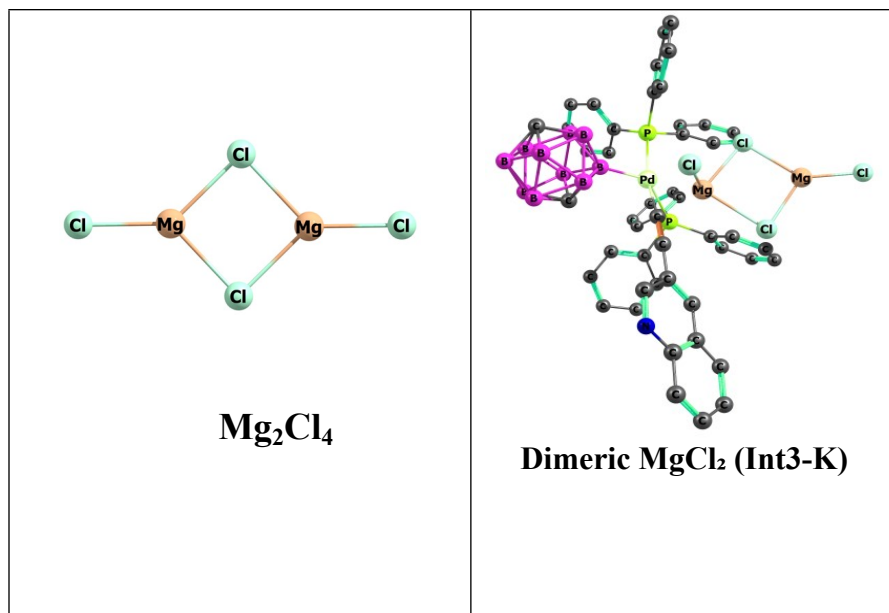
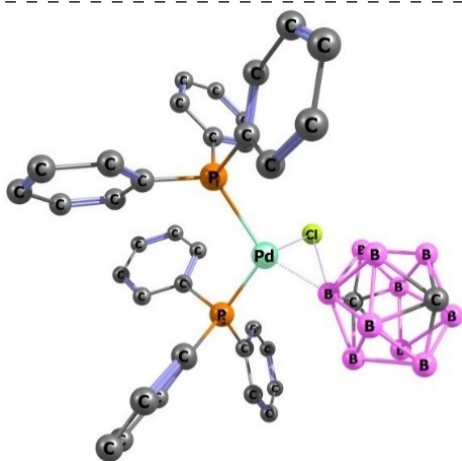


Figure S7. Optimized geometries of the transition states for 3-quinolyethynyl carborane synthesis, along with key bond lengths and Wiberg bond indices. All calculations were performed at the B3LYP-D3/BSL level of theory in 1,4-dioxane solvent. Bond lengths are reported in Angstroms (Å).



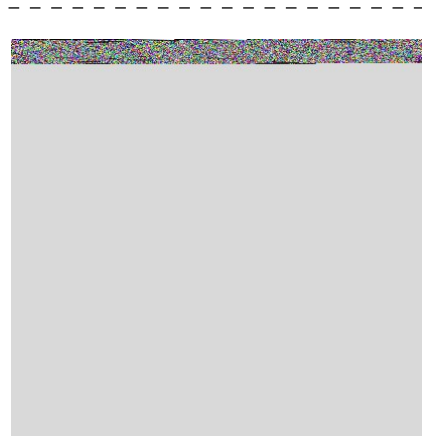
**TS1**

Pd-Cl: 3.1(0.14)  
 Pd-B: 2.0(0.56)  
 B-Cl: 3.0(0.09)



**TS2**

Pd-P1: 2.3(0.46)  
 Pd-P2: 2.5(0.39)



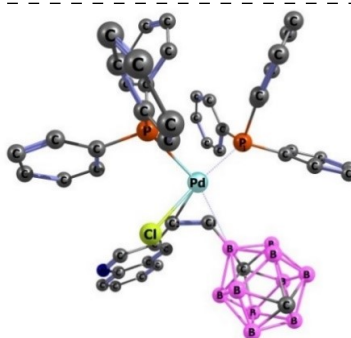
**TS3**

Pd-P1: 6.2(0.004)  
 Pd-P2: 2.4(0.48)  
 Pd-C10: 2.55(0.13)  
 Pd-C11: 2.24(0.22)



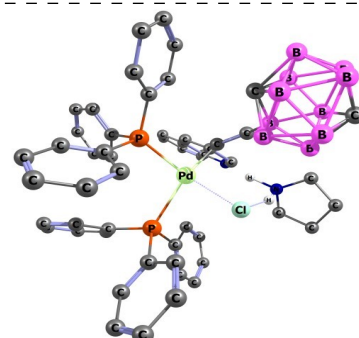
**TS1-C**

Pd-B: 2.2(0.43)  
 Pd-C10: 2.1(0.51)  
 B-C11: 2.1(0.47)  
 C10-C11: 1.29(1.14)



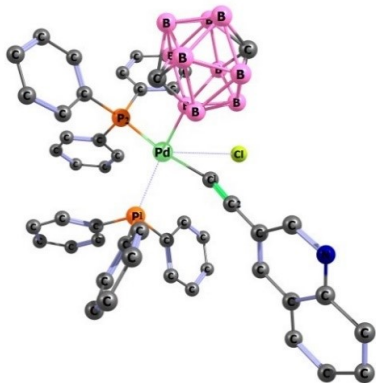
**TS2-C**

Pd-P1: 2.43(0.45)  
 Pd-B: 3.7(0.02)  
 B-C29: 1.58(0.92)



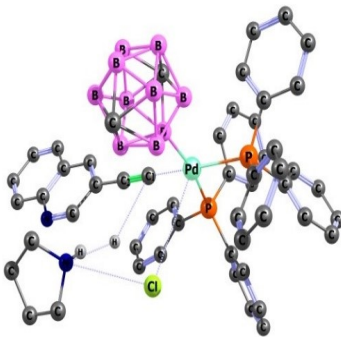
**TS1-RE-C**

Pd-Cl: 2.53(0.39)  
 Pd-C28: 2.04(0.57)  
 Cl-H48: 1.96(1.0)



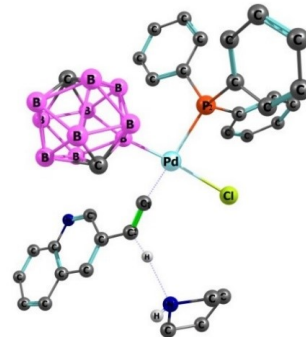
**TS1-DC**

Pd-Cl:3.73(0.08)  
Pd-P1:2.68(0.42)



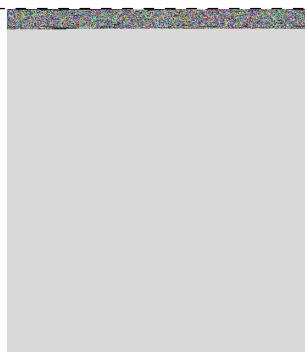
**TS2-DC**

Pd-Cl:4.1(0.05)  
Cl-H48:3.3(0.07)  
N2-H57:2.77(0.12)  
Pd-C30:3.2(0.05)  
Pd-C31:1.98(0.57)



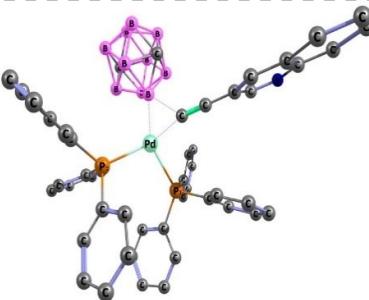
**TS1-DA**

Pd-C31:1.90(0.78)  
Pd-B:2.12(0.58)  
Pd-C30:3.18(0.05)  
H42-N2:1.87(0.9)



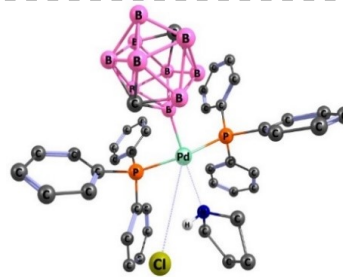
**TS2-DA**

Pd-Cl:6.3(0.00)  
Pd-P2:2.69(0.2)  
Cl-H57:1.94(0.28)



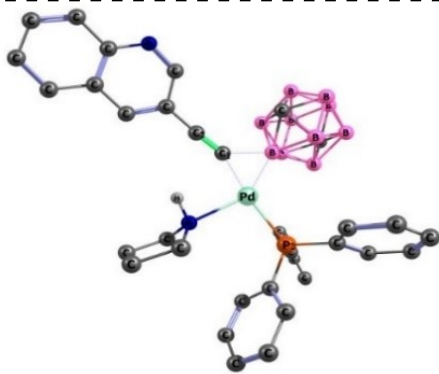
**TS1-I**

Pd-Cl:4.34(0.09)  
Pd-N1:2.39(0.15)



**TS1-RE2**

Pd-B:2.21(0.43)  
B-C31:2.04(0.2)  
Pd-C31:1.96(0.44)



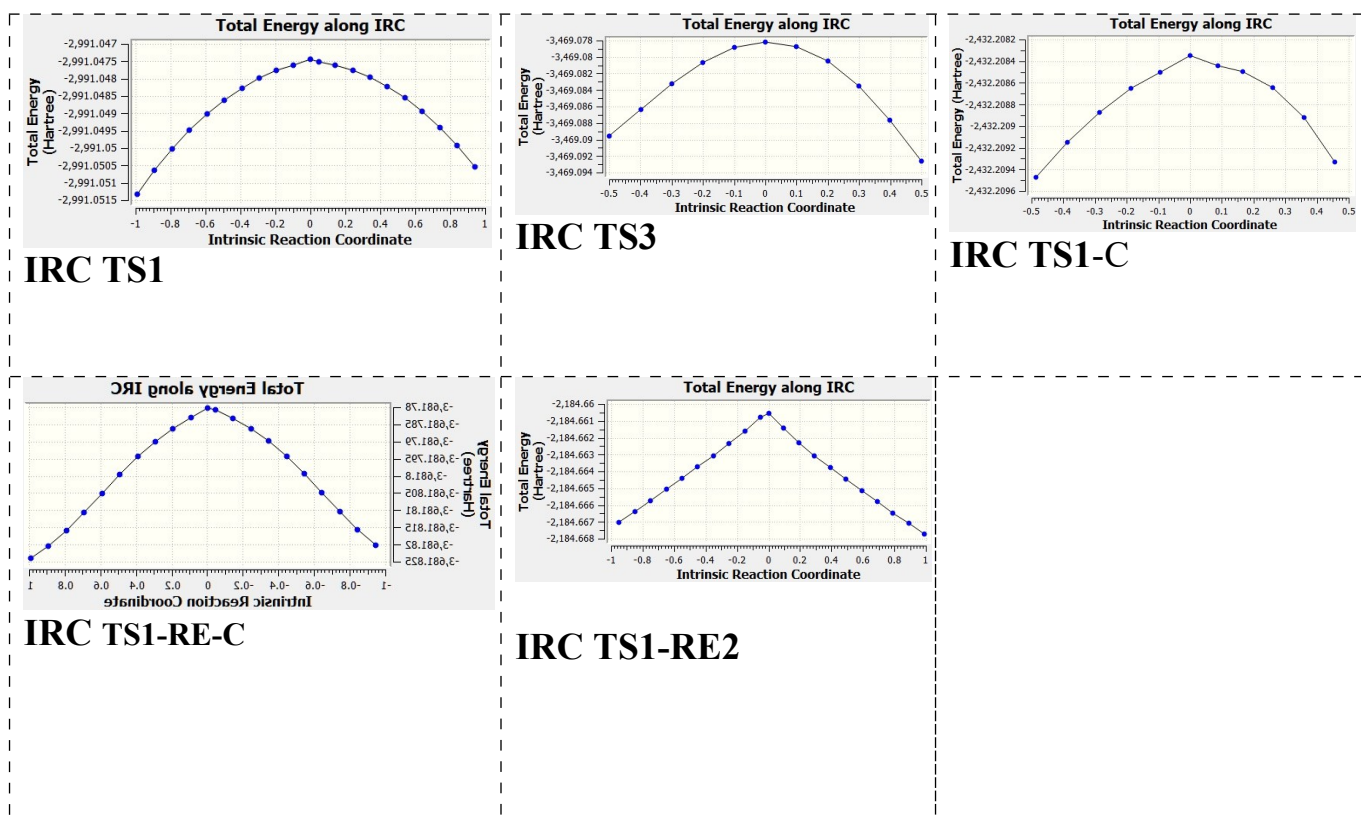
### TS-RE1

Pd-B:2.2(0.4)

Pd-C47:1.96(0.5)

B-C47:2.0(0.43)

Figure S8. Some of the intrinsic reaction coordinate (IRC) analyses for the transition states involved in the formation of 3-quinolyethynyl carborane via Sonogashira and Kumada coupling reactions. All calculations were performed at the B3LYP-D3/BSL level of theory in 1,4-dioxane solvent.



	E(Hartree)	$\Delta E = E(\text{Int3-K}) - E(\text{Int2})$ (kcal mol <sup>-1</sup> )
Monomeric MgCl <sub>2</sub> (Int3-K)	-4130.372336	-64.43
Dimeric MgCl <sub>2</sub> (Int3-K)	-5251.162856	-55.09

**Table S1.** The resulting energies are Included the Monomeric MgCl<sub>2</sub> (Int3-K) vs Dimeric MgCl<sub>2</sub> (Int3-K) comparison for the Kumada reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL level of theory with 1,4-dioxane as the solvent.

	$\Delta E$ (kcal mol <sup>-1</sup> )	$\Delta E$ (kcal mol <sup>-1</sup> )
	B3LYP-D3	Cam- B3LYP
Int3-K	-64.43	-54.6
Int4-K	-58.6	-49.3
TS-RE1	-28	-16.3
Int5	-72.2	-71

**Table S2.** The resulting energies are Included the Int3-K, Int4-K, TS-RE1 and Int5 comparison for the Kumada reaction in the synthesis of 3-quinolyethynyl carborane, calculated at the B3LYP-D3/BSL and CAM-B3LYP/BSL level of theory with 1,4-dioxane as the solvent.

## 2-Cl-p-carborane



Atom	x	y	z
H	1.753374000	1.483016000	-2.188026000
H	1.753372000	-1.483144000	-2.187940000
H	-0.635217000	-0.000066000	-2.288894000
H	-0.727477000	-2.391334000	-0.829343000
B	1.346567000	0.893207000	-1.245850000
B	1.346567000	-0.893280000	-1.245798000
C	-0.106255000	-0.000039000	-1.342003000
B	-0.137187000	-1.447122000	-0.429780000
B	1.400050000	1.444472000	0.432303000
H	1.972737000	2.398081000	0.836951000
B	2.318117000	-0.000003000	-0.070539000
H	3.499354000	0.000000000	0.003010000
C	1.357850000	0.000038000	1.342806000
H	1.875605000	0.000066000	2.295538000
B	-0.137186000	1.447096000	-0.429864000
H	-0.727475000	2.391286000	-0.829481000
B	-0.089360000	0.895786000	1.248870000
H	-0.510495000	1.480719000	2.187065000
B	1.400048000	-1.444446000	0.432387000
H	1.972733000	-2.398033000	0.837092000
B	-0.089361000	-0.895712000	1.248922000
H	-0.510496000	-1.480591000	2.187151000

B	-1.064956000	0.000003000	0.074213000
Cl	-2.864240000	0.000000000	-0.006015000

### Pd(PPh<sub>3</sub>)<sub>2</sub>



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.000073000	0.007461000	0.012440000
P	-2.328074000	0.002844000	0.004040000
P	2.327948000	0.002205000	0.004007000
C	-3.100097000	-1.604767000	-0.492127000
C	-2.431191000	-2.784395000	-0.124461000
H	-1.485130000	-2.713515000	0.407141000
C	-2.960725000	-4.033681000	-0.449135000
H	-2.431255000	-4.936549000	-0.156476000
C	-4.159730000	-4.122389000	-1.161298000
H	-4.568191000	-5.094799000	-1.423422000
C	-4.825645000	-2.956445000	-1.544220000
H	-5.754495000	-3.018300000	-2.105388000
C	-4.301214000	-1.704767000	-1.211077000
H	-4.826978000	-0.805928000	-1.518902000
C	-3.124936000	0.375258000	1.633085000

C	-4.329717000	-0.202634000	2.062188000
H	-4.842971000	-0.921612000	1.430723000
C	-4.874110000	0.133296000	3.304545000
H	-5.805630000	-0.325883000	3.625378000
C	-4.224664000	1.051730000	4.131673000
H	-4.648511000	1.309755000	5.098585000
C	-3.022356000	1.629684000	3.715628000
H	-2.505748000	2.337772000	4.358167000
C	-2.473101000	1.287694000	2.479566000
H	-1.525071000	1.718045000	2.165655000
C	-3.109836000	1.227390000	-1.143124000
C	-2.431712000	1.520417000	-2.338245000
H	-1.473552000	1.044777000	-2.534112000
C	-2.968205000	2.421594000	-3.258503000
H	-2.431411000	2.636644000	-4.178702000
C	-4.183848000	3.056148000	-2.990094000
H	-4.597921000	3.765770000	-3.701513000
C	-4.859670000	2.782893000	-1.799194000
H	-5.801777000	3.279044000	-1.580635000
C	-4.328006000	1.873356000	-0.881275000
H	-4.861364000	1.673515000	0.043273000
C	3.103074000	-1.387311000	-0.942025000
C	2.426650000	-1.851046000	-2.082902000
H	1.473582000	-1.402398000	-2.353027000
C	2.958207000	-2.884907000	-2.854386000
H	2.422901000	-3.231307000	-3.734501000
C	4.166911000	-3.482350000	-2.487347000
H	4.576971000	-4.294528000	-3.081774000

C	4.840645000	-3.038925000	-1.347619000
H	5.777173000	-3.504733000	-1.051949000
C	4.314066000	-1.997035000	-0.579695000
H	4.845904000	-1.665222000	0.306959000
C	3.111401000	1.510727000	-0.729100000
C	4.314492000	1.492547000	-1.451391000
H	4.835615000	0.554254000	-1.615826000
C	4.847429000	2.675414000	-1.970662000
H	5.777738000	2.645072000	-2.531998000
C	4.188156000	3.890120000	-1.772680000
H	4.603105000	4.808464000	-2.179587000
C	2.987316000	3.918503000	-1.058525000
H	2.462955000	4.858622000	-0.908937000
C	2.449306000	2.736717000	-0.548176000
H	1.501663000	2.753899000	-0.014937000
C	3.120315000	-0.121668000	1.672680000
C	4.331277000	0.503465000	2.008649000
H	4.851668000	1.110211000	1.273728000
C	4.872227000	0.359405000	3.289087000
H	5.808276000	0.853519000	3.536282000
C	4.213125000	-0.412437000	4.247964000
H	4.633903000	-0.520734000	5.244067000
C	3.004936000	-1.035792000	3.924919000
H	2.481123000	-1.630039000	4.668962000
C	2.459119000	-0.884795000	2.649752000
H	1.506616000	-1.348864000	2.404959000

# Int1

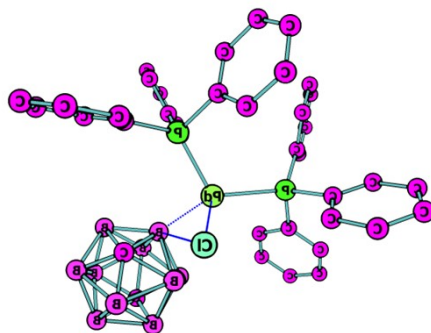


<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	-2.108039000	0.024650000	-0.006556000
P	-2.082773000	2.353055000	0.002345000
P	-2.130571000	-2.303091000	-0.007194000
C	-3.696451000	3.158725000	-0.414537000
C	-4.871582000	2.506256000	-0.005514000
C	-6.123543000	3.062007000	-0.270768000
C	-6.220207000	4.271456000	-0.963949000
C	-5.059399000	4.921681000	-1.387328000
C	-3.804696000	4.370825000	-1.113644000
C	-1.625604000	3.123955000	1.621943000
C	-2.156188000	4.337898000	2.085032000
C	-1.757468000	4.861298000	3.317775000
C	-0.822618000	4.181436000	4.100982000
C	-0.291423000	2.969879000	3.650941000
C	-0.696208000	2.441549000	2.424723000
C	-0.898098000	3.127802000	-1.190583000
C	-0.685160000	2.467916000	-2.412578000
C	0.181251000	3.000654000	-3.367601000

C	0.861263000	4.193579000	-3.108292000
C	0.668096000	4.850448000	-1.891472000
C	-0.207145000	4.322984000	-0.938368000
C	-3.580991000	-3.075885000	-0.859431000
C	-4.107159000	-2.407439000	-1.977599000
C	-5.189768000	-2.937975000	-2.679802000
C	-5.773586000	-4.137733000	-2.264638000
C	-5.267579000	-4.803604000	-1.146562000
C	-4.177192000	-4.278020000	-0.448390000
C	-0.676778000	-3.100233000	-0.830487000
C	-0.749119000	-4.306845000	-1.543580000
C	0.394474000	-4.850624000	-2.134478000
C	1.623676000	-4.198689000	-2.017988000
C	1.705737000	-2.994566000	-1.313701000
C	0.562616000	-2.445896000	-0.731603000
C	-2.153893000	-3.084989000	1.670688000
C	-1.520879000	-4.300447000	1.973517000
C	-1.587732000	-4.832253000	3.263993000
C	-2.289365000	-4.159352000	4.266249000
C	-2.919370000	-2.946263000	3.976281000
C	-2.845102000	-2.409626000	2.690532000
H	7.677383000	-2.089519000	-2.455408000
H	5.008507000	-1.085271000	-1.641583000
H	7.136039000	0.660596000	-2.217621000
H	5.405804000	1.458508000	-0.161475000
B	7.538948000	-1.571971000	-1.399849000
B	5.931081000	-0.967293000	-0.908910000
C	7.208214000	0.100832000	-1.291478000

B	6.160174000	0.558819000	-0.018053000
B	8.466474000	-1.921320000	0.063205000
H	9.236246000	-2.808810000	0.208088000
B	6.716178000	-2.260328000	0.004399000
H	6.330067000	-3.374078000	0.110886000
C	7.424610000	-1.454018000	1.333666000
H	7.501772000	-2.003897000	2.264982000
B	8.766059000	-0.421166000	-0.813090000
H	9.711440000	-0.159911000	-1.474640000
B	8.703150000	-0.392072000	0.953337000
H	9.625488000	-0.257820000	1.682045000
B	5.865831000	-0.943586000	0.856813000
H	4.919705000	-1.186231000	1.525222000
B	7.090320000	0.214255000	1.445364000
H	6.960696000	0.743907000	2.495246000
B	7.916701000	0.904940000	0.040489000
Cl	8.514648000	2.599121000	-0.091045000

Ts1



Atom	x	y	z
Cl	-1.032057000	-2.749288000	-0.618569000

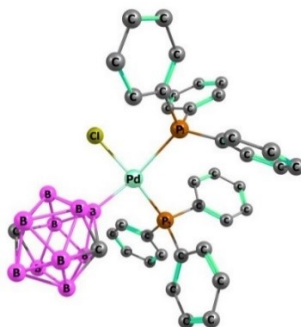
Pd	0.399542000	0.016625000	-0.479819000
P	1.683834000	0.300821000	1.787939000
P	1.733770000	-0.105189000	-2.364943000
C	3.348520000	1.108932000	1.837325000
C	3.561114000	2.381167000	2.388646000
H	2.738017000	2.922652000	2.842900000
C	4.832989000	2.960680000	2.365746000
H	4.980035000	3.946012000	2.800026000
C	5.908356000	2.277081000	1.797552000
H	6.896892000	2.727899000	1.783265000
C	5.706266000	1.007964000	1.247862000
H	6.536006000	0.465477000	0.803103000
C	4.437413000	0.429773000	1.262039000
H	4.299871000	-0.558268000	0.833494000
C	0.645731000	1.385689000	2.865820000
C	0.415063000	1.124887000	4.225051000
H	0.854584000	0.250740000	4.694059000
C	-0.383973000	1.982907000	4.984303000
H	-0.558589000	1.764030000	6.034230000
C	-0.954982000	3.115467000	4.400469000
H	-1.575934000	3.780983000	4.993735000
C	-0.731333000	3.385130000	3.048086000
H	-1.178001000	4.259777000	2.583342000
C	0.054693000	2.521060000	2.284580000
H	0.205912000	2.728214000	1.228153000
C	1.931115000	-1.234341000	2.777909000

C	1.106237000	-2.337285000	2.504554000
H	0.371168000	-2.286797000	1.705111000
C	1.234150000	-3.514505000	3.245791000
H	0.589264000	-4.359886000	3.022412000
C	2.191137000	-3.606489000	4.258217000
H	2.293899000	-4.524859000	4.830020000
C	3.021280000	-2.515701000	4.531516000
H	3.769640000	-2.582638000	5.316690000
C	2.893030000	-1.335551000	3.797444000
H	3.545744000	-0.495536000	4.015233000
C	3.153983000	-1.171610000	-1.832589000
C	2.869611000	-2.313213000	-1.061334000
H	1.845935000	-2.529031000	-0.767184000
C	3.896441000	-3.169991000	-0.660043000
H	3.658672000	-4.047888000	-0.066044000
C	5.220052000	-2.892979000	-1.010297000
H	6.019313000	-3.557092000	-0.693170000
C	5.511522000	-1.754035000	-1.763981000
H	6.538877000	-1.527030000	-2.035659000
C	4.487075000	-0.896732000	-2.172518000
H	4.738149000	-0.011674000	-2.745605000
C	1.196110000	-0.915426000	-3.937637000
C	1.039348000	-2.312365000	-3.972242000
H	1.254526000	-2.910652000	-3.094098000
C	0.599182000	-2.947854000	-5.133451000
H	0.485468000	-4.028128000	-5.140670000

C	0.306907000	-2.201620000	-6.277677000
H	-0.033122000	-2.698431000	-7.181945000
C	0.449891000	-0.814122000	-6.250306000
H	0.219623000	-0.222473000	-7.131907000
C	0.884790000	-0.173058000	-5.088162000
H	0.981774000	0.906439000	-5.086853000
C	2.454463000	1.508856000	-2.872097000
C	3.296614000	1.650473000	-3.990883000
H	3.515588000	0.795882000	-4.623344000
C	3.845499000	2.893100000	-4.308892000
H	4.493937000	2.987580000	-5.175350000
C	3.558408000	4.011095000	-3.520905000
H	3.984780000	4.977970000	-3.773223000
C	2.716774000	3.883675000	-2.415131000
H	2.481988000	4.750067000	-1.803427000
C	2.167322000	2.640593000	-2.094155000
H	1.506105000	2.539846000	-1.237970000
H	-4.022500000	-2.314488000	-2.081210000
H	-3.766113000	-0.549965000	-4.440397000
H	-1.601966469	-1.594596314	-2.710587653
H	-1.243082000	1.120695000	-4.001034000
B	-3.563839000	-1.236648000	-1.880455000
B	-3.432728000	-0.154188000	-3.371884000
C	-2.168617469	-0.822347314	-2.206269653
B	-1.970672000	0.812332000	-3.119112000
B	-3.966957000	-0.198296000	-0.506459000

H	-4.774994000	-0.347397000	0.350505000
B	-4.580095000	0.239786000	-2.091517000
H	-5.756603000	0.322789000	-2.221375000
C	-3.753924000	1.376881000	-1.130901000
H	-4.322012000	2.154557000	-0.632053000
B	-2.398723531	-1.013786686	-0.634518347
H	-2.474124531	-1.431698686	0.478804653
B	-2.441931000	0.725807000	-0.215017000
H	-2.209707000	1.261870000	0.818432000
B	-3.551414000	1.520767000	-2.790839000
H	-4.030156000	2.440716000	-3.366351000
B	-2.176322000	1.757198000	-1.651152000
H	-1.749181000	2.849770000	-1.468843000
B	-1.353529000	0.180278000	-1.529054000

### Int2



Atom	x	y	z
Cl	0.110228000	-1.470095000	-2.663172000
Pd	0.016165000	-0.034784000	-0.522909000
P	-2.361296000	-0.379415000	-0.055710000
P	2.282251000	-0.566740000	0.032920000

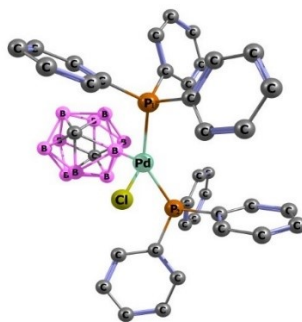
C	-2.612465000	-2.177996000	0.351145000
C	-3.386303000	-2.603515000	1.444604000
H	-3.836851000	-1.880429000	2.114550000
C	-3.590301000	-3.964766000	1.683224000
H	-4.191866000	-4.273556000	2.534180000
C	-3.031157000	-4.920492000	0.833910000
H	-3.191741000	-5.978962000	1.021219000
C	-2.267265000	-4.505948000	-0.259141000
H	-1.829476000	-5.239100000	-0.931294000
C	-2.055432000	-3.147283000	-0.501121000
H	-1.452385000	-2.839786000	-1.350608000
C	-3.099022000	0.449698000	1.422674000
C	-4.262831000	1.229178000	1.368534000
H	-4.778994000	1.371556000	0.425308000
C	-4.769952000	1.829753000	2.524467000
H	-5.671684000	2.432992000	2.462240000
C	-4.128538000	1.651966000	3.750458000
H	-4.527775000	2.114280000	4.649043000
C	-2.967284000	0.876864000	3.815894000
H	-2.458650000	0.733957000	4.765464000
C	-2.451496000	0.291089000	2.660429000
H	-1.544413000	-0.304318000	2.723487000
C	-3.565207000	-0.107475000	-1.423739000
C	-3.153495000	0.593593000	-2.564994000
H	-2.132427000	0.951259000	-2.636418000
C	-4.041599000	0.803438000	-3.622896000

H	-3.708125000	1.343570000	-4.504490000
C	-5.344169000	0.309114000	-3.552175000
H	-6.033166000	0.468342000	-4.377322000
C	-5.758791000	-0.404668000	-2.423487000
H	-6.768307000	-0.803255000	-2.369779000
C	-4.874179000	-0.617072000	-1.366937000
H	-5.199905000	-1.187424000	-0.501717000
C	2.582903000	-2.356618000	-0.315679000
C	3.744016000	-2.824864000	-0.944281000
H	4.490631000	-2.126778000	-1.307860000
C	3.947075000	-4.196999000	-1.116227000
H	4.849639000	-4.546683000	-1.610276000
C	2.997850000	-5.111430000	-0.659934000
H	3.157173000	-6.177557000	-0.796910000
C	1.838316000	-4.649960000	-0.030773000
H	1.087351000	-5.352730000	0.319452000
C	1.630275000	-3.282684000	0.137185000
H	0.715169000	-2.937256000	0.609355000
C	3.603540000	0.316350000	-0.892310000
C	3.535439000	0.272276000	-2.299190000
H	2.748280000	-0.301392000	-2.783363000
C	4.465713000	0.970770000	-3.068450000
H	4.406457000	0.924782000	-4.152259000
C	5.461857000	1.732995000	-2.449896000
H	6.180814000	2.281699000	-3.051975000
C	5.524135000	1.793451000	-1.057340000

H	6.290071000	2.390387000	-0.569978000
C	4.600939000	1.088865000	-0.278974000
H	4.659833000	1.148775000	0.802431000
C	2.743355000	-0.511166000	1.822598000
C	3.992999000	-0.982979000	2.261687000
H	4.722118000	-1.345976000	1.543236000
C	4.302652000	-1.005219000	3.621227000
H	5.273989000	-1.367988000	3.946018000
C	3.363190000	-0.574009000	4.562238000
H	3.604132000	-0.597032000	5.621513000
C	2.113461000	-0.122350000	4.137311000
H	1.376364000	0.209093000	4.863547000
C	1.805748000	-0.090678000	2.774904000
H	0.835561000	0.264551000	2.442315000
H	1.373199000	4.798849000	-2.462986000
H	2.964166000	4.734615000	0.050686000
H	2.151874000	2.405024000	-1.263200000
H	2.216479000	2.347555000	1.547136000
B	0.880066000	4.422480000	-1.453824000
B	1.832416000	4.384457000	0.048982000
C	1.368841000	2.946783000	-0.747136000
B	1.369704000	2.909852000	0.945971000
B	-0.823377000	4.550833000	-1.021548000
H	-1.655827000	5.152112000	-1.612586000
B	0.411526000	5.421339000	-0.074308000
H	0.404139000	6.605734000	-0.037474000

C	-0.820720000	4.520464000	0.682915000
H	-1.602239000	5.071984000	1.193605000
B	-0.161777000	2.969328000	-1.468955000
H	-0.352141000	2.429821000	-2.505549000
B	-1.281248000	3.086780000	-0.114849000
H	-2.417837000	2.768962000	-0.120277000
B	0.716764000	4.484488000	1.412195000
H	0.913765000	5.046620000	2.436698000
B	-0.330184000	3.035869000	1.389668000
H	-0.823585000	2.682146000	2.404604000
B	0.120470000	1.985518000	0.027765000

### TS2



Atom	x	y	z
Cl	3.238865000	0.821063000	-0.074578000
Pd	0.770934000	0.116369000	-0.240444000
P	0.552994000	-0.401312000	2.092274000
P	1.658799000	0.600899000	-2.580778000
C	0.023853000	-2.143047000	2.384604000
C	0.810637000	-3.162939000	1.817695000

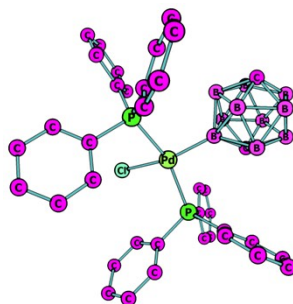
H	1.704193000	-2.909429000	1.253371000
C	0.455804000	-4.502205000	1.969706000
H	1.080049000	-5.276603000	1.532854000
C	-0.705947000	-4.845426000	2.667771000
H	-0.988145000	-5.888685000	2.777798000
C	-1.503959000	-3.841397000	3.215198000
H	-2.412244000	-4.097637000	3.753431000
C	-1.140450000	-2.497877000	3.080122000
H	-1.771605000	-1.733766000	3.520975000
C	2.102157000	-0.228442000	3.090857000
C	2.670361000	-1.285410000	3.814683000
H	2.233376000	-2.276762000	3.777573000
C	3.804996000	-1.071642000	4.603481000
H	4.234006000	-1.901777000	5.158184000
C	4.376683000	0.197563000	4.683725000
H	5.257187000	0.362420000	5.298744000
C	3.811914000	1.257138000	3.968102000
H	4.253585000	2.248334000	4.019266000
C	2.688252000	1.046107000	3.172170000
H	2.273319000	1.872839000	2.605992000
C	-0.583113000	0.672208000	3.073207000
C	-1.200831000	1.764507000	2.449994000
H	-1.036473000	1.936058000	1.391466000
C	-2.011850000	2.636067000	3.182924000
H	-2.484329000	3.477989000	2.684893000
C	-2.208364000	2.424865000	4.547345000

H	-2.838826000	3.100509000	5.118708000
C	-1.581132000	1.348024000	5.183173000
H	-1.719342000	1.188548000	6.248953000
C	-0.766522000	0.482351000	4.455450000
H	-0.263990000	-0.334264000	4.965577000
C	2.176945000	2.374318000	-2.535844000
C	3.404094000	2.851678000	-3.012751000
H	4.151872000	2.162836000	-3.388293000
C	3.691564000	4.217562000	-2.975704000
H	4.652620000	4.571194000	-3.339385000
C	2.757795000	5.123666000	-2.468896000
H	2.985467000	6.185743000	-2.442069000
C	1.533298000	4.655309000	-1.987994000
H	0.802177000	5.349708000	-1.582754000
C	1.247352000	3.289071000	-2.015641000
H	0.299859000	2.931326000	-1.619781000
C	3.083423000	-0.498762000	-3.010908000
C	3.825863000	-0.296436000	-4.186824000
H	3.592293000	0.532588000	-4.846924000
C	4.855898000	-1.171338000	-4.536418000
H	5.429271000	-0.990669000	-5.441560000
C	5.135467000	-2.280648000	-3.735993000
H	5.930998000	-2.967010000	-4.013159000
C	4.380152000	-2.509497000	-2.584155000
H	4.582961000	-3.376174000	-1.960993000
C	3.366301000	-1.621629000	-2.220249000

H	2.801163000	-1.790846000	-1.310525000
C	0.805231000	0.552077000	-4.247784000
C	0.670614000	-0.673909000	-4.922728000
H	1.063550000	-1.583225000	-4.480437000
C	0.055309000	-0.742823000	-6.172981000
H	-0.033461000	-1.702974000	-6.674248000
C	-0.433709000	0.415745000	-6.780925000
H	-0.908009000	0.363747000	-7.757220000
C	-0.296721000	1.641508000	-6.128482000
H	-0.662217000	2.552789000	-6.594323000
C	0.315233000	1.709387000	-4.874609000
H	0.411420000	2.674668000	-4.391095000
H	-4.824707000	0.191221000	0.368829000
H	-4.045032000	-2.678418000	0.455389000
H	-2.289070000	-0.633721000	1.156326000
H	-1.186162000	-2.871469000	-0.155365000
B	-4.043239000	-0.241476000	-0.410329000
B	-3.576667000	-1.955589000	-0.358692000
C	-2.489354000	-0.723673000	0.096908000
B	-1.823013000	-2.048804000	-0.715798000
B	-3.778459000	0.350852000	-2.048223000
H	-4.441874000	1.147448000	-2.622788000
B	-4.394347000	-1.300683000	-1.778226000
H	-5.469765000	-1.604695000	-2.173182000
C	-3.124240000	-0.988648000	-2.871469000
H	-3.340061000	-1.078217000	-3.930226000

B	-2.570609000	0.704861000	-0.801844000
H	-2.450536000	1.772600000	-0.303546000
B	-2.037288000	0.245226000	-2.407156000
H	-1.618225000	0.976458000	-3.229437000
B	-3.021295000	-2.424201000	-1.963410000
H	-3.183571000	-3.478057000	-2.481115000
B	-1.565032000	-1.472143000	-2.353408000
H	-0.809638000	-1.930096000	-3.135621000
B	-1.136247000	-0.392109000	-1.002420000

### Int3



Atom	x	y	z
Pd	0.020141000	0.113623000	-0.385427000
P	-2.359573000	0.404388000	-0.000348000
P	2.374679000	0.576490000	-0.026683000
C	-2.802637000	2.176345000	0.349604000
C	-2.893639000	3.069999000	-0.732079000
C	-3.222731000	4.407908000	-0.519536000
C	-3.458338000	4.881589000	0.772942000
C	-3.370096000	4.003301000	1.852683000
C	-3.047415000	2.659776000	1.643898000

C	-3.475304000	0.012187000	-1.413507000
C	-4.840381000	0.352903000	-1.391406000
C	-5.659316000	0.054703000	-2.479382000
C	-5.125816000	-0.575297000	-3.608343000
C	-3.769603000	-0.897677000	-3.648107000
C	-2.947258000	-0.602052000	-2.557308000
C	-3.065330000	-0.482780000	1.460245000
C	-2.400487000	-0.348859000	2.692811000
C	-2.896265000	-0.960545000	3.843164000
C	-4.044545000	-1.753785000	3.774709000
C	-4.690554000	-1.925949000	2.550781000
C	-4.210791000	-1.289275000	1.402114000
C	2.419813000	2.333258000	0.562874000
C	1.378200000	2.791415000	1.385300000
C	1.394661000	4.086913000	1.901844000
C	2.446239000	4.950925000	1.590609000
C	3.477209000	4.510707000	0.759551000
C	3.466602000	3.210781000	0.249383000
C	3.343387000	-0.278110000	1.306541000
C	3.086215000	0.044484000	2.649755000
C	3.748065000	-0.616986000	3.683873000
C	4.682888000	-1.614436000	3.396967000
C	4.946808000	-1.944693000	2.067507000
C	4.280306000	-1.286841000	1.031027000
C	3.466984000	0.491422000	-1.507776000
C	4.863684000	0.643370000	-1.429937000

C	5.648302000	0.585891000	-2.582428000
C	5.051017000	0.372050000	-3.827023000
C	3.666848000	0.217724000	-3.913957000
C	2.878302000	0.277013000	-2.763174000
Cl	0.021557000	2.127817000	-1.934339000
B	-0.830337000	-4.417696000	-1.311051000
B	-1.238639000	-4.535362000	0.417388000
C	-1.199927000	-3.029813000	-0.383849000
B	-0.646802000	-3.046909000	1.218832000
B	0.925569000	-4.369652000	-1.457140000
B	0.153290000	-5.405220000	-0.227841000
C	1.475581000	-4.399358000	0.153311000
B	0.009932000	-2.858032000	-1.559810000
B	1.509675000	-2.893652000	-0.645718000
B	0.265599000	-4.557481000	1.336869000
B	1.101578000	-3.002050000	1.080271000
B	0.129276000	-1.953025000	0.008963000

PPh<sub>3</sub>

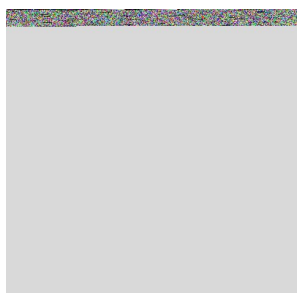


<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
P	0.000060000	-0.000150000	-1.203446000

C	-1.153156000	-1.209717000	-0.402384000
C	-1.307393000	-2.455727000	-1.034848000
H	-0.755867000	-2.665937000	-1.948480000
C	-2.162742000	-3.424699000	-0.509061000
H	-2.265915000	-4.383656000	-1.010117000
C	-2.894238000	-3.156446000	0.650696000
H	-3.568522000	-3.905942000	1.056488000
C	-2.760916000	-1.917621000	1.281208000
H	-3.330380000	-1.700612000	2.181398000
C	-1.895774000	-0.951836000	0.760626000
H	-1.801317000	0.007397000	1.260554000
C	1.624221000	-0.393808000	-0.402347000
C	1.772018000	-1.163570000	0.762231000
H	0.893979000	-1.559883000	1.263220000
C	3.040965000	-1.429654000	1.282966000
H	3.137631000	-2.029512000	2.184386000
C	4.180630000	-0.927796000	0.651041000
H	5.166827000	-1.136823000	1.056997000
C	4.047376000	-0.162491000	-0.510250000
H	4.929574000	0.225980000	-1.012372000
C	2.780535000	0.093577000	-1.036130000
H	2.686924000	0.674465000	-1.950940000
C	-0.470908000	1.603410000	-0.402642000
C	0.123169000	2.117273000	0.760795000
H	0.906223000	1.555517000	1.261015000
C	-0.280746000	3.349373000	1.281344000

H	0.191505000	3.733790000	2.181857000
C	-1.286555000	4.084484000	0.650478000
H	-1.598553000	5.043121000	1.056362000
C	-1.884094000	3.585405000	-0.509670000
H	-2.662708000	4.154419000	-1.010952000
C	-1.472466000	2.360193000	-1.035449000
H	-1.929851000	1.987828000	-1.949352000

### pyrrolidine



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	1.161477000	-0.448459000	0.171310000
C	-1.161682000	-0.448020000	0.171191000
C	-0.778616000	1.030194000	-0.056469000
C	0.779043000	1.029854000	-0.056627000
H	1.322947000	-0.629572000	1.251001000
H	2.076060000	-0.742366000	-0.355656000
H	-2.076293000	-0.741480000	-0.355977000
H	-1.323425000	-0.629213000	1.250824000
H	-1.161338000	1.380747000	-1.019838000
H	-1.199172000	1.677022000	0.719576000

H	1.161702000	1.379937000	-1.020194000
H	1.200064000	1.676722000	0.719132000
N	-0.000209000	-1.172246000	-0.357243000
H	-0.000413000	-2.147495000	-0.064592000

### 3-ethynylquinoline



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	0.841609000	0.780100000	-0.000202000
C	0.530707000	-0.617853000	0.000019000
C	1.590824000	-1.564221000	0.000020000
C	2.901418000	-1.141091000	-0.000190000
C	3.208115000	0.243252000	-0.000408000
C	2.201233000	1.184501000	-0.000415000
N	-0.130040000	1.743767000	-0.000216000
C	-1.384936000	1.359019000	-0.000018000
C	-1.812906000	-0.008423000	0.000213000
C	-0.834226000	-0.989375000	0.000228000
C	-3.205001000	-0.319972000	0.000418000
C	-4.390433000	-0.565479000	0.000591000
H	-5.434286000	-0.786049000	0.000752000
H	1.349870000	-2.624406000	0.000188000
H	3.707933000	-1.868819000	-0.000188000

H	4.247342000	0.559959000	-0.000572000
H	2.413703000	2.249061000	-0.000580000
H	-2.142411000	2.141396000	-0.000033000
H	-1.110298000	-2.040261000	0.000399000

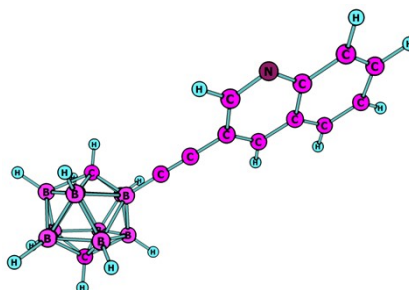
### H-Base<sup>+</sup>Cl<sup>-</sup>



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Cl	2.438361000	0.468614000	0.928839000
H	-0.791955000	0.561920000	2.195012000
C	-1.038465000	1.304646000	0.214975000
C	-0.852199000	-1.065020000	0.843848000
C	-1.746969000	0.415736000	-0.820070000
H	-1.693837000	2.025886000	0.704559000
H	-0.176113000	1.827524000	-0.204550000
C	-1.056206000	-0.950579000	-0.666790000
H	-0.040160000	-1.729099000	1.144752000
H	-1.773337000	-1.346159000	1.360612000

H	-1.656675000	0.827406000	-1.828400000
H	-2.813747000	0.331349000	-0.584022000
H	-0.083733000	-0.950409000	-1.170577000
H	-1.650052000	-1.779376000	-1.060574000
N	-0.483465000	0.340637000	1.247357000
H	0.609861000	0.416972000	1.226481000

### Product

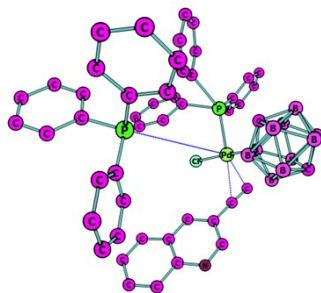


Atom	x	y	z
C	4.600910000	-0.735623000	0.008530000
C	4.101833000	0.606616000	-0.007177000
C	5.022572000	1.689314000	-0.005358000
C	6.378577000	1.449524000	0.011208000
C	6.871573000	0.120085000	0.026620000
C	6.002854000	-0.950101000	0.025328000
N	3.770142000	-1.823263000	0.007447000
C	2.474628000	-1.613871000	-0.009396000
C	1.862499000	-0.317480000	-0.025239000
C	2.699485000	0.788216000	-0.023200000
C	0.443471000	-0.197836000	-0.043475000
C	-0.771514000	-0.111058000	-0.061317000

H	4.638184000	2.706248000	-0.017293000
H	7.078112000	2.280611000	0.012416000
H	7.944308000	-0.051296000	0.039448000
H	6.358501000	-1.975656000	0.036728000
H	1.831479000	-2.492679000	-0.011951000
H	2.282778000	1.791585000	-0.034625000
H	-5.050753000	0.484073000	2.650558000
H	-5.237666000	-2.157825000	1.312585000
H	-2.766816000	-1.029320000	2.028448000
H	-2.813992000	-2.509690000	-0.354231000
B	-4.672389000	0.357712000	1.535712000
B	-4.784502000	-1.231364000	0.730962000
C	-3.280872000	-0.569246000	1.191918000
B	-3.326999000	-1.446270000	-0.273701000
B	-4.671300000	1.608916000	0.288248000
H	-5.178299000	2.675995000	0.367842000
B	-5.686956000	0.152650000	0.103507000
H	-6.865389000	0.258017000	0.060527000
C	-4.714253000	0.731365000	-1.175776000
H	-5.222047000	1.192795000	-2.015343000
B	-3.144843000	1.125506000	1.029161000
H	-2.511659000	1.755360000	1.805714000
B	-3.212619000	1.396620000	-0.716958000
H	-2.754736000	2.319502000	-1.299772000
B	-4.854038000	-0.962388000	-1.013929000
H	-5.481907000	-1.593874000	-1.794282000

B	-3.326046000	-0.195469000	-1.523829000
H	-2.942387000	-0.319030000	-2.636604000
B	-2.290166000	0.011806000	-0.094831000

Ts3

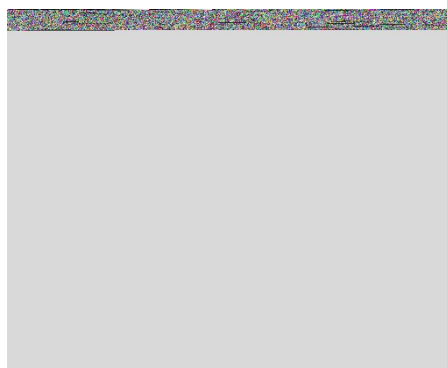


Atom	x	y	z
Pd	3.422927000	-2.968934000	0.715982000
Cl	4.963901000	-4.474805000	-0.660310000
P	-1.011614000	-2.369948000	-3.592928000
P	3.949872000	-0.995619000	-0.560224000
C	0.159314000	-7.959312000	0.421525000
C	1.288672000	-7.612447000	-0.389275000
C	1.454542000	-8.237095000	-1.656108000
C	0.538446000	-9.165049000	-2.098533000
C	-0.579148000	-9.507650000	-1.294932000
C	-0.766696000	-8.918800000	-0.061483000
N	-0.058598000	-7.397621000	1.650830000
C	0.801507000	-6.507878000	2.087345000
C	1.963076000	-6.087858000	1.359616000
C	2.198589000	-6.656718000	0.114596000

C	2.859695000	-5.143023000	1.935175000
C	3.639959000	-4.355856000	2.470530000
B	-0.320726000	-0.124515000	1.791017000
B	0.998137000	0.834588000	2.507554000
C	1.298916000	-0.346161000	1.314725000
B	2.460125000	-0.198729000	2.544982000
B	-0.644385000	-1.495143000	2.849090000
B	-0.227931000	0.098142000	3.539957000
C	0.509569000	-1.333208000	4.093694000
B	0.338157000	-1.742803000	1.390389000
B	0.816608000	-2.513802000	2.899492000
B	1.495076000	0.054011000	4.008590000
B	2.136614000	-1.563007000	3.611101000
B	2.080960000	-1.813884000	1.844308000
C	3.498549000	0.065310000	-2.423831000
C	2.117753000	0.235860000	-2.681058000
C	4.377476000	1.120785000	-2.738928000
C	1.643829000	1.437012000	-3.195412000
C	3.879523000	2.319532000	-3.250009000
C	2.515154000	2.495094000	-3.481945000
C	4.168711000	-1.582447000	-2.445814000
C	5.466204000	-1.657105000	-3.050358000
C	3.193968000	-2.521586000	-2.925899000
C	5.728412000	-2.516613000	-4.101979000
C	3.463401000	-3.371383000	-3.980780000
C	4.727164000	-3.367245000	-4.587964000

C	5.655990000	-0.467771000	-0.112706000
C	5.851002000	0.868253000	0.281390000
C	6.728095000	-1.373729000	-0.014773000
C	7.093293000	1.293147000	0.757833000
C	7.966736000	-0.944528000	0.464152000
C	8.152012000	0.387111000	0.848927000
C	-1.989628000	-0.795742000	-3.595590000
C	-2.581107000	-0.231663000	-4.737014000
C	-2.109043000	-0.114899000	-2.370565000
C	-3.278599000	0.976424000	-4.653614000
C	-2.814476000	1.086338000	-2.285490000
C	-3.399246000	1.636981000	-3.429196000
C	-2.276231000	-3.639142000	-3.129463000
C	-3.663074000	-3.451595000	-3.245884000
C	-1.802491000	-4.853452000	-2.603807000
C	-4.550706000	-4.456462000	-2.854640000
C	-2.688945000	-5.861833000	-2.221333000
C	-4.066248000	-5.663390000	-2.344636000
C	-0.737209000	-2.680911000	-5.398711000
C	0.374861000	-2.056653000	-5.992306000
C	-1.538757000	-3.517941000	-6.190284000
C	0.665273000	-2.248121000	-7.343663000
C	-1.240412000	-3.719103000	-7.540697000
C	-0.141098000	-3.083438000	-8.121455000

## Int4



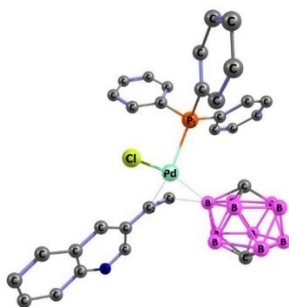
<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.029200000	0.172957000	1.167504000
Cl	-0.669571000	-1.937437000	2.373801000
P	1.583152000	-1.043113000	-0.155170000
C	-5.710459000	0.247637000	-0.232711000
C	-4.956669000	-0.884543000	0.220004000
C	-5.412563000	-2.195354000	-0.089467000
C	-6.567124000	-2.373696000	-0.817991000
C	-7.311306000	-1.252720000	-1.266330000
C	-6.894438000	0.030361000	-0.981643000
N	-5.328975000	1.535742000	0.032066000
C	-4.229291000	1.727117000	0.721851000
C	-3.401954000	0.669255000	1.221324000
C	-3.782097000	-0.642378000	0.965546000
C	-2.246543000	0.965606000	1.998480000
C	-1.273417000	1.202033000	2.710962000

H	-0.707126000	1.485079000	3.573772000
H	-4.835460000	-3.047203000	0.260468000
H	-6.914245000	-3.375892000	-1.052108000
H	-8.220484000	-1.411584000	-1.839573000
H	-7.451862000	0.899864000	-1.315375000
H	-3.944281000	2.757688000	0.925072000
H	-3.166531000	-1.460705000	1.331165000
H	-0.466805000	4.406824000	-2.593165000
H	2.438062000	3.780356000	-2.621827000
H	0.508548000	1.867865000	-1.987346000
H	2.958822000	1.739322000	-0.606724000
B	0.104446000	4.188758000	-1.578209000
B	1.846009000	3.814923000	-1.596209000
C	0.679764000	2.619552000	-1.227737000
B	2.137911000	2.552569000	-0.368104000
B	-0.296728000	4.854617000	0.001631000
H	-1.089791000	5.706223000	0.225020000
B	1.257385000	5.258423000	-0.774817000
H	1.499419000	6.380167000	-1.070310000
C	1.173421000	4.789377000	0.861277000
H	1.345052000	5.552766000	1.612052000
B	-0.659948000	3.151040000	-0.337232000
H	-1.745081000	2.730057000	-0.556113000
B	0.011740000	3.599645000	1.227729000
H	-0.568008000	3.684618000	2.254128000
B	2.517923000	4.242560000	-0.022461000

H	3.597892000	4.687301000	0.177965000
B	1.740997000	3.208651000	1.213607000
H	2.316410000	3.009933000	2.231258000
B	0.583190000	2.088431000	0.427288000
C	1.368061000	-2.884093000	-0.187852000
C	0.869038000	-3.570698000	-1.303033000
C	1.747367000	-3.619306000	0.948441000
C	0.755159000	-4.963817000	-1.284216000
C	1.640891000	-5.007999000	0.959597000
C	1.142010000	-5.685589000	-0.156024000
H	0.577856000	-3.033697000	-2.198148000
H	2.122934000	-3.108153000	1.827348000
H	0.369980000	-5.479685000	-2.159667000
H	1.939670000	-5.559947000	1.846289000
H	1.056386000	-6.768808000	-0.143901000
C	3.323878000	-0.910591000	0.428831000
C	3.631458000	-0.090225000	1.522737000
C	4.345100000	-1.682709000	-0.153670000
C	4.937991000	-0.021379000	2.011587000
C	5.650987000	-1.603642000	0.328907000
C	5.949921000	-0.771282000	1.411402000
H	2.845385000	0.491120000	1.994104000
H	4.118918000	-2.357964000	-0.973448000
H	5.160584000	0.617044000	2.861760000
H	6.432208000	-2.200817000	-0.133035000
H	6.966646000	-0.716985000	1.790597000

C	1.536671000	-0.600427000	-1.945488000
C	2.672273000	-0.303745000	-2.711086000
C	0.272067000	-0.559163000	-2.562170000
C	2.546967000	0.016959000	-4.065903000
C	0.151469000	-0.254254000	-3.918633000
C	1.291193000	0.036901000	-4.673821000
H	3.656152000	-0.308840000	-2.255535000
H	-0.622366000	-0.757243000	-1.976305000
H	3.436153000	0.253677000	-4.643390000
H	-0.831878000	-0.232088000	-4.379697000
H	1.198308000	0.285386000	-5.727186000

TS1-C



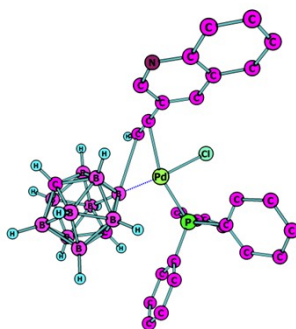
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P	2.190420000	0.160017000	0.057763000
C	-5.190520000	2.402197000	-3.209902000
C	-4.640020000	2.495886000	-1.890579000
C	-5.395571000	3.126256000	-0.864617000
C	-6.642675000	3.643124000	-1.138112000

C	-7.184781000	3.550563000	-2.444712000
C	-6.475787000	2.943066000	-3.460398000
N	-4.517562000	1.800232000	-4.241862000
C	-3.330839000	1.300592000	-3.997109000
C	-2.679870000	1.345240000	-2.717204000
C	-3.357721000	1.946139000	-1.665194000
C	-1.376276000	0.771581000	-2.575899000
C	-0.322871000	0.245701000	-3.103286000
H	0.306129000	0.229254000	-3.979160000
H	-4.971634000	3.190626000	0.133976000
H	-7.217528000	4.123909000	-0.351929000
H	-8.170116000	3.962747000	-2.643773000
H	-6.875849000	2.861773000	-4.466256000
H	-2.814404000	0.822017000	-4.828519000
H	-2.901860000	1.977490000	-0.678828000
H	0.706021000	-4.988720000	-0.308528000
H	2.238338000	-4.725134000	-2.843112000
H	1.797251000	-2.561446000	-1.154118000
H	1.778297000	-2.005197000	-3.903861000
B	0.246767000	-4.391634000	-1.222022000
B	1.167609000	-4.230693000	-2.740086000
C	0.927990000	-2.900086000	-1.702231000
B	0.892929000	-2.582831000	-3.372083000
B	-1.471913000	-4.216166000	-1.596231000
H	-2.360869000	-4.795363000	-1.071168000
B	-0.381670000	-5.079434000	-2.720414000

H	-0.551636000	-6.230716000	-2.938991000
C	-1.495994000	-3.914998000	-3.269255000
H	-2.357167000	-4.265035000	-3.827367000
B	-0.589678000	-2.840296000	-0.919574000
H	-0.703761000	-2.472914000	0.197082000
B	-1.739722000	-2.573081000	-2.232706000
H	-2.808183000	-2.073523000	-2.140135000
B	0.017423000	-3.964457000	-4.051682000
H	0.113882000	-4.367187000	-5.161022000
B	-0.825745000	-2.425108000	-3.750478000
H	-1.289695000	-1.845276000	-4.671260000
B	-0.186356000	-1.686176000	-2.249208000
C	2.805155000	1.906111000	-0.013500000
C	4.155297000	2.215764000	-0.253645000
C	1.882052000	2.946074000	0.201362000
C	4.588544000	3.551193000	-0.286496000
C	2.298594000	4.286207000	0.175544000
C	3.633777000	4.520493000	-0.071376000
H	4.879929000	1.425321000	-0.422157000
H	0.839439000	2.713634000	0.402391000
H	5.632143000	3.788356000	-0.474739000
H	1.583981000	5.087325000	0.343119000
C	3.557048000	-0.793049000	-0.745251000
C	4.276026000	-1.796556000	-0.077411000
C	3.844448000	-0.542885000	-2.100565000
C	5.261638000	-2.528034000	-0.747490000

C	4.837620000	-1.264221000	-2.761546000
C	5.547383000	-2.262437000	-2.086777000
H	4.073018000	-2.006728000	0.967359000
H	3.297319000	0.227453000	-2.637853000
H	5.808412000	-3.301686000	-0.215523000
H	5.053562000	-1.050818000	-3.804710000
H	6.316515000	-2.828951000	-2.604119000
C	2.318170000	-0.288597000	1.839848000
C	3.348612000	0.204466000	2.657467000
C	1.367327000	-1.160071000	2.389784000
C	3.430665000	-0.179637000	3.996029000
C	1.454579000	-1.547037000	3.728828000
C	2.485334000	-1.058189000	4.533026000
H	4.083831000	0.893245000	2.252429000
H	0.547495000	-1.517565000	1.776684000
H	4.229967000	0.210684000	4.620057000
H	0.709138000	-2.219630000	4.143662000
H	2.548675000	-1.353282000	5.576851000
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### Int1-C

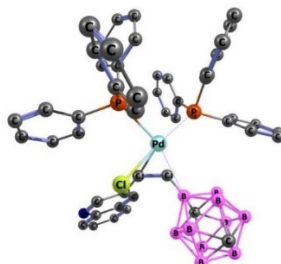


<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.557740000	-0.351279000	-2.351488000
P	2.119378000	0.197608000	-0.630937000
C	-4.801763000	2.135998000	-3.038809000
C	-3.546254000	2.825166000	-3.095571000
C	-3.505913000	4.223801000	-2.842221000
C	-4.662788000	4.907545000	-2.542288000
C	-5.904065000	4.223859000	-2.484202000
C	-5.974836000	2.868319000	-2.727064000
N	-4.910647000	0.791793000	-3.276462000
C	-3.818355000	0.120657000	-3.555713000
C	-2.513476000	0.708108000	-3.632057000
C	-2.392035000	2.073463000	-3.406023000
C	-1.387452000	-0.091291000	-3.979689000
C	-0.423947000	-0.771368000	-4.329797000
H	0.219572000	-1.329900000	-4.978469000
H	-2.550067000	4.738760000	-2.891756000
H	-4.629948000	5.975860000	-2.349483000
H	-6.807168000	4.778843000	-2.246250000
H	-6.916217000	2.329425000	-2.688202000
H	-3.926277000	-0.945323000	-3.746236000
H	-1.411690000	2.540689000	-3.456360000
H	-0.111939000	-4.349520000	1.643271000
H	1.493455000	-5.650996000	-0.486394000
H	1.575481000	-2.914597000	-0.041531000
H	1.783273000	-3.751031000	-2.714867000

B	-0.380856000	-4.168742000	0.503840000
B	0.582388000	-4.950601000	-0.775346000
C	0.665422000	-3.270241000	-0.502894000
B	0.758468000	-3.778087000	-2.118544000
B	-1.984589000	-3.827185000	-0.145296000
H	-3.006774000	-3.880486000	0.451528000
B	-1.129814000	-5.331668000	-0.588845000
H	-1.585658000	-6.383091000	-0.287363000
C	-1.892963000	-4.357005000	-1.760901000
H	-2.802313000	-4.735158000	-2.214587000
B	-0.793110000	-2.520789000	-0.056869000
H	-0.824911000	-1.642529000	0.736874000
B	-1.802192000	-2.667820000	-1.491059000
H	-2.723725000	-1.980244000	-1.773413000
B	-0.425923000	-5.097381000	-2.211667000
H	-0.414713000	-5.990403000	-2.990433000
B	-0.846615000	-3.457406000	-2.762698000
H	-1.131998000	-3.315620000	-3.901233000
B	-0.078626000	-2.239860000	-1.682672000
C	1.596400000	1.685715000	0.324614000
C	2.359147000	2.132564000	1.420800000
C	0.412681000	2.359599000	-0.014481000
C	1.960100000	3.254429000	2.161448000
C	-0.011202000	3.476758000	0.723003000
C	0.789863000	3.869775000	1.771326000
H	3.260976000	1.604263000	1.715877000

H	-0.174520000	2.025568000	-0.862600000
H	2.553044000	3.601279000	3.003054000
H	-0.930265000	3.993137000	0.460898000
C	3.710985000	0.581581000	-1.479935000
C	4.143010000	-0.295241000	-2.488699000
C	4.507838000	1.685301000	-1.149869000
C	5.359382000	-0.083365000	-3.138171000
C	5.719346000	1.901273000	-1.810323000
C	6.150602000	1.017164000	-2.800360000
H	3.520175000	-1.137477000	-2.778799000
H	4.182740000	2.392250000	-0.394928000
H	5.680398000	-0.770348000	-3.916175000
H	6.322176000	2.767408000	-1.551818000
H	7.092945000	1.189136000	-3.312915000
C	2.655992000	-0.929794000	0.739504000
C	3.813334000	-1.719022000	0.631564000
C	1.869973000	-1.040212000	1.901456000
C	4.172556000	-2.596547000	1.657776000
C	2.233556000	-1.915726000	2.924814000
C	3.384833000	-2.698412000	2.805465000
H	4.442732000	-1.647201000	-0.248714000
H	0.975530000	-0.436663000	2.013917000
H	5.073365000	-3.195539000	1.558089000
H	1.615619000	-1.984779000	3.815530000
H	3.666348000	-3.380306000	3.602803000
Cl	1.214061000	1.931766000	-3.319672000

### TS2-C



Atom	x	y	z
Pd	-0.170508000	0.871300000	-2.129057000
P	0.171041000	-1.408279000	-2.885498000
C	1.727172000	-1.740607000	-3.829346000
C	1.871559000	-2.830544000	-4.704792000
H	1.025749000	-3.477171000	-4.917968000
C	3.103603000	-3.097033000	-5.301579000
H	3.199902000	-3.937329000	-5.983852000
C	4.214318000	-2.296608000	-5.013534000
H	5.173959000	-2.511207000	-5.475806000
C	4.087349000	-1.229823000	-4.123299000
H	4.943972000	-0.604781000	-3.887220000
C	2.848743000	-0.953383000	-3.536900000
H	-1.461337000	-3.995455000	-2.678770000
C	0.222820000	-2.938372000	-1.822381000
C	-0.656126000	-4.023187000	-1.953811000
H	2.750835000	-0.117852000	-2.851386000
C	-0.500687000	-5.163274000	-1.159519000

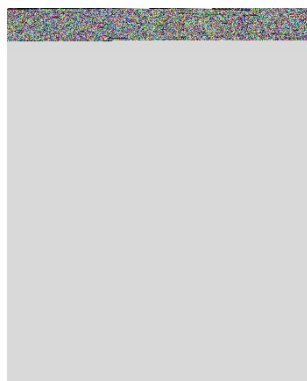
H	-1.193690000	-5.992513000	-1.274763000
C	0.538741000	-5.241913000	-0.233011000
H	0.657701000	-6.128974000	0.382931000
C	1.432189000	-4.174336000	-0.109176000
H	2.252570000	-4.227437000	0.601144000
C	1.274019000	-3.034188000	-0.895141000
H	1.981227000	-2.217193000	-0.791420000
C	-1.245381000	-1.721681000	-4.031807000
C	-2.531601000	-1.880023000	-3.478899000
H	-2.664835000	-1.897550000	-2.400755000
C	-3.650180000	-2.042189000	-4.295112000
H	-4.629945000	-2.173662000	-3.844051000
C	-3.509627000	-2.035369000	-5.685570000
H	-4.380107000	-2.159129000	-6.323717000
C	-2.244495000	-1.862914000	-6.245433000
H	-2.121335000	-1.842488000	-7.324285000
C	-1.120707000	-1.705458000	-5.428495000
H	-0.153019000	-1.557114000	-5.892071000
C	-5.529701000	3.956210000	-0.370433000
C	-5.575445000	2.532414000	-0.212622000
C	-6.800026000	1.914550000	0.164120000
C	-7.927324000	2.677159000	0.376897000
C	-7.879771000	4.083914000	0.215078000
C	-6.705336000	4.711089000	-0.152547000
N	-4.381603000	4.613853000	-0.738271000
C	-3.308563000	3.905019000	-0.976138000

C	-3.219330000	2.468854000	-0.815972000
C	-4.384320000	1.805720000	-0.416750000
C	-2.056644000	1.778565000	-1.254681000
C	-1.552492000	0.553914000	-0.675975000
H	-6.828936000	0.834768000	0.287290000
H	-8.859209000	2.201634000	0.668573000
H	-8.777782000	4.671420000	0.383553000
H	-6.649310000	5.787499000	-0.280253000
H	-2.404883000	4.433429000	-1.270645000
H	-4.399511000	0.725372000	-0.315987000
P	0.726744000	2.134027000	-4.255188000
C	-0.196161000	3.729121000	-4.472766000
C	-1.572984000	3.751406000	-4.202591000
H	-2.052510000	2.867823000	-3.792870000
C	-2.323757000	4.908312000	-4.420065000
H	-3.387846000	4.907705000	-4.199775000
C	-1.705061000	6.067731000	-4.892812000
H	-2.286225000	6.972267000	-5.050444000
C	-0.333254000	6.059830000	-5.149401000
H	0.160707000	6.959457000	-5.507000000
C	0.415852000	4.898380000	-4.946312000
H	1.481096000	4.916039000	-5.148852000
C	2.512971000	2.628709000	-4.196861000
C	3.224935000	3.029138000	-5.341691000
H	2.733960000	3.051710000	-6.309197000
C	4.570982000	3.389774000	-5.254869000

H	5.103533000	3.696828000	-6.151088000
C	5.228993000	3.354557000	-4.023398000
H	6.277362000	3.633061000	-3.956699000
C	4.531463000	2.962816000	-2.879235000
H	5.032246000	2.939132000	-1.915118000
C	3.184167000	2.603448000	-2.963602000
H	2.640410000	2.327487000	-2.066473000
C	0.577367000	1.420941000	-5.973768000
C	1.562994000	0.560483000	-6.490419000
H	2.450511000	0.336873000	-5.909709000
C	1.428221000	-0.004689000	-7.760154000
H	2.210022000	-0.657820000	-8.138778000
C	0.301433000	0.269363000	-8.539127000
H	0.199968000	-0.165877000	-9.529728000
C	-0.688105000	1.114704000	-8.034829000
H	-1.567643000	1.343255000	-8.631049000
C	-0.551516000	1.684498000	-6.767051000
H	-1.326638000	2.351599000	-6.405935000
Cl	0.386902000	3.312205000	-1.096532000
H	-2.172761000	-0.230508000	-1.148648000
H	-2.690206000	-2.513470000	3.054442000
H	-3.467054000	0.218152000	3.943097000
H	-3.520170000	-0.557879000	1.266881000
H	-2.761077000	2.101779000	1.831228000
B	-2.003312000	-1.582383000	2.796218000
B	-2.468002000	0.052525000	3.326930000

C	-2.531745000	-0.401624000	1.684203000
B	-2.040736000	1.185498000	2.017085000
B	-0.253780000	-1.612423000	2.580488000
H	0.464257000	-2.525617000	2.813446000
B	-0.978781000	-0.685135000	3.918726000
H	-0.742123000	-0.977717000	5.042199000
C	0.228507000	-0.016339000	2.916783000
H	1.212414000	0.125726000	3.349378000
B	-1.295943000	-1.437002000	1.168540000
H	-1.528798000	-2.282602000	0.374218000
B	0.168769000	-0.465987000	1.280152000
H	1.179000000	-0.618644000	0.686675000
B	-1.006177000	1.032814000	3.431991000
H	-0.790405000	1.876384000	4.235448000
B	-0.297393000	1.169014000	1.799227000
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B	-1.306921000	0.295512000	0.563660000

### Int1-RE-C



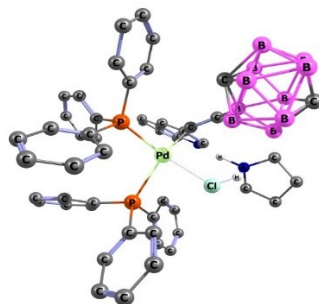
<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
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Pd	-0.227488000	1.067218000	-2.165900000
P	-0.485003000	-1.119155000	-3.081454000
C	1.083576000	-1.678245000	-3.879368000
C	1.103237000	-2.520155000	-5.001931000
C	2.317513000	-2.960351000	-5.532381000
C	3.524849000	-2.567029000	-4.949463000
C	3.514819000	-1.729547000	-3.831432000
C	2.301564000	-1.285553000	-3.301387000
C	-0.895550000	-2.547783000	-1.974457000
C	-2.119361000	-2.554327000	-1.282399000
C	-2.469091000	-3.631002000	-0.468682000
C	-1.598502000	-4.714197000	-0.319098000
C	-0.379792000	-4.716886000	-0.997074000
C	-0.031017000	-3.643822000	-1.823583000
C	-1.780680000	-1.279032000	-4.391429000
C	-2.363535000	-2.519338000	-4.707356000
C	-3.326003000	-2.613510000	-5.713562000
C	-3.723381000	-1.472957000	-6.415757000
C	-3.154618000	-0.236009000	-6.106617000
C	-2.192761000	-0.139949000	-5.098856000
C	-5.295736000	2.199693000	-0.687825000
C	-4.842680000	1.443039000	-1.812695000
C	-5.719603000	1.248081000	-2.914085000
C	-6.990876000	1.780054000	-2.895854000
C	-7.438956000	2.529319000	-1.778807000
C	-6.608741000	2.736619000	-0.697570000

N	-4.493718000	2.429357000	0.396319000
C	-3.283481000	1.917687000	0.392431000
C	-2.720043000	1.117741000	-0.661811000
C	-3.526522000	0.917371000	-1.769765000
C	-1.339897000	0.598752000	-0.506584000
C	-0.931953000	0.101846000	0.676547000
P	0.900182000	2.306814000	-4.162986000
C	0.138513000	3.988084000	-4.273125000
C	0.865688000	5.120174000	-4.666440000
C	0.233980000	6.360226000	-4.785626000
C	-1.131757000	6.481904000	-4.522763000
C	-1.864447000	5.359040000	-4.130912000
C	-1.231391000	4.122633000	-3.997855000
C	2.711470000	2.610735000	-3.945219000
C	3.562281000	2.907492000	-5.024329000
C	4.921767000	3.143782000	-4.811784000
C	5.451287000	3.087580000	-3.520567000
C	4.613616000	2.797594000	-2.441917000
C	3.253436000	2.559466000	-2.650453000
C	0.792606000	1.740730000	-5.930513000
C	-0.109650000	2.322668000	-6.836650000
C	-0.210768000	1.849986000	-8.147469000
C	0.590490000	0.791972000	-8.578662000
C	1.494143000	0.208010000	-7.688117000
C	1.591750000	0.673586000	-6.376392000
B	0.452027000	-0.288053000	1.306229000

Cl	0.154230000	3.149789000	-0.952642000
B	3.148546000	-1.377464000	1.100437000
B	2.200395000	-2.486660000	2.126066000
C	1.477686000	-1.603132000	0.850565000
B	0.555085000	-1.817317000	2.261266000
B	3.251692000	0.181606000	1.925651000
B	3.323398000	-1.337099000	2.858475000
C	2.324977000	-0.038093000	3.337425000
B	2.085943000	-0.029950000	0.615662000
B	1.602821000	0.848401000	2.064618000
B	1.713946000	-1.611940000	3.577423000
B	0.656303000	-0.263382000	3.083602000

### TS1-RE-C



Atom	x	y	z
Pd	-0.042429000	1.073554000	-2.132170000

P	-0.270243000	-1.140763000	-3.023823000
C	1.273371000	-1.564714000	-3.947842000
C	1.265146000	-2.378326000	-5.092340000
H	0.328513000	-2.757674000	-5.486929000
C	2.460442000	-2.700451000	-5.737880000
H	2.439012000	-3.328965000	-6.624023000
C	3.676836000	-2.215261000	-5.250632000
H	4.605217000	-2.463837000	-5.757366000
C	3.694463000	-1.406231000	-4.112415000
H	4.633597000	-1.015566000	-3.731680000
C	2.499995000	-1.081201000	-3.466241000
H	-2.384668000	-1.909650000	-1.124440000
C	-0.487068000	-2.603046000	-1.907229000
C	-1.647058000	-2.703464000	-1.118131000
H	2.519271000	-0.440141000	-2.590562000
C	-1.862934000	-3.820276000	-0.310816000
H	-2.766992000	-3.880491000	0.288322000
C	-0.918519000	-4.850043000	-0.264625000
H	-1.085355000	-5.716164000	0.369383000
C	0.241888000	-4.755340000	-1.034121000
H	0.984554000	-5.547683000	-1.004326000
C	0.456039000	-3.641854000	-1.852801000
H	1.359510000	-3.590800000	-2.449526000
C	-1.625115000	-1.410296000	-4.253990000
C	-2.162678000	-2.684107000	-4.508965000
H	-1.803788000	-3.548556000	-3.960026000

C	-3.167727000	-2.849128000	-5.463898000
H	-3.575764000	-3.839228000	-5.647772000
C	-3.648519000	-1.747809000	-6.176325000
H	-4.432820000	-1.878204000	-6.916887000
C	-3.121894000	-0.478494000	-5.928354000
H	-3.491429000	0.385226000	-6.472949000
C	-2.121762000	-0.310818000	-4.969696000
H	-1.731218000	0.680201000	-4.769848000
C	-5.010878000	2.470940000	-1.501863000
C	-4.683049000	1.232768000	-2.132317000
C	-5.619732000	0.622925000	-3.009572000
C	-6.840505000	1.216823000	-3.252046000
C	-7.169985000	2.445468000	-2.626504000
C	-6.275273000	3.057723000	-1.772950000
N	-4.147071000	3.115749000	-0.652014000
C	-2.958876000	2.589808000	-0.349758000
C	-2.562670000	1.308748000	-0.945292000
C	-3.414304000	0.674449000	-1.835503000
C	-1.266361000	0.712270000	-0.536709000
C	-1.004769000	0.281411000	0.707800000
H	-5.357412000	-0.319060000	-3.486966000
H	-7.554146000	0.745332000	-3.922696000
H	-8.135542000	2.904590000	-2.824096000
H	-6.507860000	3.999511000	-1.283190000
H	-3.144033000	-0.261248000	-2.316813000
P	0.943029000	2.396103000	-4.194229000

C	0.253114000	4.100897000	-3.990452000
C	0.960995000	5.261778000	-4.333929000
H	1.973961000	5.190242000	-4.716462000
C	0.374884000	6.520088000	-4.177715000
H	0.938588000	7.410647000	-4.442805000
C	-0.926192000	6.635513000	-3.683311000
H	-1.379617000	7.615829000	-3.563848000
C	-1.639668000	5.485172000	-3.336686000
H	-2.647683000	5.559284000	-2.938320000
C	-1.050241000	4.227896000	-3.481904000
H	-1.608229000	3.344731000	-3.183082000
C	2.772490000	2.633624000	-4.356433000
C	3.364421000	3.066486000	-5.556365000
H	2.748393000	3.261760000	-6.428275000
C	4.746706000	3.240151000	-5.645572000
H	5.186608000	3.575988000	-6.580839000
C	5.559403000	2.981796000	-4.539238000
H	6.635628000	3.114931000	-4.610039000
C	4.981861000	2.551876000	-3.343101000
H	5.605851000	2.351416000	-2.476240000
C	3.599113000	2.376965000	-3.250949000
H	3.156666000	2.062511000	-2.312173000
C	0.458531000	1.982582000	-5.937782000
C	-0.563234000	2.667796000	-6.613735000
H	-1.062178000	3.506531000	-6.140050000
C	-0.944174000	2.287646000	-7.903855000

H	-1.733393000	2.835902000	-8.411585000
C	-0.308930000	1.220889000	-8.540720000
H	-0.602632000	0.929096000	-9.545330000
C	0.711325000	0.533381000	-7.877960000
H	1.216350000	-0.297076000	-8.363959000
C	1.088856000	0.906557000	-6.588214000
H	1.889835000	0.365605000	-6.094629000
H	2.180522000	-0.326506000	-0.217426000
B	0.242576000	-0.261678000	1.498532000
Cl	1.168422000	2.827547000	-0.765636000
H	-1.885294000	0.360326000	1.359507000
H	3.269944000	-2.737889000	1.067006000
H	1.201868000	-3.827225000	2.897921000
H	0.534667000	-2.467877000	0.545697000
H	-1.168350000	-2.057744000	2.728278000
B	2.583339000	-2.001533000	1.692557000
B	1.344830000	-2.655308000	2.794762000
C	0.923971000	-1.852634000	1.345114000
B	-0.079820000	-1.591482000	2.686005000
B	3.044402000	-0.398510000	2.270067000
H	4.131515000	0.071515000	2.230316000
B	2.690818000	-1.706931000	3.431586000
H	3.543030000	-2.097115000	4.156541000
C	2.034909000	-0.143955000	3.619200000
H	2.427250000	0.467171000	4.424293000
B	1.916207000	-0.538866000	0.914392000

B	1.615967000	0.662896000	2.171305000
H	1.771673000	1.830655000	2.089416000
B	1.035137000	-1.455615000	4.048156000
H	0.784845000	-1.678137000	5.184954000
B	0.375932000	0.005847000	3.265400000
H	-0.308726000	0.741454000	3.894505000
H	-0.154184000	3.719026000	0.379567000
H	-0.229577000	3.118051000	2.636151000
C	-0.715703000	4.063088000	2.389809000
C	0.118352000	5.312179000	2.750396000
H	-1.697234000	4.083780000	2.877718000
C	-1.087797000	5.588370000	0.622267000
C	-0.115827000	6.310658000	1.579057000
H	1.179088000	5.053996000	2.826801000
H	-0.186895000	5.724844000	3.716883000
H	-0.884430000	5.762731000	-0.436241000
H	-2.129004000	5.865481000	0.822745000
H	0.827514000	6.529452000	1.069409000
H	-0.531058000	7.263853000	1.920301000
N	-0.939350000	4.145056000	0.928142000
H	-1.873564000	3.481448000	0.515498000

Int2-RE-C



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	2.700852000	-1.306725000	0.017222000
P	0.823429000	-2.646671000	-0.373900000
P	4.728294000	-0.238066000	0.410274000
C	0.799656000	-4.162445000	0.686744000
C	1.291689000	-4.047556000	1.997810000
H	1.689532000	-3.093064000	2.334136000
C	1.287243000	-5.145988000	2.858059000
H	1.670277000	-5.040426000	3.869558000
C	0.805188000	-6.380369000	2.414840000
H	0.810146000	-7.239075000	3.080845000
C	0.325510000	-6.508859000	1.109841000
H	-0.044696000	-7.467838000	0.756856000
C	0.320085000	-5.407121000	0.250464000
H	-0.053711000	-5.521219000	-0.762535000
C	-0.850853000	-1.906537000	-0.102778000
C	-1.919674000	-2.599007000	0.486253000
H	-1.784649000	-3.622095000	0.823155000
C	-3.162387000	-1.979947000	0.647182000
H	-3.979708000	-2.528025000	1.108936000
C	-3.356003000	-0.665782000	0.218170000
H	-4.324402000	-0.187855000	0.340070000

C	-2.296218000	0.033775000	-0.366459000
H	-2.438178000	1.060081000	-0.693942000
C	-1.052375000	-0.579150000	-0.516933000
H	-0.224450000	-0.028115000	-0.956767000
C	0.711412000	-3.317781000	-2.094895000
C	1.913970000	-3.564144000	-2.778377000
H	2.857891000	-3.332464000	-2.290378000
C	1.902723000	-4.086581000	-4.072131000
H	2.841558000	-4.272843000	-4.586906000
C	0.687885000	-4.356273000	-4.707793000
H	0.677681000	-4.754458000	-5.718888000
C	-0.513401000	-4.103716000	-4.042333000
H	-1.461705000	-4.305273000	-4.533640000
C	-0.503401000	-3.589275000	-2.743251000
H	-1.444501000	-3.394438000	-2.237816000
C	5.959597000	-1.262140000	1.336214000
C	5.971581000	-2.644255000	1.083001000
H	5.250847000	-3.063098000	0.384897000
C	6.885424000	-3.476995000	1.729006000
H	6.882898000	-4.543658000	1.521410000
C	7.790140000	-2.942880000	2.650456000
H	8.495770000	-3.592332000	3.161473000
C	7.777212000	-1.573172000	2.919953000
H	8.472566000	-1.152481000	3.641506000
C	6.869160000	-0.735902000	2.266332000
H	6.867830000	0.326532000	2.490223000

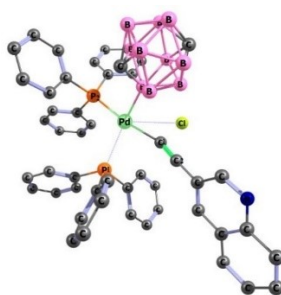
C	5.653627000	0.269415000	-1.110983000
C	7.052268000	0.373054000	-1.172343000
H	7.653856000	0.129866000	-0.301419000
C	7.682338000	0.775606000	-2.352518000
H	8.766102000	0.848393000	-2.385843000
C	6.925278000	1.077697000	-3.486590000
H	7.418106000	1.386584000	-4.404394000
C	5.533280000	0.965911000	-3.441142000
H	4.939526000	1.179246000	-4.326104000
C	4.903363000	0.557320000	-2.263708000
H	3.822929000	0.433167000	-2.234492000
C	4.646042000	1.325108000	1.404881000
C	5.505820000	2.423136000	1.221810000
H	6.276287000	2.388824000	0.457420000
C	5.372743000	3.570019000	2.012596000
H	6.034576000	4.416054000	1.850368000
C	4.383238000	3.636433000	2.996731000
H	4.266743000	4.536814000	3.591253000
C	3.526601000	2.548868000	3.190369000
H	2.747995000	2.598107000	3.946249000
C	3.651579000	1.406921000	2.396845000
H	2.967282000	0.572232000	2.529964000
C	-3.570728000	4.756309000	-0.876625000
C	-3.537190000	4.139336000	0.416452000
C	-2.512575000	4.501990000	1.333584000
C	-1.559573000	5.432505000	0.981715000

C	-1.595162000	6.042919000	-0.299297000
C	-2.579003000	5.715518000	-1.208307000
N	-4.526684000	4.448446000	-1.807040000
C	-5.434343000	3.553669000	-1.493114000
C	-5.494996000	2.868109000	-0.235831000
C	-4.532877000	3.180514000	0.713985000
C	-6.509924000	1.896676000	0.000437000
C	-7.379059000	1.061936000	0.182121000
H	-2.494745000	4.030923000	2.313589000
H	-0.761556000	5.707195000	1.664978000
H	-0.828484000	6.770779000	-0.547332000
H	-2.626713000	6.174352000	-2.191241000
H	-6.184879000	3.323864000	-2.248092000
H	-4.539099000	2.689517000	1.683265000
H	-8.662559000	-3.871207000	0.017382000
H	-10.417118000	-2.457480000	-1.913231000
H	-7.833940000	-1.536699000	-1.307430000
H	-9.775192000	0.431313000	-1.782922000
B	-9.108075000	-2.808772000	0.291110000
B	-10.163034000	-1.958176000	-0.870114000
C	-8.582858000	-1.409751000	-0.533647000
B	-9.779402000	-0.218346000	-0.793813000
B	-9.493773000	-2.228077000	1.914806000
H	-9.492391000	-2.874382000	2.906913000
B	-10.788396000	-2.454235000	0.706741000
H	-11.643259000	-3.249747000	0.901533000

C	-10.687101000	-1.035679000	1.653232000
H	-11.432952000	-0.902655000	2.428898000
B	-8.071597000	-1.594656000	1.085145000
H	-6.942742000	-1.850609000	1.334047000
B	-9.108639000	-0.487471000	1.993669000
H	-8.852302000	0.016418000	3.033464000
B	-11.201959000	-0.852680000	0.035875000
H	-12.329356000	-0.590625000	-0.213267000
B	-10.166975000	0.364329000	0.830483000
H	-10.606024000	1.428297000	1.105558000
B	-8.472212000	0.025960000	0.416416000
Cl	2.058891000	6.432257000	1.089320000
H	3.328899000	3.293567000	0.295618000
C	1.313270000	3.006779000	-0.318966000
C	3.043711000	4.186227000	-1.596602000
C	0.941946000	3.043438000	-1.813541000
H	1.486646000	1.998334000	0.060880000
H	0.575801000	3.510983000	0.308176000
C	1.729631000	4.241602000	-2.374051000
H	3.576434000	5.136558000	-1.533278000
H	3.711939000	3.406782000	-1.973122000
H	-0.136669000	3.148961000	-1.954737000
H	1.259279000	2.116257000	-2.304037000
H	1.211286000	5.180347000	-2.152040000
H	1.890026000	4.182618000	-3.453812000
N	2.599146000	3.803437000	-0.210093000

H 2.411142000 4.721785000 0.335933000

### TS1-DC



Atom	x	y	z
Pd	0.398022000	0.282459000	-0.737810000
Cl	0.310241000	0.234979000	-4.468455000
P	-1.158532000	2.370584000	-0.065439000
P	2.539189000	0.993860000	0.097876000
C	-6.267322000	-1.764756000	-3.116432000
C	-5.985619000	-0.360078000	-3.131314000
C	-7.023379000	0.553763000	-3.461906000
C	-8.285707000	0.093471000	-3.763775000
C	-8.563037000	-1.296996000	-3.748109000
C	-7.576587000	-2.207368000	-3.431710000
N	-5.314286000	-2.699711000	-2.809303000
C	-4.104996000	-2.278861000	-2.523601000
C	-3.707958000	-0.898666000	-2.500836000

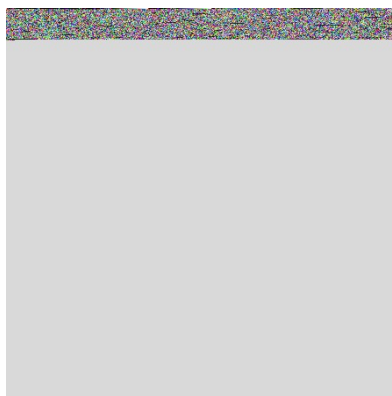
C	-4.673558000	0.053039000	-2.809530000
C	-2.375154000	-0.543198000	-2.175575000
C	-1.190735000	-0.251824000	-1.954018000
H	-0.464648000	-0.038228000	-3.123727000
H	-6.801119000	1.617789000	-3.472431000
H	-9.075683000	0.794902000	-4.016452000
H	-9.563921000	-1.644138000	-3.989121000
H	-7.769275000	-3.275541000	-3.415568000
H	-3.359275000	-3.035999000	-2.287167000
H	-4.419992000	1.109259000	-2.806370000
H	0.085206000	-4.534350000	1.947071000
H	3.014835000	-4.148887000	1.594152000
H	1.229339000	-2.003688000	1.608861000
H	3.437631000	-1.840052000	-0.122208000
B	0.519800000	-4.184829000	0.901088000
B	2.272550000	-3.956118000	0.690551000
C	1.197596000	-2.625439000	0.721665000
B	2.505737000	-2.524269000	-0.349387000
B	-0.181167000	-4.524361000	-0.680843000
H	-1.085440000	-5.258215000	-0.901173000
B	1.418901000	-5.179798000	-0.247126000
H	1.583419000	-6.351744000	-0.182188000
C	1.138051000	-4.420314000	-1.747955000
H	1.114462000	-5.048046000	-2.631635000
B	-0.310278000	-2.891106000	-0.010470000
H	-1.302940000	-2.445107000	0.453572000

B	0.065038000	-3.094894000	-1.721613000
H	-0.660743000	-2.940390000	-2.639082000
B	2.649861000	-4.148212000	-1.022321000
H	3.635673000	-4.631594000	-1.468350000
B	1.810077000	-2.853114000	-1.929687000
H	2.246041000	-2.530446000	-2.980591000
B	0.907891000	-1.805369000	-0.791418000
C	2.763676000	2.822707000	0.290858000
C	3.290770000	3.412510000	1.446641000
C	2.513684000	3.627478000	-0.833233000
C	3.575225000	4.781203000	1.472192000
C	2.800634000	4.990638000	-0.805605000
C	3.336590000	5.571030000	0.347847000
H	3.493777000	2.809247000	2.325315000
H	2.111932000	3.183500000	-1.740398000
H	3.988586000	5.225314000	2.373769000
H	2.608612000	5.598854000	-1.685183000
H	3.564557000	6.633133000	0.368352000
C	3.931196000	0.703347000	-1.084903000
C	3.657430000	0.168295000	-2.350602000
C	5.239136000	1.133416000	-0.795303000
C	4.677520000	0.029187000	-3.295823000
C	6.258064000	0.977735000	-1.734282000
C	5.979957000	0.420416000	-2.986134000
H	2.645355000	-0.125073000	-2.607893000
H	5.461994000	1.613080000	0.152914000

H	4.445060000	-0.382762000	-4.273608000
H	7.265608000	1.305674000	-1.493421000
H	6.773466000	0.307920000	-3.719854000
C	3.010666000	0.320073000	1.751844000
C	4.256850000	-0.243202000	2.062431000
C	2.022287000	0.361870000	2.752054000
C	4.511736000	-0.737331000	3.344517000
C	2.281663000	-0.122142000	4.034919000
C	3.530053000	-0.673734000	4.334366000
H	5.029426000	-0.314792000	1.305737000
H	1.039617000	0.764893000	2.522306000
H	5.480618000	-1.176863000	3.564378000
H	1.505847000	-0.077912000	4.794179000
H	3.731721000	-1.059660000	5.329590000
C	-0.725220000	3.897138000	0.901995000
C	-0.344457000	3.758976000	2.248636000
C	-0.791701000	5.186806000	0.355424000
C	-0.064222000	4.877915000	3.031135000
C	-0.507374000	6.308309000	1.139996000
C	-0.150106000	6.159411000	2.479977000
H	-0.291623000	2.772232000	2.700741000
H	-1.080730000	5.324105000	-0.681018000
H	0.216481000	4.748809000	4.073081000
H	-0.574921000	7.299653000	0.699695000
H	0.061904000	7.032648000	3.090887000
C	-2.515970000	1.709045000	1.017439000

C	-3.394722000	2.561465000	1.712090000
C	-2.663250000	0.323267000	1.179152000
C	-4.404530000	2.039367000	2.520902000
C	-3.669913000	-0.198871000	1.996026000
C	-4.546195000	0.656588000	2.664271000
H	-3.282878000	3.638314000	1.636268000
H	-1.990386000	-0.350416000	0.662270000
H	-5.075856000	2.714548000	3.044780000
H	-3.764014000	-1.275613000	2.108103000
H	-5.329630000	0.251091000	3.298739000
C	-2.005588000	3.077255000	-1.550885000
C	-3.322924000	3.563202000	-1.538784000
C	-1.268405000	3.152007000	-2.742381000
C	-3.882930000	4.120108000	-2.690725000
C	-1.826441000	3.715199000	-3.892000000
C	-3.134652000	4.201373000	-3.868571000
H	-3.920405000	3.502264000	-0.635439000
H	-0.264375000	2.741565000	-2.786646000
H	-4.904143000	4.491648000	-2.665853000
H	-1.242638000	3.752676000	-4.807006000
H	-3.572892000	4.632952000	-4.764338000

Int1-DC



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.318919000	0.218426000	-0.532970000
Cl	0.393366000	0.747816000	-3.980906000
P	-1.202066000	2.314963000	0.343557000
P	2.533185000	0.943196000	0.094434000
C	-6.107929000	-1.585452000	-3.825239000
C	-5.755867000	-0.197651000	-3.771807000
C	-6.657160000	0.772205000	-4.287525000
C	-7.859232000	0.379810000	-4.832723000
C	-8.207741000	-0.993795000	-4.884462000
C	-7.352809000	-1.957234000	-4.392542000
N	-5.285622000	-2.570234000	-3.346076000
C	-4.139635000	-2.217816000	-2.813656000
C	-3.689244000	-0.863237000	-2.718116000
C	-4.504503000	0.143900000	-3.209862000
C	-2.436095000	-0.547597000	-2.094824000
C	-1.377522000	-0.253264000	-1.494705000
H	-1.306067000	-0.935988000	-2.561879000
H	-6.379801000	1.822073000	-4.244157000

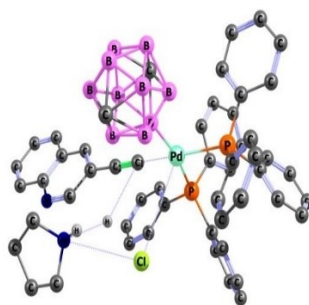
H	-8.546746000	1.122249000	-5.227231000
H	-9.159943000	-1.285796000	-5.318218000
H	-7.602363000	-3.013090000	-4.424118000
H	-3.505516000	-3.014216000	-2.428344000
H	-4.188218000	1.181620000	-3.164524000
H	0.106763000	-4.519210000	2.340860000
H	3.018242000	-4.138221000	1.857800000
H	1.226170000	-2.006563000	1.878754000
H	3.368792000	-1.897118000	0.048517000
B	0.499712000	-4.209251000	1.266511000
B	2.239680000	-3.982999000	0.978233000
C	1.162731000	-2.653152000	1.011552000
B	2.431354000	-2.590183000	-0.120896000
B	-0.262194000	-4.607281000	-0.270112000
H	-1.175204000	-5.344043000	-0.435409000
B	1.355454000	-5.241859000	0.118680000
H	1.526192000	-6.410384000	0.214557000
C	1.014056000	-4.537328000	-1.388811000
H	0.954807000	-5.200616000	-2.245014000
B	-0.369592000	-2.950784000	0.344150000
H	-1.349241000	-2.488915000	0.819382000
B	-0.053906000	-3.218238000	-1.364827000
H	-0.817451000	-3.109890000	-2.262366000
B	2.552085000	-4.237054000	-0.740731000
H	3.520468000	-4.731953000	-1.209864000
B	1.675543000	-2.974263000	-1.661099000

H	2.058830000	-2.684753000	-2.741263000
B	0.816844000	-1.885658000	-0.524832000
C	2.672355000	2.786359000	0.181171000
C	3.196101000	3.472777000	1.282868000
C	2.335700000	3.501310000	-0.982978000
C	3.395571000	4.855476000	1.217883000
C	2.535779000	4.879330000	-1.040004000
C	3.070239000	5.559309000	0.058906000
H	3.461165000	2.936827000	2.188551000
H	1.944257000	2.978148000	-1.853761000
H	3.807441000	5.377950000	2.077021000
H	2.280521000	5.420547000	-1.946915000
H	3.230859000	6.632863000	0.010022000
C	3.858461000	0.644626000	-1.157368000
C	3.537664000	0.012611000	-2.364455000
C	5.153673000	1.166012000	-0.977256000
C	4.505251000	-0.127080000	-3.363511000
C	6.119457000	1.009494000	-1.969958000
C	5.797288000	0.358011000	-3.165159000
H	2.528534000	-0.344039000	-2.539349000
H	5.405370000	1.718186000	-0.076900000
H	4.235447000	-0.607752000	-4.299323000
H	7.117817000	1.410081000	-1.816516000
H	6.548628000	0.245145000	-3.942116000
C	3.120974000	0.336567000	1.734814000
C	4.395197000	-0.196948000	1.978816000

C	2.196418000	0.382745000	2.793432000
C	4.740556000	-0.650956000	3.254408000
C	2.546199000	-0.060595000	4.069406000
C	3.822745000	-0.578403000	4.303152000
H	5.118561000	-0.276107000	1.175965000
H	1.193387000	0.758974000	2.613947000
H	5.730123000	-1.066309000	3.423084000
H	1.818980000	-0.010868000	4.875067000
H	4.095280000	-0.932193000	5.293449000
C	-0.678758000	3.873168000	1.213655000
C	-0.161376000	3.779857000	2.517712000
C	-0.807198000	5.143766000	0.634091000
C	0.191291000	4.924229000	3.231261000
C	-0.448831000	6.290124000	1.348999000
C	0.044687000	6.186164000	2.649520000
H	-0.060253000	2.809268000	2.994992000
H	-1.198649000	5.246650000	-0.371932000
H	0.577079000	4.829510000	4.242825000
H	-0.564468000	7.266096000	0.885248000
H	0.314415000	7.079477000	3.206237000
C	-2.410766000	1.654484000	1.588723000
C	-3.233123000	2.511557000	2.345290000
C	-2.513745000	0.272799000	1.801501000
C	-4.140368000	1.995430000	3.270552000
C	-3.419379000	-0.244258000	2.732180000
C	-4.236807000	0.614649000	3.466626000

H	-3.161113000	3.586919000	2.218134000
H	-1.878999000	-0.404639000	1.242569000
H	-4.768944000	2.673459000	3.841541000
H	-3.478497000	-1.318878000	2.882255000
H	-4.940366000	0.213948000	4.191236000
C	-2.247432000	2.944566000	-1.043213000
C	-3.630711000	3.166671000	-0.949875000
C	-1.597082000	3.199456000	-2.260543000
C	-4.338520000	3.660851000	-2.049031000
C	-2.303136000	3.692683000	-3.356492000
C	-3.676449000	3.931223000	-3.249872000
H	-4.160616000	2.953845000	-0.027618000
H	-0.535640000	2.947776000	-2.373827000
H	-5.407976000	3.835904000	-1.964857000
H	-1.784467000	3.869142000	-4.293584000
H	-4.230739000	4.313654000	-4.103170000

### TS2-DC



Atom	x	y	z
Pd	2.609651000	-0.265799000	-0.550663000
P	4.926445000	-0.882633000	-1.201953000

C	5.950960000	0.211193000	-2.311610000
C	6.309655000	-0.150277000	-3.618742000
H	5.974709000	-1.092062000	-4.038414000
C	7.110708000	0.691336000	-4.395436000
H	7.381003000	0.390025000	-5.403992000
C	7.565658000	1.904837000	-3.879779000
H	8.190132000	2.557246000	-4.483957000
C	7.216573000	2.272591000	-2.578128000
H	7.565634000	3.213384000	-2.161976000
C	6.418675000	1.433408000	-1.800689000
H	4.612200000	-0.356335000	1.631263000
C	6.103898000	-0.995635000	0.221266000
C	5.649010000	-0.652233000	1.502113000
H	6.172122000	1.729830000	-0.786571000
C	6.517253000	-0.662352000	2.596991000
H	6.147345000	-0.390047000	3.581758000
C	7.856117000	-1.014475000	2.422563000
H	8.532790000	-1.026721000	3.272501000
C	8.328840000	-1.331498000	1.145937000
H	9.375260000	-1.584305000	0.998974000
C	7.464298000	-1.308328000	0.051472000
H	7.858285000	-1.512104000	-0.939252000
C	4.970776000	-2.472485000	-2.145779000
C	5.925690000	-3.484963000	-1.975147000
H	6.677954000	-3.406278000	-1.198567000
C	5.908235000	-4.619620000	-2.789102000

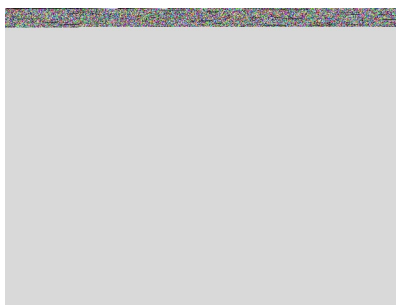
H	6.649269000	-5.399416000	-2.635785000
C	4.947048000	-4.753343000	-3.793153000
H	4.939681000	-5.634819000	-4.428265000
C	3.987349000	-3.754552000	-3.967286000
H	3.223222000	-3.855365000	-4.732861000
C	3.990634000	-2.630082000	-3.139898000
H	3.213297000	-1.879515000	-3.259061000
H	-0.373866000	-2.582645000	-0.173564000
H	0.660207000	-1.210698000	2.474930000
H	3.373769000	-1.879831000	2.605684000
H	4.494215000	-3.290462000	0.472664000
B	0.545522000	-2.977899000	0.461140000
B	1.075734000	-2.189311000	1.961034000
C	2.723978000	-2.571640000	2.085113000
B	3.360343000	-3.425141000	0.766312000
B	0.817140000	-4.722219000	0.646748000
H	0.129290000	-5.592429000	0.224223000
B	0.256374000	-3.761884000	2.031600000
H	-0.791865000	-3.982309000	2.540207000
C	1.531501000	-4.897500000	2.187944000
H	1.339826000	-5.802913000	2.752562000
B	1.970227000	-3.741295000	-0.286537000
H	2.079006000	-3.894051000	-1.457612000
B	2.561548000	-5.003663000	0.825424000
H	3.047046000	-6.045370000	0.532594000
B	1.649627000	-3.451193000	3.058087000

H	1.629105000	-3.384740000	4.238956000
B	3.072550000	-4.220275000	2.316218000
H	3.916455000	-4.618081000	3.043363000
B	2.137834000	-2.118449000	0.482055000
C	-4.284161000	1.518410000	1.500813000
C	-3.199227000	2.058979000	2.261903000
C	-3.488345000	2.911130000	3.362766000
C	-4.792040000	3.212224000	3.692123000
C	-5.865004000	2.675756000	2.936613000
C	-5.615629000	1.846355000	1.863479000
N	-4.075357000	0.689426000	0.431611000
C	-2.837147000	0.390583000	0.105037000
C	-1.670550000	0.874909000	0.789304000
C	-1.882470000	1.714794000	1.874953000
C	-0.372523000	0.488352000	0.355901000
C	0.754404000	0.145414000	0.008204000
H	-2.662551000	3.320434000	3.940173000
H	-5.003095000	3.863976000	4.535688000
H	-6.887817000	2.921679000	3.208855000
H	-6.421057000	1.422488000	1.270918000
H	-2.701361000	-0.285621000	-0.738652000
H	-1.037118000	2.112208000	2.430516000
P	2.581911000	2.220771000	-1.493829000
C	1.001150000	3.170086000	-1.293563000
C	0.846280000	4.213185000	-0.371455000
H	1.667008000	4.494111000	0.279782000

C	-0.363013000	4.911187000	-0.286378000
H	-0.464196000	5.720794000	0.431727000
C	-1.429056000	4.576109000	-1.120164000
H	-2.367549000	5.119665000	-1.054092000
C	-1.284272000	3.532530000	-2.039590000
H	-2.110758000	3.259587000	-2.690060000
C	-0.081981000	2.833101000	-2.123222000
H	0.013137000	2.022201000	-2.839601000
C	3.766802000	3.217904000	-0.479977000
C	4.565205000	4.259046000	-0.976053000
H	4.530954000	4.520185000	-2.027874000
C	5.427392000	4.958711000	-0.127990000
H	6.041141000	5.760251000	-0.530542000
C	5.501679000	4.633112000	1.227965000
H	6.172513000	5.179535000	1.885229000
C	4.711043000	3.598368000	1.733761000
H	4.762871000	3.335328000	2.786799000
C	3.856373000	2.892044000	0.885227000
H	3.252622000	2.080289000	1.283325000
C	2.934705000	2.608275000	-3.268245000
C	2.772289000	3.901581000	-3.799940000
H	2.454212000	4.717239000	-3.157614000
C	2.990189000	4.144527000	-5.155436000
H	2.864020000	5.149343000	-5.549466000
C	3.352644000	3.096281000	-6.007077000
H	3.512770000	3.284999000	-7.065156000

C	3.492211000	1.806210000	-5.496320000
H	3.758313000	0.983214000	-6.153624000
C	3.282716000	1.565286000	-4.135695000
H	3.378894000	0.557535000	-3.748064000
Cl	-0.033233000	-0.945911000	-3.617749000
H	-1.889493000	-3.190021000	-2.048259000
C	-3.677557000	-3.071930000	-1.013908000
C	-3.451546000	-2.619426000	-3.287317000
C	-4.991194000	-2.356588000	-1.404322000
H	-3.813488000	-4.167141000	-1.064692000
H	-3.337920000	-2.823825000	-0.003162000
C	-4.807226000	-1.994545000	-2.907453000
H	-2.914727000	-2.060178000	-4.060094000
H	-3.604181000	-3.649631000	-3.658874000
H	-5.130566000	-1.452681000	-0.804829000
H	-5.856378000	-3.005907000	-1.236301000
H	-4.771211000	-0.907727000	-3.034365000
H	-5.617106000	-2.373254000	-3.538865000
N	-2.712090000	-2.590860000	-2.016618000
H	-0.496087000	-0.964497000	-2.403983000

Int1-RE



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	1.541070000	0.079847000	0.394433000
P	3.972226000	0.063871000	0.817008000
C	4.888576000	0.343795000	-0.762154000
C	6.284555000	0.505887000	-0.824531000
H	6.879888000	0.477046000	0.082501000
C	6.924534000	0.675103000	-2.052318000
H	8.002638000	0.806514000	-2.082966000
C	6.185591000	0.659440000	-3.239270000
H	6.687965000	0.783299000	-4.194686000
C	4.804314000	0.466100000	-3.193207000
H	4.223438000	0.434389000	-4.110633000
C	4.161461000	0.309112000	-1.962029000
H	2.570364000	0.931430000	3.145590000
C	4.300056000	1.474889000	1.968343000
C	3.422329000	1.601597000	3.059891000
H	3.086566000	0.153760000	-1.929305000
C	3.635406000	2.575049000	4.037940000
H	2.952037000	2.651530000	4.879199000
C	4.719600000	3.448208000	3.929308000
H	4.885771000	4.209185000	4.686837000

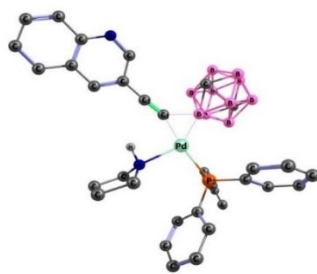
C	5.582317000	3.345542000	2.836555000
H	6.418176000	4.032032000	2.735451000
C	5.378165000	2.364316000	1.864128000
H	6.053202000	2.312908000	1.018322000
C	5.026525000	-1.265318000	1.584462000
C	5.286889000	-1.290934000	2.963552000
H	4.885758000	-0.518304000	3.610345000
C	6.070981000	-2.302152000	3.522693000
H	6.263753000	-2.299519000	4.592055000
C	6.607519000	-3.305765000	2.714631000
H	7.220260000	-4.090406000	3.149918000
C	6.355787000	-3.290513000	1.341204000
H	6.771466000	-4.063206000	0.700147000
C	5.572384000	-2.280316000	0.781142000
H	5.396756000	-2.281409000	-0.289358000
H	-1.464735000	-4.708943000	-0.284169000
H	-1.922533000	-3.900868000	2.538674000
H	-1.310568000	-2.036346000	0.541182000
H	-0.267298000	-1.537008000	3.096409000
B	-0.564167000	-4.309824000	0.375611000
B	-0.838616000	-3.825992000	2.064793000
C	-0.498878000	-2.677340000	0.855465000
B	0.167112000	-2.377596000	2.382584000
B	1.128135000	-4.765412000	0.199988000
H	1.554279000	-5.628204000	-0.492839000
B	0.234632000	-5.176790000	1.689028000

H	0.065803000	-6.312010000	1.986372000
C	1.790580000	-4.488154000	1.744090000
H	2.609596000	-5.124926000	2.059342000
B	0.606728000	-3.155398000	-0.333854000
H	0.472643000	-2.844989000	-1.470190000
B	2.127530000	-3.328675000	0.531103000
H	3.206016000	-3.284722000	0.051414000
B	0.684549000	-3.981446000	2.936462000
H	0.815849000	-4.324546000	4.063763000
B	1.855418000	-2.845002000	2.220773000
H	2.752142000	-2.473920000	2.895625000
B	1.090381000	-1.924564000	0.897697000
C	-5.730448000	1.045993000	-0.704985000
C	-5.106208000	0.048292000	-1.519492000
C	-5.893909000	-0.659389000	-2.467960000
C	-7.238461000	-0.389161000	-2.601226000
C	-7.854942000	0.599592000	-1.793807000
C	-7.116260000	1.302337000	-0.865340000
N	-5.030904000	1.763718000	0.227858000
C	-3.748558000	1.515625000	0.367302000
C	-3.012338000	0.539930000	-0.388081000
C	-3.722874000	-0.186210000	-1.334543000
C	-1.621036000	0.348990000	-0.149557000
C	-0.420280000	0.202681000	0.068204000
H	-5.417552000	-1.417806000	-3.084829000
H	-7.833338000	-0.935474000	-3.328083000

H	-8.916291000	0.801016000	-1.910427000
H	-7.566814000	2.063574000	-0.235422000
H	-3.212389000	2.100323000	1.113047000
H	-3.219482000	-0.938393000	-1.936583000
P	1.489989000	2.636659000	-0.432071000
C	2.849283000	3.903927000	-0.337526000
C	3.935524000	3.822618000	-1.227667000
H	3.966976000	3.040754000	-1.979112000
C	4.972762000	4.753788000	-1.176857000
H	5.795858000	4.676823000	-1.882461000
C	4.951091000	5.781288000	-0.230169000
H	5.756707000	6.509769000	-0.193780000
C	3.884130000	5.866230000	0.664377000
H	3.852819000	6.662539000	1.403393000
C	2.841967000	4.936828000	0.612349000
H	2.018503000	5.028338000	1.312144000
C	0.125043000	3.486397000	0.483102000
C	0.006528000	3.237227000	1.859983000
H	0.678403000	2.531501000	2.339185000
C	-0.973456000	3.879511000	2.618627000
H	-1.049544000	3.676718000	3.683493000
C	-1.862447000	4.767178000	2.006851000
H	-2.632796000	5.259952000	2.593589000
C	-1.761535000	5.010357000	0.635589000
H	-2.455348000	5.691264000	0.150113000
C	-0.772136000	4.378241000	-0.121465000

H	-0.711604000	4.576747000	-1.186398000
C	1.022362000	2.749928000	-2.221951000
C	0.541423000	1.607058000	-2.880592000
H	0.425060000	0.681241000	-2.327720000
C	0.189708000	1.659231000	-4.231644000
H	-0.179927000	0.764023000	-4.724447000
C	0.312516000	2.852714000	-4.944729000
H	0.039780000	2.892204000	-5.995901000
C	0.790242000	3.996747000	-4.300796000
H	0.889764000	4.930457000	-4.847842000
C	1.145780000	3.945845000	-2.952106000
H	1.530218000	4.839319000	-2.470686000

### TS-RE1



Atom	x	y	z
Pd	0.424975000	0.214512000	0.170273000
P	-0.579228000	-2.143250000	0.639082000
P	2.734757000	-0.261674000	-0.624493000
C	0.331059000	-3.743490000	0.429974000
C	1.568040000	-3.900670000	1.080570000
H	1.956462000	-3.103644000	1.707277000

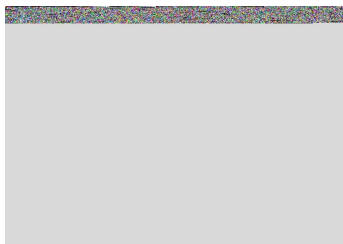
C	2.307342000	-5.074499000	0.940300000
H	3.256325000	-5.176692000	1.460053000
C	1.833724000	-6.109535000	0.129318000
H	2.411093000	-7.022951000	0.014831000
C	0.615536000	-5.959742000	-0.534134000
H	0.237819000	-6.757672000	-1.168145000
C	-0.132864000	-4.788856000	-0.383191000
H	-1.083392000	-4.697249000	-0.897604000
C	-1.078595000	-2.186893000	2.425770000
C	-0.954179000	-3.325407000	3.238102000
H	-0.541375000	-4.242956000	2.832228000
C	-1.356882000	-3.291805000	4.576085000
H	-1.250840000	-4.182447000	5.189998000
C	-1.895673000	-2.125003000	5.120322000
H	-2.207814000	-2.100443000	6.160917000
C	-2.031105000	-0.988642000	4.318724000
H	-2.450702000	-0.075410000	4.732148000
C	-1.621908000	-1.016338000	2.984948000
H	-1.728394000	-0.127677000	2.370324000
C	-2.174802000	-2.462163000	-0.238661000
C	-2.336176000	-1.959227000	-1.538482000
H	-1.545019000	-1.365446000	-1.984858000
C	-3.510575000	-2.199890000	-2.254476000
H	-3.621395000	-1.801113000	-3.259212000
C	-4.544945000	-2.936763000	-1.674221000
H	-5.463094000	-3.116571000	-2.226901000

C	-4.399101000	-3.434391000	-0.376818000
H	-5.202571000	-4.003970000	0.082532000
C	-3.222194000	-3.199752000	0.336385000
H	-3.120708000	-3.590226000	1.344481000
C	2.654992000	-1.647488000	-1.856069000
C	1.540520000	-1.670525000	-2.713131000
H	0.764734000	-0.916619000	-2.604007000
C	1.410182000	-2.653306000	-3.695522000
H	0.543797000	-2.647955000	-4.351371000
C	2.383024000	-3.646747000	-3.822437000
H	2.280843000	-4.418804000	-4.580092000
C	3.481400000	-3.649111000	-2.961003000
H	4.236721000	-4.426117000	-3.043131000
C	3.619453000	-2.656780000	-1.987491000
H	4.476809000	-2.686010000	-1.324735000
C	3.586195000	1.064572000	-1.616163000
C	3.189327000	1.311685000	-2.941421000
H	2.441218000	0.683779000	-3.414013000
C	3.755700000	2.353501000	-3.676705000
H	3.436724000	2.519344000	-4.702268000
C	4.728174000	3.174975000	-3.102116000
H	5.169477000	3.985681000	-3.675213000
C	5.128220000	2.943473000	-1.785807000
H	5.885005000	3.573043000	-1.325455000
C	4.562090000	1.900340000	-1.048656000
H	4.893870000	1.738859000	-0.029192000

C	4.015257000	-0.751478000	0.611365000
C	5.372596000	-0.943618000	0.295821000
H	5.724438000	-0.781950000	-0.718582000
C	6.284872000	-1.323362000	1.281339000
H	7.329327000	-1.469729000	1.019854000
C	5.859267000	-1.507632000	2.599839000
H	6.571974000	-1.799741000	3.366204000
C	4.518671000	-1.303501000	2.930353000
H	4.182042000	-1.430799000	3.955506000
C	3.605245000	-0.924819000	1.942944000
H	2.565105000	-0.751523000	2.206761000
C	-6.436943000	2.330090000	-1.233088000
C	-5.461294000	2.440905000	-2.275256000
C	-5.881483000	2.843775000	-3.572505000
C	-7.207397000	3.122378000	-3.822854000
C	-8.171761000	3.011215000	-2.789691000
C	-7.793993000	2.623115000	-1.521332000
N	-6.100889000	1.946876000	0.038139000
C	-4.842356000	1.675236000	0.291670000
C	-3.773686000	1.751486000	-0.667511000
C	-4.116147000	2.141593000	-1.957538000
C	-2.445504000	1.432352000	-0.283836000
C	-1.299659000	1.157309000	0.080357000
H	-5.138734000	2.928315000	-4.362305000
H	-7.519763000	3.429745000	-4.817149000
H	-9.213428000	3.234434000	-3.003183000

H	-8.514733000	2.531154000	-0.714376000
H	-4.599573000	1.369431000	1.308684000
H	-3.351033000	2.216415000	-2.726018000
H	-1.540390000	5.666828000	1.914093000
H	0.433959000	6.089431000	-0.263357000
H	-1.266709000	3.867388000	-0.205344000
H	1.326012000	3.454692000	-1.216545000
B	-0.593573000	4.959916000	1.824614000
B	0.587114000	5.208627000	0.514746000
C	-0.460208000	3.863863000	0.517056000
B	1.114066000	3.599868000	-0.061062000
B	0.218582000	4.135029000	3.151690000
H	0.013666000	4.303428000	4.306990000
B	1.074816000	5.384452000	2.205262000
H	1.441308000	6.380221000	2.733247000
C	1.795278000	3.886165000	2.575282000
H	2.597820000	3.879683000	3.304533000
B	-0.796031000	3.201086000	2.049892000
H	-1.869376000	2.797048000	2.333828000
B	0.738816000	2.526683000	2.567591000
H	0.902501000	1.659805000	3.358958000
B	2.132214000	4.546587000	1.042435000
H	3.206191000	4.981555000	0.793636000
B	1.928971000	2.791560000	1.278479000
H	2.889846000	2.109129000	1.229759000
B	0.247188000	2.302173000	0.850402000

## Int2-RE



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	2.700852000	-1.306725000	0.017222000
P	0.823429000	-2.646671000	-0.373900000
P	4.728294000	-0.238066000	0.410274000
C	0.799656000	-4.162445000	0.686744000
C	1.291689000	-4.047556000	1.997810000
H	1.689532000	-3.093064000	2.334136000
C	1.287243000	-5.145988000	2.858059000
H	1.670277000	-5.040426000	3.869558000
C	0.805188000	-6.380369000	2.414840000
H	0.810146000	-7.239075000	3.080845000
C	0.325510000	-6.508859000	1.109841000
H	-0.044696000	-7.467838000	0.756856000
C	0.320085000	-5.407121000	0.250464000
H	-0.053711000	-5.521219000	-0.762535000
C	-0.850853000	-1.906537000	-0.102778000
C	-1.919674000	-2.599007000	0.486253000
H	-1.784649000	-3.622095000	0.823155000
C	-3.162387000	-1.979947000	0.647182000

H	-3.979708000	-2.528025000	1.108936000
C	-3.356003000	-0.665782000	0.218170000
H	-4.324402000	-0.187855000	0.340070000
C	-2.296218000	0.033775000	-0.366459000
H	-2.438178000	1.060081000	-0.693942000
C	-1.052375000	-0.579150000	-0.516933000
H	-0.224450000	-0.028115000	-0.956767000
C	0.711412000	-3.317781000	-2.094895000
C	1.913970000	-3.564144000	-2.778377000
H	2.857891000	-3.332464000	-2.290378000
C	1.902723000	-4.086581000	-4.072131000
H	2.841558000	-4.272843000	-4.586906000
C	0.687885000	-4.356273000	-4.707793000
H	0.677681000	-4.754458000	-5.718888000
C	-0.513401000	-4.103716000	-4.042333000
H	-1.461705000	-4.305273000	-4.533640000
C	-0.503401000	-3.589275000	-2.743251000
H	-1.444501000	-3.394438000	-2.237816000
C	5.959597000	-1.262140000	1.336214000
C	5.971581000	-2.644255000	1.083001000
H	5.250847000	-3.063098000	0.384897000
C	6.885424000	-3.476995000	1.729006000
H	6.882898000	-4.543658000	1.521410000
C	7.790140000	-2.942880000	2.650456000
H	8.495770000	-3.592332000	3.161473000
C	7.777212000	-1.573172000	2.919953000

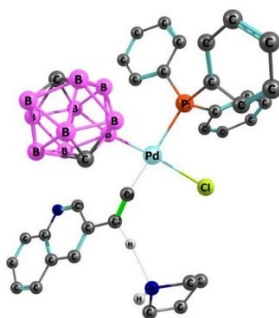
H	8.472566000	-1.152481000	3.641506000
C	6.869160000	-0.735902000	2.266332000
H	6.867830000	0.326532000	2.490223000
C	5.653627000	0.269415000	-1.110983000
C	7.052268000	0.373054000	-1.172343000
H	7.653856000	0.129866000	-0.301419000
C	7.682338000	0.775606000	-2.352518000
H	8.766102000	0.848393000	-2.385843000
C	6.925278000	1.077697000	-3.486590000
H	7.418106000	1.386584000	-4.404394000
C	5.533280000	0.965911000	-3.441142000
H	4.939526000	1.179246000	-4.326104000
C	4.903363000	0.557320000	-2.263708000
H	3.822929000	0.433167000	-2.234492000
C	4.646042000	1.325108000	1.404881000
C	5.505820000	2.423136000	1.221810000
H	6.276287000	2.388824000	0.457420000
C	5.372743000	3.570019000	2.012596000
H	6.034576000	4.416054000	1.850368000
C	4.383238000	3.636433000	2.996731000
H	4.266743000	4.536814000	3.591253000
C	3.526601000	2.548868000	3.190369000
H	2.747995000	2.598107000	3.946249000
C	3.651579000	1.406921000	2.396845000
H	2.967282000	0.572232000	2.529964000
C	-3.570728000	4.756309000	-0.876625000

C	-3.537190000	4.139336000	0.416452000
C	-2.512575000	4.501990000	1.333584000
C	-1.559573000	5.432505000	0.981715000
C	-1.595162000	6.042919000	-0.299297000
C	-2.579003000	5.715518000	-1.208307000
N	-4.526684000	4.448446000	-1.807040000
C	-5.434343000	3.553669000	-1.493114000
C	-5.494996000	2.868109000	-0.235831000
C	-4.532877000	3.180514000	0.713985000
C	-6.509924000	1.896676000	0.000437000
C	-7.379059000	1.061936000	0.182121000
H	-2.494745000	4.030923000	2.313589000
H	-0.761556000	5.707195000	1.664978000
H	-0.828484000	6.770779000	-0.547332000
H	-2.626713000	6.174352000	-2.191241000
H	-6.184879000	3.323864000	-2.248092000
H	-4.539099000	2.689517000	1.683265000
H	-8.662559000	-3.871207000	0.017382000
H	-10.417118000	-2.457480000	-1.913231000
H	-7.833940000	-1.536699000	-1.307430000
H	-9.775192000	0.431313000	-1.782922000
B	-9.108075000	-2.808772000	0.291110000
B	-10.163034000	-1.958176000	-0.870114000
C	-8.582858000	-1.409751000	-0.533647000
B	-9.779402000	-0.218346000	-0.793813000
B	-9.493773000	-2.228077000	1.914806000

H	-9.492391000	-2.874382000	2.906913000
B	-10.788396000	-2.454235000	0.706741000
H	-11.643259000	-3.249747000	0.901533000
C	-10.687101000	-1.035679000	1.653232000
H	-11.432952000	-0.902655000	2.428898000
B	-8.071597000	-1.594656000	1.085145000
H	-6.942742000	-1.850609000	1.334047000
B	-9.108639000	-0.487471000	1.993669000
H	-8.852302000	0.016418000	3.033464000
B	-11.201959000	-0.852680000	0.035875000
H	-12.329356000	-0.590625000	-0.213267000
B	-10.166975000	0.364329000	0.830483000
H	-10.606024000	1.428297000	1.105558000
B	-8.472212000	0.025960000	0.416416000
Cl	2.058891000	6.432257000	1.089320000
H	3.328899000	3.293567000	0.295618000
C	1.313270000	3.006779000	-0.318966000
C	3.043711000	4.186227000	-1.596602000
C	0.941946000	3.043438000	-1.813541000
H	1.486646000	1.998334000	0.060880000
H	0.575801000	3.510983000	0.308176000
C	1.729631000	4.241602000	-2.374051000
H	3.576434000	5.136558000	-1.533278000
H	3.711939000	3.406782000	-1.973122000
H	-0.136669000	3.148961000	-1.954737000
H	1.259279000	2.116257000	-2.304037000

H	1.211286000	5.180347000	-2.152040000
H	1.890026000	4.182618000	-3.453812000
N	2.599146000	3.803437000	-0.210093000
H	2.411142000	4.721785000	0.335933000

### TS1-DA



Atom	x	y	z
Pd	0.423242000	-0.153848000	0.052033000
P	2.896611000	-0.365403000	-0.067921000
C	3.440646000	-2.097285000	-0.416175000
C	4.515677000	-2.702305000	0.247803000
H	5.017482000	-2.187768000	1.060849000
C	4.945229000	-3.979119000	-0.124873000
H	5.776583000	-4.439750000	0.402039000

C	4.311278000	-4.658260000	-1.165812000
H	4.646636000	-5.650830000	-1.453981000
C	3.239184000	-4.058964000	-1.832894000
H	2.734032000	-4.584588000	-2.638534000
C	2.802974000	-2.789578000	-1.457320000
H	2.054879000	1.030177000	-2.474315000
C	3.841650000	0.515734000	-1.385668000
C	3.139512000	1.059050000	-2.470009000
H	1.954422000	-2.341835000	-1.966487000
C	3.823632000	1.633790000	-3.544221000
H	3.264029000	2.051061000	-4.376762000
C	5.218206000	1.672302000	-3.544834000
H	5.751562000	2.122385000	-4.377612000
C	5.928647000	1.118777000	-2.475486000
H	7.015102000	1.132704000	-2.476587000
C	5.247271000	0.534101000	-1.408292000
H	5.813756000	0.083075000	-0.599293000
C	3.657426000	0.051986000	1.555633000
C	4.537879000	1.125303000	1.754432000
H	4.859561000	1.734373000	0.917171000
C	5.008603000	1.425380000	3.035937000
H	5.690731000	2.259990000	3.172919000
C	4.606716000	0.660043000	4.130772000
H	4.975634000	0.894282000	5.125560000
C	3.722151000	-0.405906000	3.942567000
H	3.398318000	-1.003446000	4.790287000

C	3.243429000	-0.706011000	2.667718000
H	2.541328000	-1.524647000	2.532330000
H	-0.787529000	4.212098000	3.101203000
H	-2.615790000	4.533800000	0.780572000
H	-1.612047000	2.035718000	1.543767000
H	-1.948418000	2.496691000	-1.211540000
B	-0.385051000	4.047906000	1.998922000
B	-1.480137000	4.242417000	0.609213000
C	-0.900573000	2.706833000	1.078445000
B	-1.068101000	2.979461000	-0.588080000
B	1.264103000	4.330821000	1.443042000
H	2.132904000	4.853344000	2.056168000
B	-0.083164000	5.303998000	0.794436000
H	-0.111334000	6.474237000	0.978167000
C	1.090918000	4.613659000	-0.229592000
H	1.802184000	5.284377000	-0.698504000
B	0.696963000	2.665003000	1.651536000
H	1.013386000	1.954807000	2.544613000
B	1.668045000	3.081150000	0.238583000
H	2.805593000	2.821695000	0.063831000
B	-0.508991000	4.641802000	-0.807705000
H	-0.822077000	5.372046000	-1.686550000
B	0.572695000	3.262589000	-1.150572000
H	0.972015000	3.126636000	-2.256136000
B	0.292448000	1.963583000	0.039202000
C	-5.361319000	0.948368000	-3.420641000

C	-5.929827000	0.568238000	-2.163445000
C	-7.337496000	0.644612000	-1.988736000
C	-8.144232000	1.080614000	-3.017130000
C	-7.579772000	1.457635000	-4.261650000
C	-6.217082000	1.392768000	-4.460642000
N	-4.013847000	0.892319000	-3.654341000
C	-3.230308000	0.483975000	-2.684467000
C	-3.685031000	0.091807000	-1.385076000
C	-5.045426000	0.132829000	-1.146045000
C	-2.733094000	-0.354637000	-0.358148000
C	-1.464180000	-0.143599000	-0.197154000
H	-7.766286000	0.354912000	-1.032451000
H	-9.220016000	1.137535000	-2.877276000
H	-8.230164000	1.799591000	-5.061794000
H	-5.763493000	1.675572000	-5.405554000
H	-2.163792000	0.432350000	-2.901441000
H	-5.445215000	-0.154551000	-0.177646000
Cl	0.330264000	-2.501363000	0.989206000
H	-4.437452000	-1.227106000	2.374073000
C	-5.231902000	-2.855093000	1.343885000
C	-3.135950000	-2.845707000	2.482991000
C	-4.623420000	-4.277995000	1.224650000
H	-6.051171000	-2.842983000	2.076463000
H	-5.636304000	-2.491948000	0.393292000
C	-3.140097000	-4.114456000	1.628112000
H	-2.153465000	-2.366222000	2.517672000

H	-3.461511000	-3.065205000	3.513322000
H	-4.730899000	-4.684829000	0.214972000
H	-5.138556000	-4.962992000	1.906063000
H	-2.507252000	-3.955557000	0.749566000
H	-2.748436000	-4.980890000	2.168661000
N	-4.109316000	-1.984397000	1.777962000
H	-3.163140000	-1.026825000	0.465688000

### Int1-DA

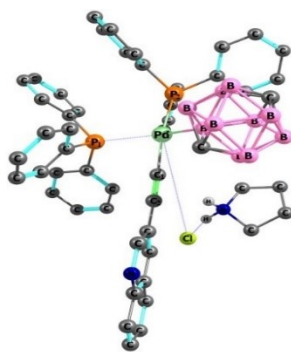


<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.462195000	-0.845118000	0.541678000
P	2.888732000	-1.015069000	0.903859000
C	3.528093000	-2.734948000	1.179002000
C	4.312312000	-3.097276000	2.280622000
C	4.833927000	-4.390970000	2.383184000
C	4.585131000	-5.331420000	1.384303000
C	3.806346000	-4.975244000	0.278810000
C	3.278251000	-3.689767000	0.180195000
C	4.107869000	-0.499884000	-0.385883000
C	3.653413000	-0.309421000	-1.697241000
C	4.553373000	-0.035876000	-2.730801000

C	5.919716000	0.051090000	-2.462970000
C	6.386115000	-0.154663000	-1.160945000
C	5.489456000	-0.440047000	-0.131627000
C	3.299123000	-0.125158000	2.465929000
C	4.182427000	0.959789000	2.553021000
C	4.371559000	1.623131000	3.769102000
C	3.684446000	1.211018000	4.910802000
C	2.795981000	0.134491000	4.832246000
C	2.596518000	-0.523737000	3.619302000
B	-0.560793000	3.775931000	0.952620000
B	-1.363558000	3.482255000	-0.607586000
C	-0.947344000	2.199367000	0.435537000
B	-0.784385000	1.907538000	-1.230004000
B	1.172662000	3.902045000	0.663980000
B	0.013921000	4.580890000	-0.509571000
C	1.332057000	3.623635000	-1.008762000
B	0.508886000	2.379556000	1.285544000
B	1.744418000	2.337249000	0.030602000
B	-0.126368000	3.423191000	-1.860656000
B	0.940803000	2.033209000	-1.523159000
B	0.387786000	1.170112000	-0.053506000
C	-6.920097000	-0.660076000	-0.362942000
C	-6.414404000	-0.416481000	0.954330000
C	-7.331940000	-0.151393000	2.007456000
C	-8.687574000	-0.129579000	1.763257000
C	-9.186345000	-0.371707000	0.458213000

C	-8.321092000	-0.631535000	-0.583174000
N	-6.091873000	-0.919365000	-1.421511000
C	-4.796872000	-0.939323000	-1.203815000
C	-4.171491000	-0.719336000	0.070069000
C	-5.012742000	-0.458133000	1.144025000
C	-2.749664000	-0.773838000	0.193523000
C	-1.520696000	-0.780152000	0.298014000
Cl	0.250462000	-3.170028000	1.814658000
H	-1.232394000	-3.814260000	0.623204000
C	-3.191500000	-4.664499000	0.553783000
C	-1.635728000	-4.521347000	-1.348477000
C	-3.164186000	-5.994744000	-0.203991000
H	-3.035241000	-4.746510000	1.630333000
H	-4.113475000	-4.109758000	0.366777000
C	-2.709778000	-5.583802000	-1.614856000
H	-1.558346000	-3.752321000	-2.118013000
H	-0.650063000	-4.964087000	-1.189939000
H	-4.141221000	-6.484575000	-0.192876000
H	-2.436938000	-6.676687000	0.251215000
H	-3.546415000	-5.148414000	-2.172871000
H	-2.312953000	-6.418480000	-2.198414000
N	-2.049175000	-3.874152000	-0.043109000
H	-2.291438000	-2.873922000	-0.160678000

TS2-DA



Atom	x	y	z
Pd	1.558339000	0.125539000	0.216736000
P	3.998774000	0.098971000	0.405039000
C	4.733702000	0.527243000	-1.240108000
C	6.124943000	0.518977000	-1.450106000
H	6.798366000	0.273613000	-0.634529000
C	6.654280000	0.800201000	-2.709460000
H	7.731403000	0.797784000	-2.852036000
C	5.804171000	1.067899000	-3.786777000
H	6.218867000	1.278706000	-4.768561000
C	4.421826000	1.045535000	-3.599766000
H	3.749858000	1.234037000	-4.432203000
C	3.891994000	0.776386000	-2.334297000
H	3.175528000	0.641944000	3.096073000
C	4.637406000	1.307306000	1.647232000
C	4.014636000	1.304812000	2.908182000
H	2.815129000	0.754415000	-2.202132000
C	4.467086000	2.143505000	3.927627000
H	3.979367000	2.121505000	4.898306000
C	5.536439000	3.011599000	3.696267000
H	5.886480000	3.669412000	4.486967000

C	6.145944000	3.037518000	2.441015000
H	6.967756000	3.721170000	2.247613000
C	5.703207000	2.190010000	1.422768000
H	6.182685000	2.235681000	0.452154000
C	4.995522000	-1.426967000	0.760658000
C	5.862664000	-1.535697000	1.856374000
H	5.951824000	-0.719695000	2.565358000
C	6.622953000	-2.693640000	2.045696000
H	7.291635000	-2.761060000	2.899575000
C	6.529495000	-3.752906000	1.142610000
H	7.124598000	-4.650141000	1.288627000
C	5.668113000	-3.652496000	0.046371000
H	5.589525000	-4.471389000	-0.663494000
C	4.905350000	-2.500414000	-0.140536000
H	4.241662000	-2.433488000	-0.998179000
H	-2.134085000	-3.684038000	2.242702000
H	-1.394421000	-1.851114000	4.466969000
H	-1.242156000	-1.070306000	1.775334000
H	0.726231000	-0.062648000	3.516329000
B	-1.003505000	-3.371807000	2.411531000
B	-0.560976000	-2.275768000	3.739422000
C	-0.491594000	-1.772106000	2.113516000
B	0.722578000	-1.184733000	3.133962000
B	0.410364000	-4.345282000	2.005865000
H	0.401705000	-5.478799000	1.658612000
B	0.057865000	-3.930385000	3.705578000

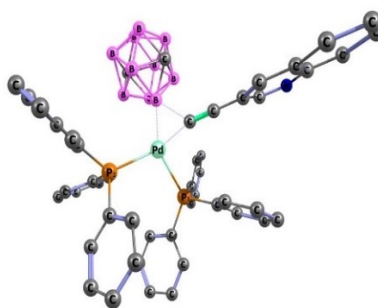
H	-0.180490000	-4.787032000	4.489024000
C	1.621824000	-3.766283000	3.049223000
H	2.378403000	-4.470502000	3.376920000
B	0.011068000	-2.944144000	1.002305000
H	-0.478347000	-3.022862000	-0.070293000
B	1.692284000	-3.251830000	1.413148000
H	2.524160000	-3.698943000	0.700950000
B	1.123970000	-2.575247000	4.159824000
H	1.596682000	-2.527348000	5.245696000
B	2.131083000	-2.166087000	2.747826000
H	3.259446000	-1.878745000	2.944329000
B	1.106895000	-1.566961000	1.405970000
C	-5.511547000	-0.021387000	-2.077637000
C	-4.497377000	0.003598000	-3.086647000
C	-4.879268000	0.026800000	-4.456009000
C	-6.212401000	0.028310000	-4.804215000
C	-7.217086000	0.006884000	-3.803563000
C	-6.875141000	-0.018051000	-2.467913000
N	-5.205979000	-0.048987000	-0.743062000
C	-3.938923000	-0.056300000	-0.398574000
C	-2.836022000	-0.033640000	-1.317474000
C	-3.143829000	0.002249000	-2.671781000
C	-1.494938000	-0.045963000	-0.823325000
C	-0.350236000	-0.018049000	-0.369543000
H	-4.101019000	0.037255000	-5.214955000
H	-6.500033000	0.045150000	-5.851831000

H	-8.263546000	0.009236000	-4.096406000
H	-7.628040000	-0.036015000	-1.685616000
H	-3.722266000	-0.077453000	0.669281000
H	-2.360695000	0.029137000	-3.426313000
P	1.335311000	2.742148000	-0.396956000
C	2.642916000	4.025068000	-0.073650000
C	3.698446000	4.158746000	-0.994256000
H	3.738516000	3.523229000	-1.873220000
C	4.689840000	5.121374000	-0.808162000
H	5.489014000	5.215724000	-1.538703000
C	4.653253000	5.963626000	0.306415000
H	5.423482000	6.716841000	0.448934000
C	3.617438000	5.832949000	1.231374000
H	3.574396000	6.485417000	2.099479000
C	2.618642000	4.873090000	1.043350000
H	1.812295000	4.801692000	1.765188000
C	-0.028131000	3.251155000	0.744064000
C	0.049651000	2.845870000	2.087843000
H	0.893088000	2.250234000	2.425611000
C	-0.950911000	3.192661000	2.996324000
H	-0.871283000	2.874533000	4.032371000
C	-2.056693000	3.933720000	2.570929000
H	-2.842163000	4.195307000	3.274594000
C	-2.149726000	4.329271000	1.235868000
H	-3.009370000	4.899513000	0.894427000
C	-1.141087000	3.995108000	0.327978000

H	-1.231202000	4.310876000	-0.705743000
C	0.772095000	3.250530000	-2.082151000
C	0.373322000	2.273556000	-3.006059000
H	0.368417000	1.228085000	-2.716962000
C	-0.040835000	2.631080000	-4.292494000
H	-0.337443000	1.848556000	-4.986078000
C	-0.063169000	3.975395000	-4.666582000
H	-0.382877000	4.256070000	-5.666659000
C	0.328576000	4.960283000	-3.755142000
H	0.312939000	6.008645000	-4.041576000
C	0.747624000	4.602151000	-2.473878000
H	1.061981000	5.375972000	-1.780455000
Cl	-0.686683000	-0.759637000	-5.627917000
H	-0.445015000	-1.773228000	-2.176834000
C	-1.208716000	-3.440066000	-3.250094000
C	1.113211000	-2.809189000	-3.157353000
C	-0.477741000	-4.628742000	-2.612191000
H	-2.178036000	-3.205952000	-2.808101000
H	-1.331170000	-3.554594000	-4.330066000
C	1.034333000	-4.271451000	-2.669852000
H	1.398048000	-2.734754000	-4.209224000
H	1.771047000	-2.171345000	-2.564872000
H	-0.706515000	-5.553122000	-3.148794000
H	-0.798797000	-4.762107000	-1.575992000
H	1.578902000	-4.923859000	-3.357462000
H	1.492584000	-4.377882000	-1.683471000

N	-0.286219000	-2.268362000	-3.068554000
H	-0.447444000	-1.581908000	-3.876888000

TS1-I



Atom	x	y	z
Cl	-0.168915000	-3.548686000	-2.268068000
Pd	0.353982000	-0.042268000	0.237773000
P	2.075986000	0.553326000	1.893343000
P	-1.058671000	0.820188000	-1.573293000
C	3.462100000	1.225240000	0.857343000
C	3.157174000	2.180754000	-0.129665000
H	2.125976000	2.465817000	-0.314133000
C	4.163050000	2.750739000	-0.910565000
H	3.903734000	3.492147000	-1.661150000
C	5.491226000	2.352248000	-0.744508000
H	6.274421000	2.789068000	-1.357555000

C	5.801339000	1.376340000	0.202812000
H	6.828082000	1.044182000	0.329070000
C	4.797572000	0.817988000	0.999132000
H	5.066572000	0.060995000	1.726190000
C	1.753987000	1.957956000	3.075398000
C	1.604456000	1.736130000	4.454317000
H	1.715686000	0.739415000	4.862986000
C	1.320838000	2.791954000	5.323691000
H	1.215570000	2.593099000	6.386724000
C	1.178376000	4.090311000	4.834668000
H	0.960279000	4.911362000	5.511759000
C	1.325774000	4.325286000	3.466162000
H	1.229720000	5.332859000	3.070675000
C	1.607499000	3.271095000	2.596373000
H	1.726733000	3.489957000	1.542413000
C	2.837197000	-0.732688000	2.973225000
C	2.342369000	-2.043685000	2.917077000
H	1.522112000	-2.280070000	2.248283000
C	2.889493000	-3.047162000	3.720068000
H	2.492312000	-4.056436000	3.662864000
C	3.937317000	-2.750711000	4.592150000
H	4.363834000	-3.530357000	5.217069000
C	4.432691000	-1.445574000	4.666217000
H	5.243191000	-1.206716000	5.349094000
C	3.884939000	-0.441780000	3.867524000
H	4.269057000	0.570472000	3.949538000

C	-0.178174000	0.800194000	-3.209343000
C	-0.299534000	-0.281503000	-4.096224000
H	-0.910695000	-1.140172000	-3.847847000
C	0.397471000	-0.283750000	-5.306761000
H	0.289417000	-1.130894000	-5.978020000
C	1.228331000	0.784518000	-5.649036000
H	1.765731000	0.779585000	-6.593362000
C	1.368489000	1.856847000	-4.765388000
H	2.016325000	2.692446000	-5.016554000
C	0.676123000	1.862721000	-3.553967000
H	0.795981000	2.707971000	-2.884956000
C	-2.730334000	0.124295000	-1.965259000
C	-2.839803000	-1.262810000	-2.177289000
H	-1.970199000	-1.917535000	-2.101346000
C	-4.077966000	-1.831868000	-2.484528000
H	-4.137612000	-2.903469000	-2.652891000
C	-5.222816000	-1.036853000	-2.563488000
H	-6.185503000	-1.483691000	-2.796420000
C	-5.124663000	0.335902000	-2.329570000
H	-6.010702000	0.963361000	-2.374991000
C	-3.889287000	0.915095000	-2.031068000
H	-3.842060000	1.981311000	-1.844151000
C	-1.328235000	2.635760000	-1.339009000
C	-1.846043000	3.431406000	-2.378662000
H	-2.097855000	2.982131000	-3.334267000
C	-2.030868000	4.802160000	-2.200021000

H	-2.434863000	5.399795000	-3.012402000
C	-1.693581000	5.404260000	-0.984241000
H	-1.836048000	6.472700000	-0.847563000
C	-1.170386000	4.627783000	0.049572000
H	-0.903640000	5.084901000	0.998366000
C	-0.989479000	3.253123000	-0.127282000
H	-0.587233000	2.653533000	0.682397000
H	-3.751076000	-3.026002000	2.180135000
H	-5.138458000	-0.472623000	1.541417000
H	-2.794219000	-1.260239000	0.251734000
H	-3.127896000	1.495460000	0.754362000
B	-3.260824000	-1.990071000	2.477828000
B	-4.091861000	-0.462319000	2.095631000
C	-2.670238000	-0.931968000	1.275811000
B	-2.849437000	0.722741000	1.602183000
B	-2.192996000	-1.703844000	3.850346000
H	-1.945396000	-2.466545000	4.722636000
B	-3.788184000	-0.910628000	3.774137000
H	-4.608753000	-1.148947000	4.595060000
C	-2.379924000	-0.041361000	4.181141000
H	-2.267396000	0.278877000	5.210907000
B	-1.509945000	-1.731995000	2.214007000
H	-0.869688000	-2.623703000	1.768078000
B	-0.968152000	-0.511521000	3.358438000
H	0.058292000	-0.518054000	3.937450000
B	-3.533707000	0.769241000	3.229809000

H	-4.186668000	1.645903000	3.687393000
B	-1.783428000	1.018357000	2.969383000
H	-1.306863000	2.055731000	3.280933000
B	-1.215777000	-0.038637000	1.650306000
H	1.144873000	-1.750747000	-1.700905000
C	2.653286000	-2.254496000	-0.483465000
C	2.818924000	-0.673147000	-2.223092000
C	3.487181000	-2.946113000	-1.569703000
H	3.300520000	-1.770919000	0.255486000
H	1.966877000	-2.932661000	0.026847000
C	3.860317000	-1.790035000	-2.524209000
H	2.258759000	-0.373872000	-3.106754000
H	3.310015000	0.211963000	-1.816153000
H	2.856485000	-3.679453000	-2.081060000
H	4.361851000	-3.464127000	-1.161627000
H	3.823943000	-2.104104000	-3.571835000
H	4.874352000	-1.424651000	-2.327244000
N	1.871836000	-1.212309000	-1.201490000

### Int1-I



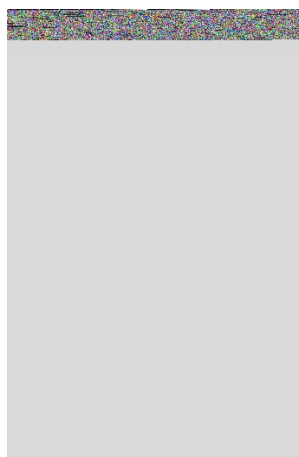
<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.318816000	-0.201273000	0.396722000
P	2.031376000	0.435276000	2.020047000
P	-1.110934000	0.514428000	-1.471979000
C	3.316133000	1.269968000	0.973551000
C	2.887399000	2.165173000	-0.022844000
H	1.825906000	2.333505000	-0.181463000
C	3.810902000	2.843285000	-0.820305000
H	3.459837000	3.539976000	-1.576608000
C	5.179529000	2.624161000	-0.647922000
H	5.899518000	3.147063000	-1.270705000
C	5.615594000	1.727281000	0.328744000
H	6.677585000	1.545972000	0.467815000
C	4.693261000	1.056263000	1.135283000
H	5.057586000	0.357322000	1.878780000
C	1.694514000	1.725945000	3.309623000
C	1.621058000	1.414312000	4.676603000
H	1.799612000	0.402468000	5.020055000
C	1.325425000	2.403200000	5.617897000
H	1.280971000	2.140405000	6.671048000
C	1.093819000	3.717354000	5.211642000
H	0.865886000	4.485384000	5.945016000
C	1.163836000	4.038927000	3.854295000
H	0.994584000	5.060331000	3.525156000
C	1.460016000	3.053801000	2.912443000
H	1.518605000	3.335548000	1.867129000

C	2.895300000	-0.920795000	2.911837000
C	2.523377000	-2.245558000	2.633714000
H	1.721360000	-2.440671000	1.928318000
C	3.162773000	-3.313556000	3.266882000
H	2.859450000	-4.332287000	3.043355000
C	4.180485000	-3.070059000	4.190275000
H	4.676818000	-3.899440000	4.685720000
C	4.553664000	-1.755578000	4.483560000
H	5.339590000	-1.559735000	5.207169000
C	3.915688000	-0.686996000	3.852885000
H	4.207698000	0.327715000	4.104991000
C	-0.223387000	0.368726000	-3.099227000
C	-0.676876000	-0.430065000	-4.159763000
H	-1.603516000	-0.985350000	-4.073424000
C	0.047760000	-0.503860000	-5.353510000
H	-0.324792000	-1.122730000	-6.164786000
C	1.232434000	0.215611000	-5.508086000
H	1.791052000	0.156992000	-6.437562000
C	1.691333000	1.020152000	-4.461206000
H	2.607166000	1.593630000	-4.572261000
C	0.971059000	1.096233000	-3.268941000
H	1.338240000	1.735179000	-2.471350000
C	-2.761539000	-0.230922000	-1.820612000
C	-2.850539000	-1.629011000	-1.967693000
H	-1.961721000	-2.247619000	-1.871497000
C	-4.076736000	-2.240667000	-2.229647000

H	-4.125844000	-3.319324000	-2.346486000
C	-5.236641000	-1.467337000	-2.329930000
H	-6.192947000	-1.943036000	-2.526080000
C	-5.161450000	-0.083563000	-2.168416000
H	-6.059746000	0.523061000	-2.236519000
C	-3.933274000	0.533950000	-1.916610000
H	-3.896059000	1.610425000	-1.793568000
C	-1.377152000	2.338569000	-1.385558000
C	-1.778948000	3.054264000	-2.528547000
H	-1.942195000	2.535987000	-3.468679000
C	-1.965922000	4.434809000	-2.467234000
H	-2.279899000	4.974494000	-3.356013000
C	-1.744790000	5.121217000	-1.269543000
H	-1.887068000	6.197177000	-1.225574000
C	-1.336837000	4.421402000	-0.133523000
H	-1.160299000	4.947969000	0.800003000
C	-1.153946000	3.037246000	-0.190007000
H	-0.837562000	2.498679000	0.696706000
H	-2.844691000	-1.441955000	0.435639000
B	-3.264057000	-2.208069000	2.655755000
B	-4.096955000	-0.670657000	2.315787000
C	-2.693827000	-1.131607000	1.460476000
B	-2.859653000	0.518190000	1.814062000
B	-2.165952000	-1.950067000	4.010261000
B	-3.759184000	-1.148390000	3.980045000
C	-2.338192000	-0.292439000	4.371113000

H	-2.203734000	0.010305000	5.403552000
B	-1.517591000	-1.952320000	2.360173000
B	-0.944243000	-0.755745000	3.512926000
B	-3.510044000	0.540166000	3.457584000
B	-1.764128000	0.786742000	3.167550000
B	-1.232036000	-0.249287000	1.823783000
C	1.295681000	-2.630027000	-1.387900000
C	3.318035000	-1.489240000	-0.982503000
C	2.421387000	-3.469745000	-2.056683000
H	0.993151000	-3.069350000	-0.432540000
H	0.402852000	-2.535974000	-2.010396000
C	3.659899000	-2.541362000	-2.047127000
H	3.852186000	-0.545844000	-1.100427000
H	3.514345000	-1.874292000	0.022980000
H	2.150721000	-3.773977000	-3.071719000
H	2.606577000	-4.382345000	-1.481854000
H	3.783435000	-2.053883000	-3.021471000
H	4.588879000	-3.074796000	-1.824590000
N	1.853044000	-1.267263000	-1.124219000

In1-RE2



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	0.702087000	1.104661000	-1.214817000
P	2.634564000	0.351679000	0.103898000
C	3.203773000	-1.391616000	-0.226690000
C	2.864920000	-2.475676000	0.595995000
H	2.271376000	-2.319855000	1.490147000
C	3.295329000	-3.768925000	0.283752000
H	3.026644000	-4.593627000	0.938418000
C	4.069983000	-3.999940000	-0.853282000
H	4.405706000	-5.005058000	-1.092751000
C	4.419162000	-2.926264000	-1.676958000
H	5.031980000	-3.090526000	-2.559151000
C	3.991417000	-1.635185000	-1.365682000
H	3.414702000	2.555616000	-1.608776000
C	4.238945000	1.232731000	-0.124763000
C	4.310275000	2.262922000	-1.071868000
H	4.291234000	-0.809884000	-2.004985000

C	5.522540000	2.908313000	-1.332981000
H	5.559015000	3.705472000	-2.070158000
C	6.677868000	2.527518000	-0.650800000
H	7.620463000	3.029689000	-0.850553000
C	6.623767000	1.485217000	0.280249000
H	7.524285000	1.171388000	0.800939000
C	5.417376000	0.833704000	0.533186000
H	5.399882000	0.000574000	1.229250000
C	2.253140000	0.304042000	1.911709000
C	3.115321000	0.752967000	2.922246000
H	4.073184000	1.193649000	2.671054000
C	2.742919000	0.658776000	4.265312000
H	3.420372000	1.019546000	5.034398000
C	1.509892000	0.108678000	4.619205000
H	1.224422000	0.034695000	5.664818000
C	0.638976000	-0.333089000	3.620847000
H	-0.330095000	-0.747919000	3.883747000
C	1.002206000	-0.223634000	2.277761000
H	0.302962000	-0.540431000	1.507720000
H	-2.254510000	4.611589000	1.997478000
H	-2.117916000	5.977057000	-0.637951000
H	-1.908004000	3.196795000	-0.403128000
H	-0.351513000	4.427038000	-2.393433000
B	-1.234698000	4.644158000	1.393770000
B	-1.152110000	5.461604000	-0.183471000
C	-1.053760000	3.763420000	-0.055832000

B	-0.087415000	4.491096000	-1.243657000
B	0.383249000	4.639228000	2.095786000
H	0.649991000	4.748920000	3.245800000
B	-0.194221000	6.053671000	1.175686000
H	-0.309114000	7.104810000	1.711734000
C	1.348051000	5.381947000	0.907098000
H	2.207755000	5.950016000	1.244736000
B	-0.219134000	3.175146000	1.297749000
H	-0.587702000	2.209717000	1.874287000
B	1.446388000	3.684198000	1.030182000
H	2.420890000	3.203707000	1.496042000
B	0.513689000	5.958049000	-0.459911000
H	0.869727000	6.946032000	-1.010146000
B	1.524532000	4.490552000	-0.548574000
H	2.547137000	4.565729000	-1.139297000
B	0.510162000	3.021504000	-0.344899000
C	-5.327681000	2.455797000	-5.310645000
C	-5.473514000	1.523038000	-4.234687000
C	-6.731052000	0.890644000	-4.035922000
C	-7.793927000	1.171660000	-4.866419000
C	-7.647578000	2.095986000	-5.931397000
C	-6.439921000	2.724718000	-6.148922000
N	-4.145399000	3.099920000	-5.558083000
C	-3.124250000	2.843069000	-4.773406000
C	-3.146920000	1.929825000	-3.665030000
C	-4.345809000	1.276286000	-3.415908000

C	-1.973565000	1.730548000	-2.879661000
C	-0.945670000	1.606812000	-2.215463000
H	-6.839439000	0.183186000	-3.217148000
H	-8.751974000	0.684447000	-4.707076000
H	-8.495347000	2.307251000	-6.577286000
H	-6.304381000	3.436312000	-6.957860000
H	-2.194091000	3.368180000	-4.987717000
H	-4.423391000	0.574568000	-2.589313000
H	-0.487525000	-0.525031000	-2.843362000
C	1.278295000	-1.102130000	-3.677439000
C	0.139268000	-2.231837000	-1.942511000
C	0.977491000	-2.538014000	-4.199563000
H	1.084376000	-0.317703000	-4.413461000
H	2.319805000	-1.018418000	-3.361444000
C	-0.028403000	-3.129499000	-3.180064000
H	1.000624000	-2.543939000	-1.347449000
H	-0.738809000	-2.200897000	-1.290875000
H	1.898419000	-3.129420000	-4.229743000
H	0.564925000	-2.525602000	-5.212776000
H	0.160007000	-4.185478000	-2.961887000
H	-1.053590000	-3.048026000	-3.560730000
N	0.402753000	-0.880211000	-2.492865000

## TS1-RE2



Atom	x	y	z
Pd	0.458548000	1.017737000	-1.187826000
P	2.465797000	0.315004000	0.050021000
C	2.971237000	-1.463538000	-0.152471000
C	2.634616000	-2.455838000	0.779794000
H	2.115434000	-2.190381000	1.694951000
C	2.969720000	-3.793637000	0.549425000
H	2.703882000	-4.546070000	1.287195000
C	3.648222000	-4.161104000	-0.613301000
H	3.911328000	-5.200539000	-0.788949000
C	3.992644000	-3.180209000	-1.547379000
H	4.528120000	-3.452206000	-2.453134000
C	3.655373000	-1.845610000	-1.320077000
H	3.045693000	2.635687000	-1.579387000
C	4.050343000	1.170652000	-0.363514000
C	4.004009000	2.293160000	-1.202453000
H	3.942044000	-1.094418000	-2.050795000
C	5.176256000	2.964042000	-1.561694000
H	5.121811000	3.831124000	-2.214216000

C	6.410386000	2.516641000	-1.088722000
H	7.323080000	3.035897000	-1.368256000
C	6.471202000	1.390011000	-0.262785000
H	7.430627000	1.030016000	0.098820000
C	5.301707000	0.717718000	0.092605000
H	5.365351000	-0.170720000	0.714059000
C	2.263049000	0.468151000	1.883919000
C	3.267837000	0.911002000	2.756552000
H	4.237282000	1.205451000	2.370037000
C	3.028353000	0.994564000	4.130261000
H	3.815944000	1.347211000	4.790807000
C	1.786597000	0.629331000	4.653384000
H	1.603597000	0.693948000	5.722421000
C	0.776513000	0.192028000	3.793526000
H	-0.197759000	-0.082140000	4.188749000
C	1.009275000	0.124117000	2.418915000
H	0.207588000	-0.186270000	1.753324000
H	-2.631041000	4.758255000	1.993579000
H	-2.741336000	6.137882000	-0.636468000
H	-2.640206000	3.356888000	-0.419549000
H	-1.273143000	4.550249000	-2.589754000
B	-1.687126000	4.752139000	1.276752000
B	-1.751896000	5.581849000	-0.294978000
C	-1.720663000	3.877405000	-0.185496000
B	-0.866663000	4.579859000	-1.480691000
B	-0.001176000	4.671776000	1.780611000

H	0.404668000	4.752876000	2.891230000
B	-0.617850000	6.118872000	0.942910000
H	-0.625900000	7.169639000	1.491078000
C	0.848995000	5.381696000	0.490720000
H	1.769411000	5.905255000	0.724585000
B	-0.757499000	3.240021000	1.051911000
H	-1.098338000	2.282945000	1.659794000
B	0.885451000	3.679769000	0.593407000
H	1.886569000	3.169138000	0.955107000
B	-0.107876000	6.005021000	-0.764536000
H	0.220030000	6.981419000	-1.351185000
B	0.812475000	4.487993000	-0.983345000
H	1.759276000	4.510660000	-1.695097000
B	-0.242421000	3.059184000	-0.682315000
C	-5.761609000	2.175667000	-4.856423000
C	-4.915388000	1.061444000	-5.159151000
C	-5.318763000	0.142057000	-6.165727000
C	-6.507517000	0.320865000	-6.838695000
C	-7.344493000	1.424816000	-6.536727000
C	-6.979294000	2.333457000	-5.566274000
N	-5.432396000	3.097638000	-3.900207000
C	-4.304515000	2.938954000	-3.247829000
C	-3.376670000	1.861364000	-3.455122000
C	-3.710876000	0.929258000	-4.429176000
C	-2.184066000	1.778067000	-2.680136000
C	-1.167006000	1.784808000	-1.979991000

H	-4.674226000	-0.703544000	-6.393884000
H	-6.809301000	-0.386352000	-7.606310000
H	-8.278763000	1.551314000	-7.076638000
H	-7.603811000	3.186388000	-5.318521000
H	-4.066536000	3.690990000	-2.496994000
H	-3.048556000	0.091903000	-4.633816000
H	-0.865910000	-0.605736000	-2.779349000
C	0.828039000	-1.248431000	-3.710370000
C	-0.214593000	-2.350212000	-1.930358000
C	0.230782000	-2.523037000	-4.346179000
H	0.801544000	-0.370446000	-4.361495000
H	1.865403000	-1.420340000	-3.406890000
C	-0.354832000	-3.313820000	-3.141599000
H	0.647107000	-2.625183000	-1.316902000
H	-1.096285000	-2.326957000	-1.283738000
H	0.980389000	-3.094841000	-4.902569000
H	-0.563283000	-2.254036000	-5.052091000
H	0.187073000	-4.247739000	-2.961915000
H	-1.402720000	-3.576581000	-3.318880000
N	0.030402000	-0.998624000	-2.488842000

Int2-RE2



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	2.700852000	-1.306725000	0.017222000
P	0.823429000	-2.646671000	-0.373900000
P	4.728294000	-0.238066000	0.410274000
C	0.799656000	-4.162445000	0.686744000
C	1.291689000	-4.047556000	1.997810000
H	1.689532000	-3.093064000	2.334136000
C	1.287243000	-5.145988000	2.858059000
H	1.670277000	-5.040426000	3.869558000
C	0.805188000	-6.380369000	2.414840000
H	0.810146000	-7.239075000	3.080845000
C	0.325510000	-6.508859000	1.109841000
H	-0.044696000	-7.467838000	0.756856000
C	0.320085000	-5.407121000	0.250464000
H	-0.053711000	-5.521219000	-0.762535000
C	-0.850853000	-1.906537000	-0.102778000
C	-1.919674000	-2.599007000	0.486253000
H	-1.784649000	-3.622095000	0.823155000
C	-3.162387000	-1.979947000	0.647182000
H	-3.979708000	-2.528025000	1.108936000
C	-3.356003000	-0.665782000	0.218170000
H	-4.324402000	-0.187855000	0.340070000
C	-2.296218000	0.033775000	-0.366459000
H	-2.438178000	1.060081000	-0.693942000
C	-1.052375000	-0.579150000	-0.516933000
H	-0.224450000	-0.028115000	-0.956767000

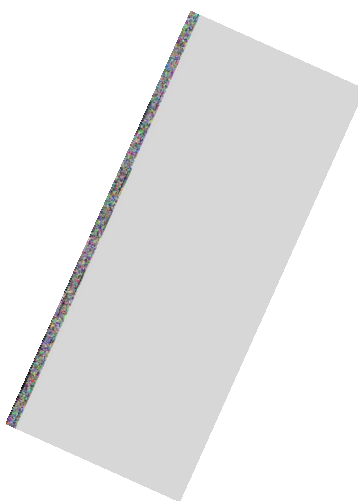
C	0.711412000	-3.317781000	-2.094895000
C	1.913970000	-3.564144000	-2.778377000
H	2.857891000	-3.332464000	-2.290378000
C	1.902723000	-4.086581000	-4.072131000
H	2.841558000	-4.272843000	-4.586906000
C	0.687885000	-4.356273000	-4.707793000
H	0.677681000	-4.754458000	-5.718888000
C	-0.513401000	-4.103716000	-4.042333000
H	-1.461705000	-4.305273000	-4.533640000
C	-0.503401000	-3.589275000	-2.743251000
H	-1.444501000	-3.394438000	-2.237816000
C	5.959597000	-1.262140000	1.336214000
C	5.971581000	-2.644255000	1.083001000
H	5.250847000	-3.063098000	0.384897000
C	6.885424000	-3.476995000	1.729006000
H	6.882898000	-4.543658000	1.521410000
C	7.790140000	-2.942880000	2.650456000
H	8.495770000	-3.592332000	3.161473000
C	7.777212000	-1.573172000	2.919953000
H	8.472566000	-1.152481000	3.641506000
C	6.869160000	-0.735902000	2.266332000
H	6.867830000	0.326532000	2.490223000
C	5.653627000	0.269415000	-1.110983000
C	7.052268000	0.373054000	-1.172343000
H	7.653856000	0.129866000	-0.301419000
C	7.682338000	0.775606000	-2.352518000

H	8.766102000	0.848393000	-2.385843000
C	6.925278000	1.077697000	-3.486590000
H	7.418106000	1.386584000	-4.404394000
C	5.533280000	0.965911000	-3.441142000
H	4.939526000	1.179246000	-4.326104000
C	4.903363000	0.557320000	-2.263708000
H	3.822929000	0.433167000	-2.234492000
C	4.646042000	1.325108000	1.404881000
C	5.505820000	2.423136000	1.221810000
H	6.276287000	2.388824000	0.457420000
C	5.372743000	3.570019000	2.012596000
H	6.034576000	4.416054000	1.850368000
C	4.383238000	3.636433000	2.996731000
H	4.266743000	4.536814000	3.591253000
C	3.526601000	2.548868000	3.190369000
H	2.747995000	2.598107000	3.946249000
C	3.651579000	1.406921000	2.396845000
H	2.967282000	0.572232000	2.529964000
C	-3.570728000	4.756309000	-0.876625000
C	-3.537190000	4.139336000	0.416452000
C	-2.512575000	4.501990000	1.333584000
C	-1.559573000	5.432505000	0.981715000
C	-1.595162000	6.042919000	-0.299297000
C	-2.579003000	5.715518000	-1.208307000
N	-4.526684000	4.448446000	-1.807040000
C	-5.434343000	3.553669000	-1.493114000

C	-5.494996000	2.868109000	-0.235831000
C	-4.532877000	3.180514000	0.713985000
C	-6.509924000	1.896676000	0.000437000
C	-7.379059000	1.061936000	0.182121000
H	-2.494745000	4.030923000	2.313589000
H	-0.761556000	5.707195000	1.664978000
H	-0.828484000	6.770779000	-0.547332000
H	-2.626713000	6.174352000	-2.191241000
H	-6.184879000	3.323864000	-2.248092000
H	-4.539099000	2.689517000	1.683265000
H	-8.662559000	-3.871207000	0.017382000
H	-10.417118000	-2.457480000	-1.913231000
H	-7.833940000	-1.536699000	-1.307430000
H	-9.775192000	0.431313000	-1.782922000
B	-9.108075000	-2.808772000	0.291110000
B	-10.163034000	-1.958176000	-0.870114000
C	-8.582858000	-1.409751000	-0.533647000
B	-9.779402000	-0.218346000	-0.793813000
B	-9.493773000	-2.228077000	1.914806000
H	-9.492391000	-2.874382000	2.906913000
B	-10.788396000	-2.454235000	0.706741000
H	-11.643259000	-3.249747000	0.901533000
C	-10.687101000	-1.035679000	1.653232000
H	-11.432952000	-0.902655000	2.428898000
B	-8.071597000	-1.594656000	1.085145000
H	-6.942742000	-1.850609000	1.334047000

B	-9.108639000	-0.487471000	1.993669000
H	-8.852302000	0.016418000	3.033464000
B	-11.201959000	-0.852680000	0.035875000
H	-12.329356000	-0.590625000	-0.213267000
B	-10.166975000	0.364329000	0.830483000
H	-10.606024000	1.428297000	1.105558000
B	-8.472212000	0.025960000	0.416416000
Cl	2.058891000	6.432257000	1.089320000
H	3.328899000	3.293567000	0.295618000
C	1.313270000	3.006779000	-0.318966000
C	3.043711000	4.186227000	-1.596602000
C	0.941946000	3.043438000	-1.813541000
H	1.486646000	1.998334000	0.060880000
H	0.575801000	3.510983000	0.308176000
C	1.729631000	4.241602000	-2.374051000
H	3.576434000	5.136558000	-1.533278000
H	3.711939000	3.406782000	-1.973122000
H	-0.136669000	3.148961000	-1.954737000
H	1.259279000	2.116257000	-2.304037000
H	1.211286000	5.180347000	-2.152040000
H	1.890026000	4.182618000	-3.453812000
N	2.599146000	3.803437000	-0.210093000
H	2.411142000	4.721785000	0.335933000

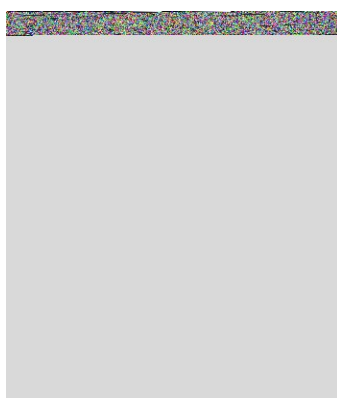
### 3-quinolyethynyl magnesium bromide



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
C	-2.947818000	0.749374000	-0.000015000
C	-2.518262000	-0.616641000	0.000137000
C	-3.495331000	-1.648778000	0.000062000
C	-4.837341000	-1.338336000	-0.000204000
C	-5.260752000	0.014723000	-0.000403000
C	-4.336460000	1.037341000	-0.000301000

N	-2.061170000	1.792113000	0.000084000
C	-0.778864000	1.513839000	0.000236000
C	-0.230956000	0.187691000	0.000327000
C	-1.126424000	-0.871307000	0.000299000
C	1.182871000	0.008976000	0.000328000
C	2.405913000	-0.105406000	0.000309000
H	-3.165729000	-2.684929000	0.000226000
H	-5.579158000	-2.131986000	-0.000263000
H	-6.323060000	0.242482000	-0.000646000
H	-4.637402000	2.080387000	-0.000434000
H	-0.090271000	2.357795000	0.000343000
H	-0.763881000	-1.895676000	0.000405000
Mg	4.434598000	-0.135932000	-0.000024000
Cl	6.672533000	-0.145326000	-0.000270000

### Monomeric MgCl<sub>2</sub> (Int3-K)



Atom	x	y	z
Pd	-0.740052000	0.759982000	-0.036383000
P	0.250188000	-1.865737000	0.409769000

P	-3.144366000	0.332603000	0.130460000
C	-0.632201000	-3.202942000	1.353983000
C	-1.615888000	-3.948073000	0.678865000
H	-1.823993000	-3.752456000	-0.368372000
C	-2.327581000	-4.949898000	1.338269000
H	-3.080204000	-5.515179000	0.795896000
C	-2.080362000	-5.220092000	2.686637000
H	-2.637282000	-5.999392000	3.199631000
C	-1.111075000	-4.483227000	3.368463000
H	-0.903012000	-4.689701000	4.415015000
C	-0.389967000	-3.483917000	2.708264000
H	0.369324000	-2.934090000	3.253373000
C	1.003873000	-2.843919000	-0.963909000
C	1.553852000	-4.121980000	-0.756119000
H	1.540205000	-4.565046000	0.235324000
C	2.113350000	-4.832996000	-1.817852000
H	2.536276000	-5.818524000	-1.642392000
C	2.123168000	-4.283364000	-3.103682000
H	2.553565000	-4.841664000	-3.930677000
C	1.566604000	-3.022550000	-3.322993000
H	1.551171000	-2.593124000	-4.320873000
C	1.008836000	-2.306462000	-2.259046000
H	0.563779000	-1.336598000	-2.452531000
C	1.662223000	-1.443048000	1.528163000
C	1.390470000	-0.628433000	2.642610000
H	0.375687000	-0.284036000	2.826704000

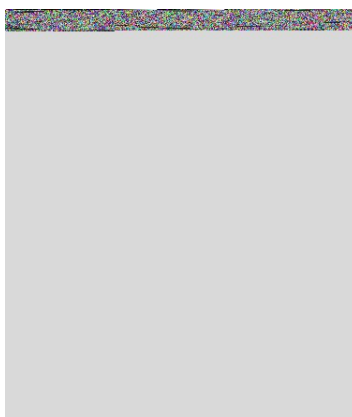
C	2.409525000	-0.251872000	3.518513000
H	2.177641000	0.368036000	4.380507000
C	3.724447000	-0.663262000	3.280997000
H	4.520943000	-0.362449000	3.955769000
C	4.007263000	-1.457871000	2.169788000
H	5.026994000	-1.778010000	1.973815000
C	2.983861000	-1.849818000	1.301351000
H	3.223917000	-2.469853000	0.444502000
C	-3.855646000	0.170253000	1.823352000
C	-4.819953000	1.046919000	2.340933000
H	-5.224833000	1.841211000	1.724094000
C	-5.270833000	0.907652000	3.656644000
H	-6.017475000	1.596900000	4.041114000
C	-4.768747000	-0.108279000	4.470063000
H	-5.122432000	-0.215596000	5.491675000
C	-3.807811000	-0.987545000	3.963045000
H	-3.411070000	-1.785377000	4.584672000
C	-3.349227000	-0.845803000	2.653839000
H	-2.602997000	-1.539040000	2.278153000
C	-4.253875000	1.476376000	-0.804602000
C	-5.644002000	1.267105000	-0.841475000
H	-6.090723000	0.456738000	-0.273300000
C	-6.461488000	2.090270000	-1.614814000
H	-7.534602000	1.920962000	-1.629563000
C	-5.902103000	3.121213000	-2.376041000
H	-6.540393000	3.757267000	-2.982940000

C	-4.522046000	3.323594000	-2.361665000
H	-4.076469000	4.114878000	-2.957601000
C	-3.703426000	2.505067000	-1.579363000
H	-2.631840000	2.668437000	-1.570642000
C	-3.573909000	-1.263802000	-0.702034000
C	-4.554930000	-2.139775000	-0.214851000
H	-5.041880000	-1.943982000	0.734800000
C	-4.910431000	-3.275714000	-0.946647000
H	-5.673306000	-3.945589000	-0.559041000
C	-4.291276000	-3.548851000	-2.168106000
H	-4.571021000	-4.431965000	-2.736027000
C	-3.313785000	-2.678915000	-2.659404000
H	-2.828961000	-2.878679000	-3.610805000
C	-2.955940000	-1.542367000	-1.932198000
H	-2.205291000	-0.869168000	-2.337299000
C	6.280822000	1.650233000	-2.338549000
C	5.597445000	0.439881000	-2.684318000
C	6.283518000	-0.557261000	-3.429179000
C	7.591038000	-0.360477000	-3.814384000
C	8.266700000	0.838238000	-3.471677000
C	7.627161000	1.822960000	-2.749343000
N	5.678955000	2.651104000	-1.624873000
C	4.431062000	2.485234000	-1.253847000
C	3.651595000	1.315759000	-1.538395000
C	4.256413000	0.296184000	-2.259147000
C	2.300512000	1.221395000	-1.077455000

C	1.147057000	1.133632000	-0.645429000
H	5.758749000	-1.472944000	-3.689776000
H	8.111138000	-1.124377000	-4.385220000
H	9.297623000	0.977917000	-3.784591000
H	8.125782000	2.748243000	-2.478170000
H	3.968842000	3.295827000	-0.693180000
H	3.704620000	-0.609397000	-2.497163000
H	2.061207000	4.891431000	2.530801000
H	0.394798000	3.466085000	4.537188000
H	1.238249000	2.239752000	2.163248000
H	-1.318878000	1.554793000	3.119492000
B	0.934286000	4.621228000	2.285339000
B	-0.062711000	3.766657000	3.486095000
C	0.466766000	2.993119000	2.055463000
B	-1.092881000	2.599494000	2.609684000
B	-0.140350000	5.520586000	1.213443000
H	0.080852000	6.578351000	0.729599000
B	-0.501981000	5.394227000	2.957473000
H	-0.520558000	6.368769000	3.630828000
C	-1.698870000	5.130714000	1.775083000
H	-2.471195000	5.883945000	1.666694000
B	0.519147000	3.975892000	0.672799000
H	1.380834000	3.880203000	-0.124251000
B	-1.167984000	4.349663000	0.340208000
H	-1.630793000	4.669320000	-0.700227000
B	-1.755630000	4.145117000	3.164003000

H	-2.610706000	4.283177000	3.972305000
B	-2.166888000	3.511293000	1.550122000
H	-3.296923000	3.270853000	1.311427000
B	-0.748694000	2.690591000	0.844911000
Mg	0.384317000	2.011617000	-2.630741000
Cl	-0.633214000	0.515398000	-4.066235000
Cl	0.841539000	4.138132000	-3.345187000

### Dimeric MgCl<sub>2</sub> (Int3-K)



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	-0.822045000	0.737503000	-0.156585000
P	0.202661000	-1.900737000	0.254848000
P	-3.213718000	0.298326000	0.167830000
C	-0.647728000	-3.147889000	1.335711000
C	-1.721108000	-3.887306000	0.806534000
H	-2.011617000	-3.759691000	-0.231101000
C	-2.416403000	-4.801163000	1.598688000

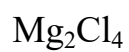
H	-3.237932000	-5.364807000	1.165801000
C	-2.065086000	-4.984411000	2.938269000
H	-2.609834000	-5.693809000	3.555114000
C	-1.006829000	-4.251002000	3.476934000
H	-0.717966000	-4.389923000	4.515369000
C	-0.300927000	-3.342852000	2.682934000
H	0.526277000	-2.793413000	3.118593000
C	0.788868000	-2.934672000	-1.163780000
C	0.959771000	-4.326954000	-1.083585000
H	0.719714000	-4.853199000	-0.165581000
C	1.434507000	-5.048083000	-2.181600000
H	1.556444000	-6.125076000	-2.103588000
C	1.755548000	-4.390679000	-3.371050000
H	2.126294000	-4.953004000	-4.223438000
C	1.597810000	-3.005575000	-3.459610000
H	1.856829000	-2.481508000	-4.375365000
C	1.109675000	-2.285472000	-2.367058000
H	0.991949000	-1.210062000	-2.445495000
C	1.755384000	-1.557397000	1.204241000
C	1.706190000	-0.599336000	2.231547000
H	0.775464000	-0.078492000	2.439233000
C	2.839413000	-0.308893000	2.992857000
H	2.779766000	0.428336000	3.789054000
C	4.047419000	-0.958887000	2.725478000
H	4.933293000	-0.726455000	3.309807000
C	4.109489000	-1.905769000	1.702260000

H	5.044907000	-2.415314000	1.487376000
C	2.971122000	-2.207913000	0.949313000
H	3.035910000	-2.952659000	0.162804000
C	-3.855408000	0.162511000	1.893568000
C	-4.857012000	0.993891000	2.415713000
H	-5.321916000	1.748890000	1.791952000
C	-5.265818000	0.862223000	3.745586000
H	-6.041458000	1.516812000	4.133229000
C	-4.684204000	-0.101603000	4.569579000
H	-5.005180000	-0.203177000	5.602542000
C	-3.685006000	-0.934525000	4.058976000
H	-3.224769000	-1.690604000	4.688840000
C	-3.268544000	-0.799273000	2.734862000
H	-2.490730000	-1.454728000	2.356691000
C	-4.363472000	1.427397000	-0.736500000
C	-5.753402000	1.209917000	-0.730067000
H	-6.177940000	0.394744000	-0.151960000
C	-6.599954000	2.030774000	-1.473628000
H	-7.671998000	1.855135000	-1.454784000
C	-6.070940000	3.067895000	-2.248464000
H	-6.732156000	3.702890000	-2.831546000
C	-4.692296000	3.275395000	-2.280504000
H	-4.270050000	4.068717000	-2.890528000
C	-3.843440000	2.458114000	-1.529068000
H	-2.772225000	2.616846000	-1.566563000
C	-3.694743000	-1.314674000	-0.606353000

C	-4.665826000	-2.164156000	-0.056117000
H	-5.111690000	-1.934906000	0.906084000
C	-5.064066000	-3.316686000	-0.738379000
H	-5.819583000	-3.963836000	-0.301001000
C	-4.496973000	-3.636124000	-1.973653000
H	-4.809101000	-4.532350000	-2.502552000
C	-3.528861000	-2.794728000	-2.528991000
H	-3.084958000	-3.032364000	-3.491782000
C	-3.130464000	-1.641707000	-1.850518000
H	-2.389290000	-0.988582000	-2.301219000
C	6.287459000	1.919813000	-1.957658000
C	5.760446000	0.601603000	-2.148669000
C	6.627913000	-0.438243000	-2.580456000
C	7.960677000	-0.180110000	-2.811885000
C	8.481532000	1.125122000	-2.621660000
C	7.664397000	2.153737000	-2.203783000
N	5.507622000	2.966469000	-1.546196000
C	4.233823000	2.741554000	-1.323288000
C	3.600088000	1.464505000	-1.476643000
C	4.384742000	0.399406000	-1.894183000
C	2.208305000	1.311203000	-1.181731000
C	1.021775000	1.167958000	-0.863541000
H	6.221121000	-1.435744000	-2.726466000
H	8.619973000	-0.977087000	-3.143568000
H	9.535101000	1.311691000	-2.809746000
H	8.043020000	3.159978000	-2.054276000

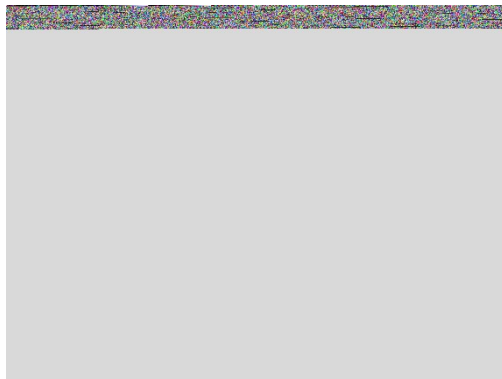
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H	3.946539000	-0.585294000	-2.027953000
H	2.090896000	4.996792000	2.092677000
H	0.788567000	3.430710000	4.259168000
H	1.375489000	2.312277000	1.756345000
H	-0.992245000	1.452487000	3.019696000
B	0.958182000	4.665687000	1.990089000
B	0.179670000	3.727028000	3.286602000
C	0.555078000	3.019343000	1.777627000
B	-0.891981000	2.521022000	2.517871000
B	-0.299642000	5.522915000	1.098578000
H	-0.204153000	6.602499000	0.621637000
B	-0.416826000	5.336515000	2.869499000
H	-0.400790000	6.293518000	3.567650000
C	-1.744821000	5.029219000	1.847299000
H	-2.565038000	5.738193000	1.864709000
B	0.365936000	4.032217000	0.427311000
H	1.117075000	4.006464000	-0.479217000
B	-1.366169000	4.313208000	0.331673000
H	-1.977844000	4.633094000	-0.628093000
B	-1.559841000	4.009677000	3.201421000
H	-2.305852000	4.078996000	4.119141000
B	-2.147665000	3.391974000	1.635736000
H	-3.283434000	3.090595000	1.538473000
B	-0.792585000	2.668811000	0.728312000
Mg	-0.117171000	0.094711000	-5.787003000

Mg	0.547013000	2.000697000	-3.007180000
Cl	1.903649000	0.738053000	-4.734492000
Cl	-1.495193000	0.996334000	-4.076897000
Cl	-0.511438000	-1.295533000	-7.527689000
Cl	0.554533000	4.222547000	-3.589954000



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Mg	-0.151146000	-0.176038000	-5.804098000
Mg	0.444625000	2.428312000	-3.770335000
Cl	1.842079000	0.973996000	-5.083918000
Cl	-1.548389000	1.278109000	-4.489965000
Cl	-0.477522000	-1.911695000	-7.192356000
Cl	0.771746000	4.164125000	-2.382543000

## Int4-K



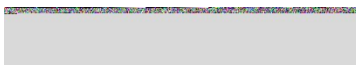
Atom	x	y	z
Pd	0.029267000	0.172819000	1.167525000
Cl	-0.669462000	-1.937893000	2.373443000
P	1.583572000	-1.042719000	-0.155131000
C	-5.710539000	0.246672000	-0.232437000
C	-4.956385000	-0.885449000	0.219821000
C	-5.411919000	-2.196281000	-0.090091000
C	-6.566477000	-2.374700000	-0.818597000
C	-7.311020000	-1.253782000	-1.266482000
C	-6.894508000	0.029316000	-0.981362000
N	-5.329406000	1.534791000	0.032769000
C	-4.229714000	1.726230000	0.722516000
C	-3.402015000	0.668420000	1.221548000
C	-3.781820000	-0.643219000	0.965357000
C	-2.246638000	0.964916000	1.998700000
C	-1.273566000	1.201651000	2.711152000
H	-0.707283000	1.484732000	3.573954000
H	-4.834537000	-3.048083000	0.259497000
H	-6.913320000	-3.376912000	-1.053057000

H	-8.220192000	-1.412710000	-1.839717000
H	-7.452206000	0.898781000	-1.314739000
H	-3.944982000	2.756805000	0.926098000
H	-3.165991000	-1.461505000	1.330628000
H	-0.469254000	4.406432000	-2.592798000
H	2.435731000	3.780922000	-2.622627000
H	0.507114000	1.867894000	-1.987296000
H	2.958016000	1.740162000	-0.607579000
B	0.102435000	4.188607000	-1.578037000
B	1.844136000	3.815348000	-1.596744000
C	0.678406000	2.619642000	-1.227766000
B	2.136927000	2.553146000	-0.368686000
B	-0.298336000	4.854377000	0.001940000
H	-1.091539000	5.705773000	0.225635000
B	1.255353000	5.258663000	-0.775065000
H	1.496934000	6.380473000	-1.070685000
C	1.172166000	4.789638000	0.860963000
H	1.343836000	5.553107000	1.611649000
B	-0.661139000	3.150727000	-0.336735000
H	-1.746203000	2.729363000	-0.555204000
B	0.011020000	3.599544000	1.227959000
H	-0.568297000	3.684348000	2.254615000
B	2.516523000	4.243227000	-0.023267000
H	3.596406000	4.688369000	0.176730000
B	1.740414000	3.209115000	1.213137000
H	2.316251000	3.010735000	2.230615000

B	0.582648000	2.088517000	0.427308000
C	1.369203000	-2.883810000	-0.187468000
C	0.870232000	-3.570829000	-1.302420000
C	1.748955000	-3.618663000	0.948900000
C	0.756841000	-4.963983000	-1.283291000
C	1.642978000	-5.007391000	0.960368000
C	1.144127000	-5.685391000	-0.155016000
H	0.578756000	-3.034148000	-2.197628000
H	2.124528000	-3.107208000	1.827634000
H	0.371684000	-5.480161000	-2.158571000
H	1.942127000	-5.559041000	1.847121000
H	1.058867000	-6.768636000	-0.142646000
C	3.324312000	-0.909455000	0.428645000
C	3.631725000	-0.088784000	1.522367000
C	4.345752000	-1.681322000	-0.153818000
C	4.938279000	-0.019396000	2.011082000
C	5.651655000	-1.601718000	0.328618000
C	5.950408000	-0.769057000	1.410935000
H	2.845493000	0.492385000	1.993694000
H	4.119723000	-2.356810000	-0.973446000
H	5.160734000	0.619267000	2.861110000
H	6.433034000	-2.198716000	-0.133284000
H	6.967153000	-0.714332000	1.790014000
C	1.536746000	-0.600409000	-1.945545000
C	2.672174000	-0.303649000	-2.711369000
C	0.272044000	-0.559560000	-2.562043000

C	2.546597000	0.016697000	-4.066244000
C	0.151179000	-0.254986000	-3.918560000
C	1.290728000	0.036225000	-4.673983000
H	3.656121000	-0.308397000	-2.255961000
H	-0.622256000	-0.757708000	-1.975999000
H	3.435645000	0.253479000	-4.643916000
H	-0.832243000	-0.233136000	-4.379477000
H	1.197639000	0.284434000	-5.727395000

### MgCl2



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Mg	0.000000000	0.000000000	-0.000216000
Cl	0.000000000	0.000000000	2.240768000
Cl	0.000000000	0.000000000	-2.240615000

### Int5



<b>Atom</b>	<b>x</b>	<b>y</b>	<b>z</b>
Pd	5.033741000	0.071932000	-0.159844000

P	4.086605000	2.195799000	-0.029139000
P	5.970706000	-2.050704000	-0.340306000
C	4.364302000	3.265194000	-1.513979000
C	4.460638000	2.628423000	-2.762591000
H	4.395577000	1.543947000	-2.810052000
C	4.654302000	3.371317000	-3.927735000
H	4.726146000	2.863298000	-4.885801000
C	4.770502000	4.762039000	-3.859972000
H	4.931256000	5.341100000	-4.765487000
C	4.689780000	5.404438000	-2.622754000
H	4.787341000	6.485289000	-2.562207000
C	4.486576000	4.662237000	-1.456570000
H	4.430878000	5.174077000	-0.500583000
C	2.247108000	2.209320000	0.178455000
C	1.395088000	3.129982000	-0.450253000
H	1.806624000	3.890156000	-1.107202000
C	0.013677000	3.072301000	-0.244843000
H	-0.634759000	3.787254000	-0.744823000
C	-0.533172000	2.101831000	0.596851000
H	-1.608045000	2.055674000	0.751954000
C	0.308037000	1.180538000	1.228623000
H	-0.109881000	0.417357000	1.879612000
C	1.685224000	1.227315000	1.011980000
H	2.335470000	0.492354000	1.480431000
C	4.675022000	3.246225000	1.376367000
C	6.001000000	3.073441000	1.806548000

H	6.620458000	2.320908000	1.324325000
C	6.516560000	3.843347000	2.849909000
H	7.544638000	3.697855000	3.170859000
C	5.708562000	4.787196000	3.488997000
H	6.106081000	5.380678000	4.308057000
C	4.384672000	4.957699000	3.078667000
H	3.748608000	5.684557000	3.577208000
C	3.870075000	4.193374000	2.028440000
H	2.837145000	4.331109000	1.722633000
C	7.424561000	-2.164930000	-1.480502000
C	8.269670000	-1.045786000	-1.565582000
H	8.029755000	-0.155930000	-0.988384000
C	9.394177000	-1.064130000	-2.391315000
H	10.038169000	-0.190357000	-2.445174000
C	9.681906000	-2.196659000	-3.157506000
H	10.551966000	-2.208500000	-3.808620000
C	8.841109000	-3.309448000	-3.091568000
H	9.054628000	-4.190558000	-3.691165000
C	7.719990000	-3.295648000	-2.257687000
H	7.071749000	-4.165988000	-2.219971000
C	6.605139000	-2.775557000	1.240180000
C	7.724606000	-3.618489000	1.318102000
H	8.279400000	-3.869963000	0.419170000
C	8.140437000	-4.132358000	2.549165000
H	9.012069000	-4.780157000	2.594799000
C	7.442843000	-3.813556000	3.715950000

H	7.769521000	-4.212317000	4.672698000
C	6.329949000	-2.971179000	3.649971000
H	5.788119000	-2.710178000	4.555171000
C	5.919565000	-2.449927000	2.422548000
H	5.069095000	-1.774042000	2.373253000
C	4.825192000	-3.357182000	-0.981349000
C	4.871229000	-4.700929000	-0.579582000
H	5.599435000	-5.022672000	0.158857000
C	3.980145000	-5.633333000	-1.118134000
H	4.027365000	-6.670535000	-0.796473000
C	3.034548000	-5.236108000	-2.066377000
H	2.344478000	-5.962891000	-2.486783000
C	2.975782000	-3.898121000	-2.468048000
H	2.237498000	-3.580039000	-3.199420000
C	3.858862000	-2.965298000	-1.923126000
H	3.798944000	-1.919767000	-2.216097000
C	-2.502990000	-3.592551000	1.501445000
C	-1.769832000	-2.678248000	0.677846000
C	-0.498675000	-3.064480000	0.172333000
C	0.021847000	-4.304204000	0.471632000
C	-0.705938000	-5.208151000	1.286481000
C	-1.941324000	-4.862117000	1.790957000
N	-3.730405000	-3.282917000	2.022590000
C	-4.239270000	-2.103860000	1.752244000
C	-3.597022000	-1.109589000	0.943083000
C	-2.355233000	-1.419019000	0.408192000

C	-4.237745000	0.142700000	0.716433000
C	-4.812739000	1.202713000	0.540153000
H	0.056132000	-2.367154000	-0.450367000
H	0.993260000	-4.592873000	0.080972000
H	-0.281188000	-6.182118000	1.513621000
H	-2.514180000	-5.539417000	2.416724000
H	-5.216045000	-1.877044000	2.177119000
H	-1.827381000	-0.697935000	-0.209337000
H	-4.847554000	6.260484000	1.227761000
H	-7.204347000	5.174483000	2.667318000
H	-4.861323000	3.667972000	2.308639000
H	-7.278140000	2.247347000	2.216333000
B	-5.485779000	5.388031000	0.744524000
B	-6.902955000	4.734638000	1.610156000
C	-5.471935000	3.823604000	1.426184000
B	-6.950349000	2.972429000	1.340448000
B	-5.713730000	5.099373000	-0.984042000
H	-5.381082000	5.819897000	-1.862807000
B	-7.102943000	5.536601000	0.047953000
H	-7.688950000	6.546050000	-0.150102000
C	-7.189850000	4.246318000	-1.067949000
H	-7.799004000	4.395821000	-1.952423000
B	-4.657486000	4.029768000	-0.060547000
H	-3.474839000	4.002296000	-0.106661000
B	-5.759937000	3.336513000	-1.256473000
H	-5.458288000	2.891405000	-2.310809000

B	-8.007060000	4.042281000	0.416965000
H	-9.189954000	4.064656000	0.463271000
B	-7.180285000	2.682187000	-0.389088000
H	-7.812413000	1.806727000	-0.873392000
B	-5.552944000	2.514363000	0.305291000
Mg	-12.153062927	-0.357922860	-0.932796397
Cl	-10.239115927	-0.972688860	0.042477603
Cl	-14.066899927	0.257421140	-1.908530397