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Theoretical study of formation mechanism for 4-methyl-3-phenylbenzonitrile in the course of the Hiyama and Suzuki–Miyaura reactions

Zeinab Ahmadvand and Mehdi Bayat

Figure S1. Optimized structures of the reactants, transition states, intermediates and product in Suzuki-Miyaura cross-coupling reaction for preparation of 4-methyl-3-phenylbenzonitrile at Cam-B3LYP/DEF2-SVP level of theory in the presence of ethylene glycol as solvent.

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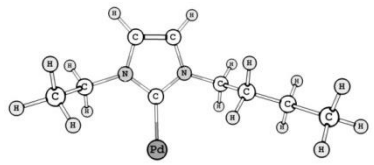
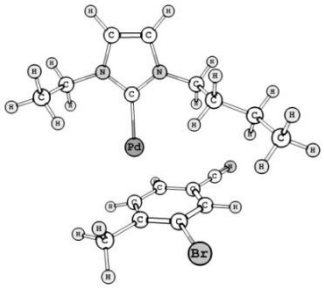
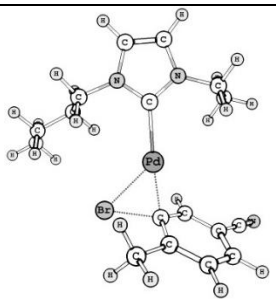
<tr><td> 
Pd0-NHC</td><td> 
Int1</td><td> 
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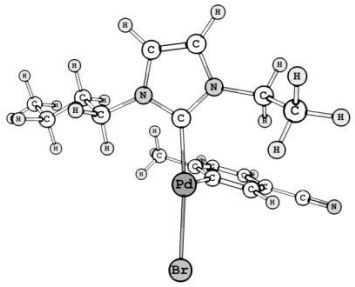
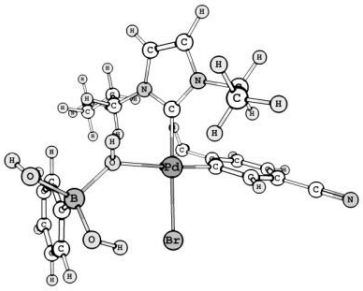
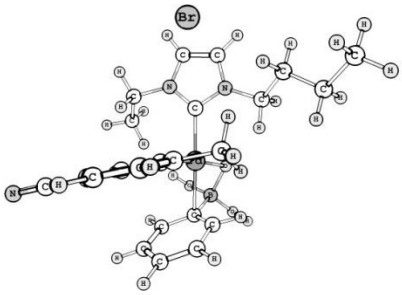
<tr><td> 
Int2</td><td> 
Int3</td><td> 
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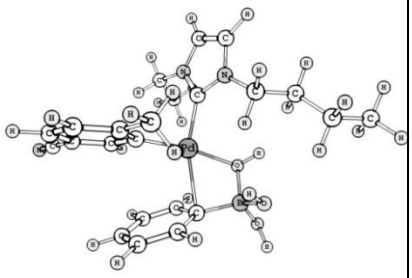
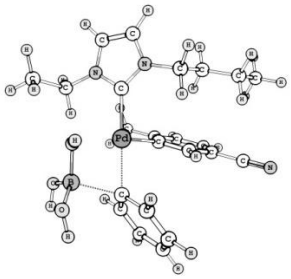
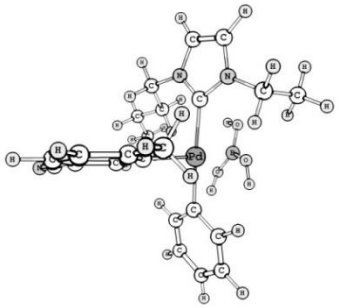
<tr><td> 
Int5</td><td> 
TS2</td><td> 
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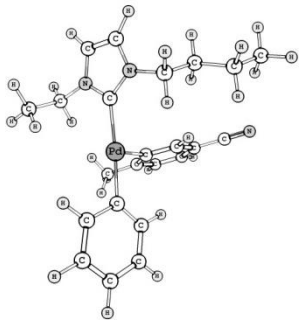
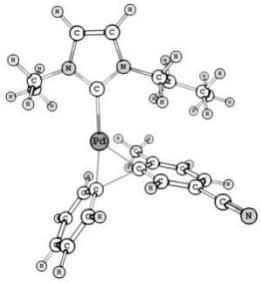
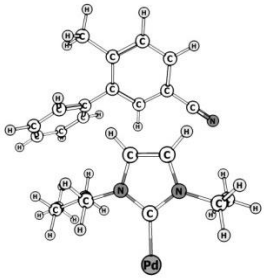
<tr><td> 
Int7</td><td> 
TS3</td><td> 
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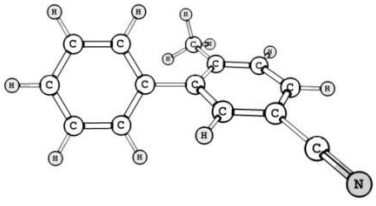
<tr><td> 
4-methyl-3-phenylbenzonitrile</td><td></td><td></td></tr>
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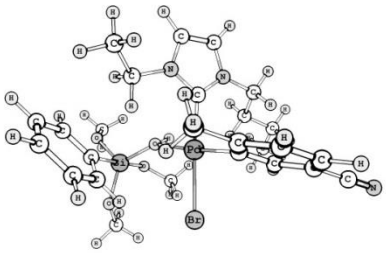
Figure S2 Optimized structures of transition state and intermediates in Hiyama−Denmark cross-coupling reaction (except the common point structures with Suzuki-Miyaura cross-coupling reaction) for preparation of 4-methyl-3-phenylbenzonitrile at Cam-B3LYP/DEF2-SVP level of theory in the presence of ethylene glycol as solvent.



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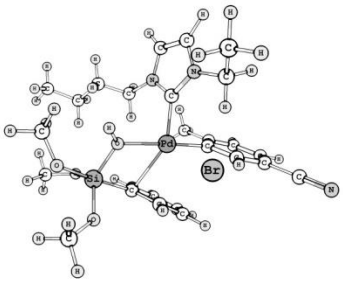

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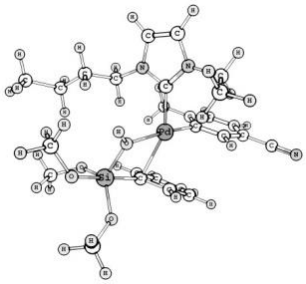

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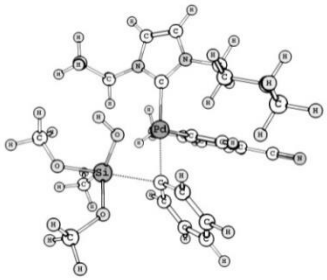
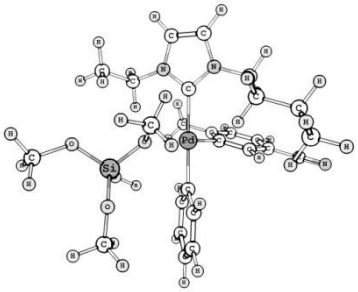


TS2′



Int6′

Table S1. Energies (E) and Gibbs free energies (G) of optimized structures of the reactants and products in the Suzuki−Miyaura cross-coupling reaction for preparation of 4-methyl-3-phenylbenzonitrile -B3LYP-D3/DEF2-SVP level in the presence of 1,2-ethanediol as solvent. All energies are in hartree atomic unit.

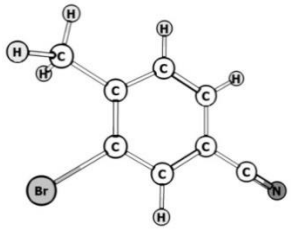
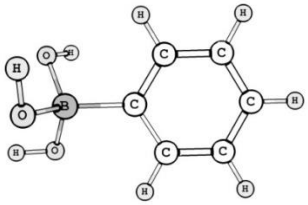
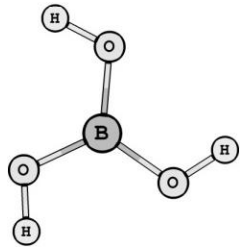
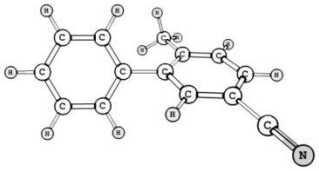
	E	**G**	**sp(G)**
	-2936.71945	-2936.636592	-2937.350723
	-483.6634874	-483.559352	-484.124337
	-252.2262276	-252.203723	-252.5121294
	-594.1132717	-593.942196	-594.5898032
Br^-	-2574.1342397	-2574.150415	-2574.48329

Table S2. Energies (E) and Gibbs free energies (G) of optimized structures of the Pd compounds in the Suzuki−Miyaura cross-coupling reaction for preparation of 4-methyl-3-phenylbenzonitrile at Cam-B3LYP-D3/DEF2-SVP level of theory and corresponding values at Cam-B3LYP-D3/DEF2-TZVP//Cam-B3LYP-D3/DEF2-SVP level in the presence of 1,2-ethanediol as solvent. All energies are in hartree atomic unit.

	E	**G**	**$sp_{(G)}$**
Pd(0)-NHC	-589.3676135	-589.166229	-589.702103
Int1	-3526.1259185	-3525.820370	-3527.068022
TS1	-3526.1100885	-3525.807192	-3527.056091
Int2	-3526.1741875	-3525.868302	-3527.118238
Int3	-4009.8888388	-4009.454603	-4011.255149
Int4	-4009.8662129	-4009.433179	-4011.24229
Int5	-1435.7241237	-1435.285650	-1436.765637
TS2	-1435.7113974	-1435.271514	-1436.751577
Int6	-1435.7364352	-1435.299755	-1436.779915
Int7	-1183.4796643	-1183.085612	-1184.269361
TS3	-1183.4615719	-1183.069218	-1184.252023
Int8	-1183.4952367	-1183.103575	-1184.283315

Table S3. Energies (E) and Gibbs free energies (G) of optimized structures of the reactants in the Hiyama−Denmark cross-coupling reaction for preparation of 4-methyl-3-phenylbenzonitrile at Cam-B3LYP-D3/DEF2-SVP level of theory and corresponding values at Cam-B3LYP-D3/DEF2-TZVP//Cam-B3LYP-D3/DEF2-SVP level in the presence of 1,2-ethanediol as solvent. All energies are in hartree atomic unit.

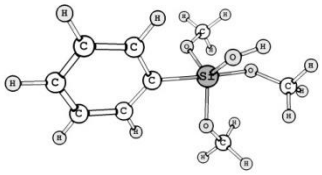
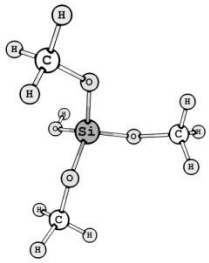
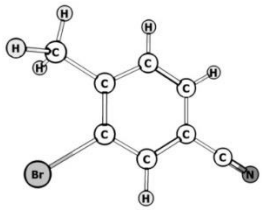
	E	**G**	**sp(G)**
	-941.7574742	-941.567462	-942.4414036
	-710.3266852	-710.224090	-710.8547771

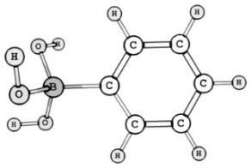
Table S4. Energies (E) and Gibbs free energies (G) of optimized structures of the Pd compounds in the Hiyama−Denmark cross-coupling reaction for preparation of 4-methyl-3-phenylbenzonitrile at Cam-B3LYP-D3/DEF2-SVP level of theory and corresponding values at Cam-B3LYP-D3/DEF2-TZVP//Cam-B3LYP-D3/DEF2-SVP level in the presence of 1,2-ethanediol as solvent. All energies are in hartree atomic unit.

	E	**G**	**sp(G)**
Pd(0)-NHC	-589.3676135	-589.166229	-589.702103
Int1′	-3526.1259185	-3525.820370	-3527.068022
TS1′	-3526.1100885	-3525.807192	-3527.056091
Int2′	-3526.1741875	-3525.868302	-3527.118238
Int3′	-4467.9792766	-4467.457657	-4469.566825
Int4′	-4467.9693784	-4467.445450	-4469.559848
Int5′	-1893.8197352	-1893.292442	-1895.08475
TS2′	-1893.8058355	-1893.281116	-1895.077516
Int6′	-1893.8497901	-1893.328934	-1895.129679
Int7′	-1183.4796643	-1183.085612	-1184.269361
TS3′	-1183.4615719	-1183.069218	-1184.252023
Int8′	-1183.4952367	-1183.103575	-1184.283315

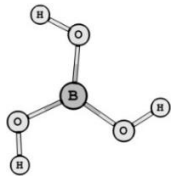
Table S5. Optimized coordinates of reactants, transition states, intermediates and products in the Suzuki−Miyaura and Hiyama−Denmark cross-coupling reactions for preparation of 4-methyl-3-phenylbenzonitrile at Cam-B3LYP/def2-SVP level of theory in the presence of 1,2-ethanediol as solvent. For transition state structures, one imaginary frequency was observed and given below. For all minimum structures, no imaginary frequency was observed**.**



Atom	X	Y	Z
C	-0.735898000	-3.296677000	0.000000000
C	-0.010131000	-2.056501000	0.000000000
C	-0.709046000	-0.844644000	0.000000000
C	0.000000000	0.349137000	0.000000000
C	1.403159000	0.382605000	0.000000000
C	2.070624000	-0.848076000	0.000000000
C	1.388739000	-2.056284000	0.000000000
N	-1.317983000	-4.294312000	0.000000000
C	2.169488000	1.671296000	0.000000000
Br	-0.989056000	1.968624000	0.000000000
H	-1.798884000	-0.837258000	0.000000000
H	3.162209000	-0.851847000	0.000000000
H	1.937179000	-2.998845000	0.000000000
H	1.914830000	2.276950000	0.882838000
H	3.251064000	1.487264000	0.000000000
H	1.914830000	2.276950000	-0.882838000

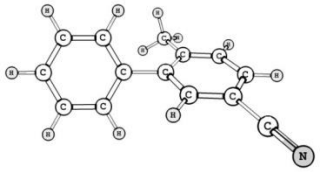


Atom	X	Y	Z
C	0.072521000	-0.010818000	-0.037619000
C	0.817668000	-1.200702000	-0.013985000
C	2.211954000	-1.205446000	0.020316000
C	2.915520000	0.000339000	0.030431000
C	2.205135000	1.199454000	-0.001252000
C	0.809191000	1.183145000	-0.037285000
B	-1.572852000	-0.019162000	0.000425000
O	-2.014854000	-1.204559000	-0.740003000
O	-2.107385000	1.238039000	-0.568125000
O	-2.092186000	-0.111889000	1.376991000
H	-2.976698000	-1.219588000	-0.672096000
H	-1.654486000	1.401280000	-1.402342000
H	-2.030081000	0.763689000	1.772706000
H	4.008366000	0.003936000	0.058176000
H	2.743590000	2.151919000	-0.001036000
H	0.262472000	2.130831000	-0.073683000
H	0.276530000	-2.151329000	-0.035365000
H	2.758026000	-2.153481000	0.036983000



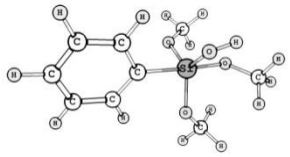
Atom	X	Y	Z
O	1.293685000	-0.429786000	-0.000071000
B	-0.000029000	-0.000014000	0.000494000

O	-1.019062000	-0.905453000	-0.000070000
O	-0.274617000	1.335249000	-0.000071000
H	-1.887925000	-0.485710000	-0.000260000
H	1.364711000	-1.392124000	-0.000259000
H	0.523311000	1.877821000	-0.000259000



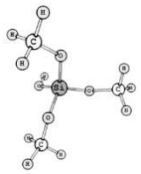
Atom	**X**	**Y**	**Z**
C	-2.152440000	0.420223000	0.924107000
C	-1.257568000	-0.143715000	0.006857000
C	-1.728121000	-1.128436000	-0.870183000
C	-3.060507000	-1.532917000	-0.837956000
C	-3.942536000	-0.962155000	0.076960000
C	-3.483398000	0.013800000	0.959864000
C	0.177182000	0.258104000	-0.022458000
C	1.146048000	-0.738817000	0.104812000
C	2.509050000	-0.428149000	0.084253000
C	2.915583000	0.900958000	-0.072237000
C	1.952678000	1.888981000	-0.213093000
C	0.583285000	1.598987000	-0.193506000
H	0.832337000	-1.775849000	0.233583000
C	-0.405728000	2.718462000	-0.374841000
H	3.976409000	1.154147000	-0.090508000
H	-1.041658000	-1.574661000	-1.593210000
H	-1.799234000	1.174841000	1.629023000
C	3.484978000	-1.472837000	0.225537000
H	2.271368000	2.923970000	-0.353553000
H	-4.165870000	0.460130000	1.686313000
H	-4.987325000	-1.278849000	0.103716000

H	-3.411309000	-2.297668000	-1.534236000
H	0.066064000	3.577059000	-0.871005000
H	-1.272989000	2.400687000	-0.968965000
H	-0.791417000	3.069561000	0.594472000
N	4.270371000	-2.312615000	0.339381000



Atom	**X**	**Y**	**Z**
C	-1.241855000	0.010448000	-0.149282000
C	-2.061583000	-1.019634000	-0.642596000
Si	0.717698000	-0.160476000	-0.147435000
C	-1.912803000	1.109583000	0.410744000
C	-3.454437000	-0.966934000	-0.578085000
C	-3.305573000	1.180877000	0.484391000
H	-3.785276000	2.058375000	0.928535000
C	-4.087641000	0.138587000	-0.010445000
H	-5.178550000	0.188255000	0.041945000
H	-4.052167000	-1.792450000	-0.976333000
H	-1.585957000	-1.889023000	-1.104029000
H	-1.316153000	1.942019000	0.792372000
O	0.866183000	1.550905000	-0.122273000
O	2.491283000	-0.393591000	-0.095165000
O	0.589412000	-1.022671000	1.327730000
C	1.910844000	2.352477000	0.326890000
H	2.413078000	2.876234000	-0.509593000
H	1.527548000	3.132044000	1.012370000
H	2.687591000	1.781169000	0.862050000
C	3.331985000	-0.028810000	-1.130556000
H	4.343777000	0.214728000	-0.751744000

H	3.474447000	-0.837010000	-1.884079000
H	2.983683000	0.859708000	-1.695952000
C	1.597545000	-1.614868000	2.088203000
H	2.205268000	-2.332465000	1.510082000
H	2.305793000	-0.878480000	2.510043000
H	1.137429000	-2.158948000	2.933492000
O	0.634381000	-0.953815000	-1.670478000
H	1.482755000	-1.334477000	-1.919161000



Atom	**X**	**Y**	**Z**
Si	0.012589000	0.000981000	0.325624000
O	-0.369298000	-1.141908000	-0.789310000
O	1.449984000	0.638934000	-0.140448000
O	-1.050128000	1.246617000	0.415970000
O	0.023818000	-0.754075000	1.784538000
H	0.020632000	-0.196045000	2.571369000
C	-1.437088000	-2.057568000	-0.680458000
H	-1.318532000	-2.835233000	-1.448852000
H	-1.453461000	-2.543221000	0.309193000
H	-2.409613000	-1.561383000	-0.838860000
C	2.573122000	-0.106591000	-0.557085000
H	3.304192000	0.577119000	-1.012329000
H	3.057806000	-0.612323000	0.295293000
H	2.296120000	-0.870979000	-1.301555000
C	-1.197986000	2.250988000	-0.565119000
H	-1.817749000	3.060514000	-0.153269000
H	-0.222758000	2.670619000	-0.861475000
H	-1.696171000	1.859677000	-1.468276000

Suzuki-Miyaura Hiyama-Denmark

Pd(0)-NHC

Atom	X	Y	Z
Pd	-0.654125000	-1.643661000	-0.229060000
N	0.318951000	1.160155000	-0.673696000
N	-1.758365000	1.147471000	-0.138972000
C	-0.708066000	0.313760000	-0.380548000
C	-0.077960000	2.482523000	-0.596863000
H	0.599575000	3.306422000	-0.802824000
C	-1.388601000	2.474558000	-0.259739000
H	-2.090498000	3.290323000	-0.110460000
C	1.683064000	0.739653000	-0.953204000
H	2.136116000	1.484621000	-1.624041000
H	1.627285000	-0.213935000	-1.496584000
C	2.518928000	0.574979000	0.308345000
H	2.022325000	-0.168760000	0.954187000
H	2.527808000	1.526678000	0.866547000
C	3.946840000	0.134679000	0.009773000
H	3.921894000	-0.811242000	-0.558160000
H	4.426094000	0.874778000	-0.653977000
C	4.785412000	-0.045235000	1.268714000
H	4.850996000	0.895098000	1.838652000
H	5.810622000	-0.364910000	1.029824000
H	4.342979000	-0.804190000	1.933177000
C	-3.085997000	0.712372000	0.273088000
H	-3.810168000	1.447013000	-0.107258000
H	-3.282998000	-0.245137000	-0.227487000
C	-3.207011000	0.560131000	1.780330000
H	-2.990259000	1.508983000	2.293426000
H	-4.225949000	0.246726000	2.050806000
H	-2.499830000	-0.201975000	2.140237000

Int1

Atom	X	Y	Z
C	-2.379358000	-0.714975000	0.057150000
C	-1.620485000	-1.831372000	0.401054000
C	-2.371275000	0.460234000	0.820169000
C	-0.827664000	-1.758573000	1.584260000
C	-1.554463000	0.544372000	1.938356000
C	-0.751401000	-0.566296000	2.333560000
H	-0.426994000	-2.689858000	1.992647000
C	-1.508883000	1.760115000	2.695463000
H	-0.288472000	-0.557257000	3.321997000
Br	-3.468878000	-0.742704000	-1.500330000
H	-2.986590000	1.308907000	0.522935000
Pd	0.943215000	-0.691064000	0.914055000
N	2.607770000	1.499168000	-0.436355000
N	3.692649000	-0.344930000	-0.483845000
C	2.550239000	0.211261000	-0.013219000
C	3.754560000	1.737360000	-1.168866000
H	3.987800000	2.712155000	-1.587905000
C	4.441027000	0.569110000	-1.201092000
H	5.393782000	0.314703000	-1.656787000
C	1.557652000	2.482467000	-0.203095000
H	2.009650000	3.481688000	-0.280250000
H	1.205814000	2.354612000	0.830093000

C	0.390879000	2.341561000	-1.170919000
H	0.004316000	1.311466000	-1.095455000
H	0.754486000	2.472935000	-2.204135000
C	-0.730061000	3.331877000	-0.880399000
H	-1.068302000	3.197674000	0.161313000
H	-0.337270000	4.361432000	-0.939234000
C	-1.911239000	3.175699000	-1.829637000
H	-1.606094000	3.352709000	-2.873056000
H	-2.718596000	3.883985000	-1.591107000
H	-2.329571000	2.158065000	-1.778992000
C	4.040526000	-1.751898000	-0.326673000
H	5.136515000	-1.829116000	-0.351353000
H	3.704943000	-2.059848000	0.672919000
C	3.407254000	-2.628051000	-1.394811000
H	3.724014000	-2.316748000	-2.401290000
H	3.701654000	-3.677448000	-1.248972000
H	2.310238000	-2.562936000	-1.337538000
C	-1.657852000	-3.104451000	-0.391155000
H	-1.363461000	-2.924606000	-1.435243000
H	-0.981445000	-3.854453000	0.037407000
H	-2.677457000	-3.518650000	-0.415319000
N	-1.457970000	2.747695000	3.294692000

TS1

Atom	X	Y	Z
C	-1.754468000	-0.855371000	-0.209638000
C	-2.335456000	-0.180075000	0.876562000
C	-2.467830000	-1.060416000	-1.420662000
C	-3.618193000	0.373581000	0.733058000
H	-1.815909000	-0.125037000	1.833604000
C	-3.738558000	-0.492825000	-1.514509000
C	-4.318690000	0.218882000	-0.465057000
C	-4.206672000	1.089676000	1.830126000
H	-4.296761000	-0.612005000	-2.445902000
H	-5.316569000	0.644461000	-0.575540000
Br	-0.274043000	-2.334021000	0.302442000
Pd	-0.081078000	0.226184000	-0.403090000
N	2.886744000	1.113433000	-0.596141000
N	1.640184000	2.842944000	-0.434382000
C	1.587106000	1.492839000	-0.527911000
C	3.735237000	2.201332000	-0.526461000
H	4.816209000	2.102787000	-0.570435000
C	2.945335000	3.298202000	-0.423747000
H	3.195689000	4.353309000	-0.357945000
C	3.320729000	-0.276010000	-0.653585000
H	4.308239000	-0.304165000	-1.136328000
H	2.616687000	-0.814260000	-1.303093000
C	3.364784000	-0.934665000	0.718119000
H	2.379284000	-0.803536000	1.192874000
H	4.101988000	-0.414310000	1.352880000
C	3.692352000	-2.420439000	0.638760000
H	2.958253000	-2.909710000	-0.023971000
H	4.678529000	-2.557602000	0.162742000
C	3.674720000	-3.099277000	2.002020000
H	4.402972000	-2.636991000	2.687085000
H	3.918494000	-4.169313000	1.924799000
H	2.679873000	-3.014015000	2.467309000

C	0.468437000	3.696282000	-0.279565000
H	0.710174000	4.677349000	-0.711886000
H	-0.337079000	3.255874000	-0.882532000
C	0.036137000	3.830442000	1.171152000
H	0.841030000	4.259516000	1.786185000
H	-0.842990000	4.486727000	1.246024000
H	-0.230705000	2.845098000	1.581069000
C	-1.906287000	-1.885093000	-2.543471000
H	-1.887096000	-2.947188000	-2.250771000
H	-2.519070000	-1.786271000	-3.448952000
H	-0.872249000	-1.603648000	-2.782034000
N	-4.675499000	1.668888000	2.713427000

Int2

Atom	X	Y	Z
C	-1.182857000	-0.029776000	0.741870000
C	-0.672328000	0.065818000	2.049909000
C	-2.526193000	0.256464000	0.501771000
C	-1.537388000	0.456107000	3.081415000
C	-3.371575000	0.651940000	1.548481000
C	-2.872757000	0.753748000	2.850481000
H	-1.145289000	0.529451000	4.098376000
C	-4.749095000	0.953072000	1.275169000
H	-3.524171000	1.060238000	3.669867000
Br	-1.165557000	-2.876830000	-1.036383000
H	-2.936411000	0.180562000	-0.506229000
Pd	-0.121226000	-0.633605000	-0.791295000
N	2.258280000	1.174329000	-0.662243000
N	0.502607000	2.361589000	-1.020678000
C	0.910520000	1.098078000	-0.773224000
C	2.689897000	2.472445000	-0.852166000
H	3.736974000	2.754988000	-0.811366000
C	1.582821000	3.219177000	-1.077868000
H	1.469450000	4.281944000	-1.270969000
C	3.146249000	0.037133000	-0.426922000
H	3.649302000	-0.217367000	-1.372439000
H	2.503799000	-0.811805000	-0.159259000
C	4.169598000	0.282272000	0.671392000
H	3.653157000	0.625607000	1.582361000
H	4.857990000	1.090845000	0.377130000
C	4.973279000	-0.977112000	0.978379000
H	4.281775000	-1.778929000	1.288382000
H	5.458204000	-1.333386000	0.053700000
C	6.023524000	-0.757572000	2.058980000
H	6.748166000	0.014868000	1.756917000
H	6.584200000	-1.680607000	2.267470000
H	5.558746000	-0.426455000	3.000987000
C	-0.876392000	2.776802000	-1.275363000
H	-1.506225000	2.357748000	-0.482950000
H	-0.902513000	3.869074000	-1.170632000
C	-1.372757000	2.353171000	-2.646842000
H	-1.374153000	1.257047000	-2.739509000
H	-2.400618000	2.712870000	-2.797526000
H	-0.738843000	2.770377000	-3.443002000
C	0.768571000	-0.224649000	2.365195000
H	1.417650000	0.537696000	1.910959000
H	0.951612000	-0.225126000	3.447936000

H	1.078683000	-1.197681000	1.957529000
N	-5.856498000	1.198399000	1.053107000

Int3

Atom	X	Y	Z
O	-1.666545000	-2.844016000	2.043362000
H	-1.062573000	-3.014251000	1.305663000
B	-2.315364000	-1.579410000	1.789084000
O	-1.249499000	-0.476353000	1.597743000
H	-1.028573000	-0.178635000	2.489256000
O	-3.074022000	-1.226820000	2.980638000
H	-3.782196000	-0.621978000	2.739331000
C	-3.241160000	-1.559475000	0.439624000
C	-3.870827000	-0.386608000	-0.004420000
C	-3.479484000	-2.717995000	-0.311140000
C	-4.687088000	-0.360809000	-1.135476000
H	-3.716802000	0.541783000	0.551967000
C	-4.293705000	-2.713381000	-1.444527000
H	-2.999405000	-3.647890000	0.004659000
C	-4.901017000	-1.530315000	-1.864829000
H	-5.154208000	0.576030000	-1.452049000
H	-4.454028000	-3.637170000	-2.007881000
H	-5.536383000	-1.519491000	-2.754147000
C	2.102317000	-0.006503000	-0.826561000
C	2.075550000	0.769897000	-2.005403000
C	3.300500000	-0.643074000	-0.490042000
C	3.231226000	0.889960000	-2.789224000
C	4.453457000	-0.510972000	-1.278733000
C	4.420818000	0.265435000	-2.441434000
H	3.194932000	1.491669000	-3.700842000
C	5.663538000	-1.178865000	-0.889887000
H	5.311402000	0.372648000	-3.062361000
Br	0.345536000	-2.664304000	-0.610976000
H	3.352326000	-1.269706000	0.402624000
Pd	0.498179000	-0.300682000	0.318644000
N	-0.292683000	2.522116000	0.969995000
N	1.624965000	2.096246000	1.838266000
C	0.660865000	1.565282000	1.052487000
C	0.066407000	3.636715000	1.704220000
H	-0.562133000	4.518859000	1.773781000
C	1.273972000	3.367113000	2.252438000
H	1.914024000	3.964527000	2.895091000
C	-1.573673000	2.375405000	0.286775000
H	-2.358580000	2.286573000	1.051979000
H	-1.540363000	1.415254000	-0.238960000
C	-1.893337000	3.511332000	-0.671908000
H	-1.063507000	3.636826000	-1.385853000
H	-1.979789000	4.463965000	-0.123769000
C	-3.189244000	3.246681000	-1.431853000
H	-3.098500000	2.293414000	-1.978918000
H	-4.010609000	3.100453000	-0.709453000
C	-3.547390000	4.366650000	-2.399249000
H	-3.677857000	5.323225000	-1.868915000
H	-4.482565000	4.150623000	-2.936686000
H	-2.754013000	4.509605000	-3.149828000
C	2.827738000	1.403092000	2.293991000
H	3.296316000	0.933394000	1.422802000

Int3′

Atom	X	Y	Z
Pd	0.532424000	0.129457000	0.181529000
N	-0.071818000	1.782412000	-2.278198000
N	1.548390000	0.425701000	-2.663798000
C	0.724897000	0.867155000	-1.683326000
C	0.239460000	1.905598000	-3.619134000
H	-0.287703000	2.583692000	-4.282479000
C	1.259632000	1.050355000	-3.861638000
H	1.807238000	0.833927000	-4.774180000
C	2.318170000	0.858098000	0.652846000
C	3.397292000	-0.023433000	0.756841000
C	2.542519000	2.220045000	0.945694000
C	4.677784000	0.419524000	1.119338000
H	3.251878000	-1.087538000	0.562066000
C	3.824254000	2.649374000	1.317143000
C	4.896012000	1.771644000	1.402475000
C	5.757901000	-0.523126000	1.197528000
H	3.984533000	3.706077000	1.545296000
H	5.887555000	2.125751000	1.688091000
Br	0.416889000	-0.984541000	2.465937000
C	1.425100000	3.223521000	0.857226000
H	1.106853000	3.342587000	-0.188164000
H	0.539936000	2.888105000	1.417699000
H	1.729370000	4.209043000	1.235865000
N	6.623185000	-1.288248000	1.252504000
C	-1.191236000	2.473789000	-1.640086000
H	-2.122509000	2.021853000	-2.004774000
H	-1.141375000	2.246506000	-0.570176000
C	-1.185106000	3.971349000	-1.885926000
H	-1.301878000	4.219948000	-2.950689000
H	-2.026798000	4.419801000	-1.341477000
H	-0.255580000	4.435002000	-1.525026000
C	2.567628000	-0.610006000	-2.521325000
H	3.140791000	-0.625762000	-3.458020000
H	3.256043000	-0.309135000	-1.722501000
C	1.984413000	-1.985470000	-2.232791000
H	1.406634000	-1.932249000	-1.295265000
H	1.270860000	-2.252977000	-3.030354000
C	3.056751000	-3.059825000	-2.103508000
H	3.625562000	-3.128787000	-3.046401000
H	3.784387000	-2.754987000	-1.331603000
C	2.473709000	-4.421262000	-1.747293000
H	3.258208000	-5.186837000	-1.655796000
H	1.931281000	-4.377847000	-0.789525000
H	1.760533000	-4.759616000	-2.515534000
C	-3.239033000	0.753803000	0.578759000
C	-4.055486000	1.656064000	-0.117642000
Si	-3.034334000	-1.119492000	0.081948000
C	-2.508629000	1.283575000	1.656757000
C	-4.124185000	3.010941000	0.216951000
C	-2.555168000	2.635471000	1.994861000
H	-1.957733000	3.008798000	2.831911000
C	-3.364184000	3.512298000	1.270875000

H	3.517979000	2.172742000	2.663588000
C	2.535526000	0.374988000	3.373756000
H	1.871868000	-0.413051000	2.988921000
H	3.472232000	-0.095167000	3.705923000
H	2.053971000	0.842891000	4.245165000
C	0.819370000	1.477718000	-2.436037000
H	0.551124000	2.253123000	-1.704839000
H	0.935773000	1.958323000	-3.417245000
H	-0.032567000	0.782872000	-2.485140000
N	6.636843000	-1.716723000	-0.572845000
H	-3.404634000	4.573543000	1.529859000
H	-4.770558000	3.681921000	-0.356462000
H	-4.645852000	1.282420000	-0.956736000
H	-1.873052000	0.616218000	2.241337000
O	-3.439964000	-1.550950000	1.684477000
O	-2.697835000	-2.792732000	-0.405537000
O	-4.280886000	-1.022725000	-1.069787000
C	-3.626820000	-2.811461000	2.250548000
H	-2.697388000	-3.200828000	2.706130000
H	-4.381369000	-2.745012000	3.054847000
H	-3.971159000	-3.562800000	1.520441000
C	-1.618044000	-3.546577000	0.045682000
H	-1.946548000	-4.548629000	0.382183000
H	-0.868025000	-3.716628000	-0.756901000
H	-1.076641000	-3.082295000	0.890288000
C	-4.708122000	-1.989837000	-1.979827000
H	-3.902705000	-2.316778000	-2.660538000
H	-5.089856000	-2.900211000	-1.485525000
H	-5.523534000	-1.567786000	-2.593711000
O	-1.393450000	-0.721148000	-0.513614000
H	-1.117002000	-1.449943000	-1.083627000

Int4

Atom	X	Y	Z
O	-3.451228000	2.629250000	1.487868000
H	-3.188053000	1.822957000	1.941206000
B	-2.881818000	2.691871000	0.165191000
O	-1.337846000	2.787413000	0.268087000
H	-1.100737000	3.242098000	1.086464000
O	-3.418847000	3.857999000	-0.480336000
H	-3.123996000	3.890233000	-1.395978000
C	-3.071190000	1.297062000	-0.702923000
C	-2.379830000	1.066699000	-1.912834000
C	-3.990494000	0.300323000	-0.299804000
C	-2.616085000	-0.082355000	-2.692983000
H	-1.715278000	1.839297000	-2.312951000
C	-4.219732000	-0.833171000	-1.060360000
H	-4.536247000	0.447895000	0.635629000
C	-3.530312000	-1.027618000	-2.267239000
H	-2.071224000	-0.223209000	-3.628983000
H	-4.938171000	-1.583801000	-0.721794000
H	-3.712126000	-1.925633000	-2.861626000
C	-0.563736000	-1.190253000	-0.401520000
C	0.305213000	-1.626479000	-1.423776000
C	-1.384206000	-2.127443000	0.224715000
C	0.326043000	-2.981571000	-1.775079000
C	-1.355025000	-3.482721000	-0.140075000
C	-0.488731000	-3.914975000	-1.147578000
H	0.999995000	-3.313284000	-2.568467000
C	-2.226068000	-4.413491000	0.519466000
H	-0.457898000	-4.966275000	-1.437357000
Br	4.085644000	-1.824971000	0.235923000
H	-2.083976000	-1.815806000	1.001895000
Pd	-0.837136000	0.727189000	0.012264000
N	1.765707000	1.613521000	1.114400000
N	0.858046000	0.227072000	2.483970000
C	0.723371000	0.766142000	1.253363000

Int4′

Atom	X	Y	Z
Pd	-0.347969000	0.134639000	0.128644000
N	-1.341670000	2.454606000	-1.586938000
N	0.358229000	2.957144000	-0.367972000
C	-0.488149000	1.947670000	-0.674497000
C	-1.040825000	3.779502000	-1.844428000
H	-1.613276000	4.379220000	-2.545472000
C	0.030241000	4.095292000	-1.078714000
H	0.583101000	5.024158000	-0.974100000
C	-2.101460000	0.463860000	1.002257000
C	-2.286977000	1.273046000	2.141322000
C	-3.191338000	-0.254169000	0.504337000
C	-3.547985000	1.322256000	2.752793000
C	-4.446046000	-0.192810000	1.127482000
H	-3.066584000	-0.893002000	-0.375075000
C	-4.628245000	0.602018000	2.264249000
H	-3.682810000	1.944641000	3.640898000
C	-5.541402000	-0.954299000	0.595751000
H	-5.601131000	0.652828000	2.755454000
C	-1.162129000	2.088942000	2.719529000
H	-0.266608000	1.471446000	2.872253000
H	-0.885227000	2.903441000	2.033912000
H	-1.443630000	2.539429000	3.681196000
N	-6.421582000	-1.568051000	0.164914000
C	1.496760000	2.861239000	0.538575000
H	1.425419000	3.682072000	1.267787000
H	1.387817000	1.918140000	1.086966000
C	2.834926000	2.897378000	-0.182875000
H	2.825805000	2.136362000	-0.978045000
H	2.967518000	3.877157000	-0.671804000
C	3.989481000	2.626015000	0.776762000
H	3.874906000	3.258880000	1.673673000
H	3.915993000	1.581072000	1.121175000
C	5.356897000	2.878744000	0.154714000

C	2.544536000	1.615877000	2.254244000
H	3.439781000	2.222688000	2.347124000
C	1.971463000	0.744563000	3.117474000
H	2.259933000	0.440877000	4.119403000
C	2.086601000	2.365793000	-0.095880000
H	1.991455000	3.441021000	0.118342000
H	1.315548000	2.108849000	-0.832166000
C	3.470991000	2.024481000	-0.631826000
H	3.616190000	0.933344000	-0.573285000
H	4.244630000	2.471412000	0.014958000
C	3.671634000	2.498167000	-2.066305000
H	2.897321000	2.039378000	-2.705000000
H	3.511676000	3.588441000	-2.127702000
C	5.052214000	2.142309000	-2.603096000
H	5.845101000	2.624959000	-2.010091000
H	5.175444000	2.458421000	-3.649574000
H	5.220284000	1.054749000	-2.554570000
C	-0.037754000	-0.754354000	3.093594000
H	-0.155820000	-1.584683000	2.387782000
H	0.484130000	-1.148780000	3.974674000
C	-1.386396000	-0.178538000	3.487963000
H	-1.944226000	0.152058000	2.600366000
H	-1.983754000	-0.948278000	3.996600000
H	-1.269461000	0.677992000	4.167636000
C	1.209953000	-0.663499000	-2.140683000
H	2.015805000	-0.339154000	-1.466254000
H	1.682281000	-1.130794000	-3.015905000
H	0.660087000	0.227879000	-2.476983000
N	-2.933794000	-5.156014000	1.053218000
H	6.168634000	2.640402000	0.858201000
H	5.506061000	2.263980000	-0.746095000
H	5.468919000	3.932944000	-0.144057000
C	-2.412384000	1.719284000	-2.258040000
H	-2.389708000	0.695126000	-1.873296000
H	-3.372011000	2.178411000	-1.977263000
C	-2.233977000	1.690010000	-3.765026000
H	-3.039986000	1.091732000	-4.211643000
H	-2.264748000	2.695206000	-4.210611000
H	-1.279830000	1.211947000	-4.027709000
C	1.133996000	-1.545614000	1.423491000
C	-0.105483000	-2.172835000	1.154916000
Si	2.548183000	-1.535746000	0.036453000
C	1.304401000	-1.039118000	2.731377000
C	-1.095058000	-2.316189000	2.143524000
C	0.324472000	-1.173625000	3.707004000
H	0.498177000	-0.774046000	4.709854000
C	-0.883666000	-1.818376000	3.418640000
H	-1.651414000	-1.922699000	4.188535000
H	-2.034282000	-2.816016000	1.896552000
H	-0.268429000	-2.648975000	0.183720000
H	2.249859000	-0.552717000	2.976417000
O	3.697699000	-0.967955000	1.155664000
O	3.637089000	-1.514026000	-1.338216000
O	2.298185000	-3.199696000	-0.164678000
C	5.091340000	-1.070548000	1.118359000
H	5.557417000	-0.070354000	1.059404000
H	5.460534000	-1.553405000	2.040483000
H	5.448270000	-1.657095000	0.256675000
C	4.234232000	-0.376016000	-1.860147000
H	5.166146000	-0.638733000	-2.392907000
H	3.591823000	0.149878000	-2.599666000
H	4.501400000	0.369646000	-1.089761000
C	2.843932000	-4.056312000	-1.126491000
H	2.598948000	-3.741536000	-2.154698000
H	3.944136000	-4.117379000	-1.064812000
H	2.435013000	-5.069418000	-0.969769000
O	1.552070000	-0.307050000	-0.764914000
H	1.745931000	-0.108299000	-1.688777000
Br	-1.789390000	-1.982159000	-2.671932000

Int5

Atom	X	Y	Z
Pd	0.055795000	-0.158208000	-0.378019000
N	0.268751000	2.858845000	-0.746777000
N	1.857327000	2.064105000	0.462326000
C	0.732329000	1.714265000	-0.201616000
C	1.098175000	3.917769000	-0.429868000
H	0.899771000	4.929211000	-0.771769000
C	2.097355000	3.418812000	0.334362000
H	2.949964000	3.903643000	0.800352000
C	-1.588958000	0.371359000	0.594313000
C	-1.636332000	0.523969000	1.996270000
C	-2.781222000	0.463539000	-0.125566000
C	-2.868987000	0.747176000	2.623756000
C	-4.007984000	0.691705000	0.515696000
H	-2.779772000	0.344321000	-1.209961000

Int5′

Atom	X	Y	Z
Pd	-0.479949000	0.047238000	-0.277312000
N	-1.302705000	2.802790000	-1.284934000
N	0.199755000	2.884301000	0.249971000
C	-0.581258000	2.030331000	-0.447252000
C	-0.974297000	4.135098000	-1.118233000
H	-1.445489000	4.923191000	-1.698128000
C	-0.030627000	4.187414000	-0.148906000
H	0.489439000	5.030993000	0.294968000
C	-2.305670000	0.070059000	0.500924000
C	-2.606439000	0.416419000	1.833868000
C	-3.337147000	-0.408739000	-0.309789000
C	-3.914999000	0.251274000	2.309823000
C	-4.642400000	-0.564565000	0.177874000
H	-3.134616000	-0.699683000	-1.342346000

C	-4.053368000	0.834235000	1.905006000
H	-2.899407000	0.853857000	3.710708000
C	-5.212609000	0.766129000	-0.261850000
H	-5.002632000	1.008658000	2.413337000
O	1.737052000	-1.050273000	-1.360919000
H	2.633132000	-0.708605000	-1.256794000
B	1.643606000	-2.426758000	-0.699509000
O	2.134490000	-3.384948000	-1.655432000
H	2.347305000	-4.205046000	-1.196971000
O	2.456389000	-2.471669000	0.504773000
H	2.025460000	-2.054009000	1.256347000
C	0.021522000	-2.545321000	-0.383792000
C	-0.918098000	-2.327789000	-1.415087000
C	-0.499546000	-2.960689000	0.863976000
C	-2.290399000	-2.544449000	-1.225463000
H	-0.559782000	-2.054923000	-2.411826000
C	-1.857269000	-3.161452000	1.063320000
H	0.191418000	-3.149532000	1.690297000
C	-2.758913000	-2.956788000	0.012245000
H	-2.987147000	-2.380716000	-2.050514000
H	-2.225632000	-3.483106000	2.040229000
H	-3.827762000	-3.117100000	0.170030000
C	-0.391634000	0.436285000	2.837362000
H	0.129997000	-0.517022000	2.666574000
H	0.312302000	1.240468000	2.579237000
H	-0.620756000	0.516125000	3.908433000
N	-6.179000000	0.823132000	-0.893844000
C	2.758979000	1.150694000	1.154114000
H	2.909002000	1.518568000	2.179687000
H	2.248906000	0.183902000	1.218988000
C	4.092876000	0.991018000	0.438616000
H	3.904244000	0.746449000	-0.621110000
H	4.630523000	1.953547000	0.432052000
C	4.955562000	-0.091971000	1.076433000
H	5.108150000	0.148921000	2.142397000
H	4.398780000	-1.042220000	1.042213000
C	6.302995000	-0.252185000	0.385069000
H	6.905581000	-1.041632000	0.858053000
H	6.172566000	-0.521114000	-0.675228000
H	6.885323000	0.682204000	0.420715000
C	-0.896103000	2.979325000	-1.622470000
H	-1.739851000	2.484579000	-1.129953000
H	-1.134683000	4.048911000	-1.683707000
C	-0.652300000	2.400140000	-3.005124000
H	-1.543489000	2.547205000	-3.631721000
H	0.200918000	2.892319000	-3.494486000
H	-0.446455000	1.321370000	-2.946734000

C	-4.935346000	-0.232745000	1.504069000
H	-4.137616000	0.511784000	3.347346000
C	-5.668645000	-1.075233000	-0.686613000
H	-5.946424000	-0.353627000	1.895318000
C	-1.557644000	0.964541000	2.762278000
H	-0.663475000	0.326229000	2.767285000
H	-1.244014000	1.967370000	2.437422000
H	-1.933204000	1.046932000	3.791177000
N	-6.490913000	-1.486929000	-1.387336000
C	1.192568000	2.505378000	1.249819000
H	0.974148000	3.054880000	2.177555000
H	1.047760000	1.438560000	1.455168000
C	2.621389000	2.764064000	0.799580000
H	2.778660000	2.281556000	-0.177402000
H	2.777300000	3.845925000	0.653603000
C	3.624058000	2.219947000	1.812118000
H	3.348813000	2.570352000	2.821628000
H	3.534372000	1.121221000	1.831278000
C	5.060372000	2.628138000	1.511584000
H	5.762359000	2.188381000	2.235644000
H	5.368334000	2.300045000	0.507045000
H	5.177619000	3.722477000	1.550817000
C	-2.236691000	2.312238000	-2.296139000
H	-2.888464000	1.573128000	-1.817806000
H	-2.865404000	3.163359000	-2.588386000
C	-1.529391000	1.719375000	-3.502627000
H	-2.270429000	1.385678000	-4.242791000
H	-0.873012000	2.461829000	-3.979777000
H	-0.920621000	0.851894000	-3.208710000
C	0.597353000	-2.030863000	0.328158000
C	-0.469005000	-2.495855000	-0.475384000
Si	2.330267000	-1.558478000	-0.520564000
C	0.404630000	-2.123610000	1.728762000
C	-1.621966000	-3.078890000	0.077650000
C	-0.741829000	-2.678558000	2.279295000
H	-0.850265000	-2.738322000	3.365252000
C	-1.758181000	-3.172278000	1.452084000
H	-2.654467000	-3.618289000	1.889090000
H	-2.410309000	-3.451115000	-0.580123000
H	-0.350145000	-2.512442000	-1.562773000
H	1.206360000	-1.770957000	2.379807000
O	3.083306000	-1.331364000	0.987187000
O	3.718603000	-1.102880000	-1.482352000
O	2.313856000	-3.093499000	-1.238596000
C	4.423674000	-1.569558000	1.311792000
H	4.871263000	-0.677221000	1.784275000
H	4.503975000	-2.402667000	2.032655000
H	5.030912000	-1.821222000	0.427372000
C	4.360463000	0.124922000	-1.424416000
H	5.385023000	0.042316000	-1.829199000
H	3.853621000	0.910832000	-2.026324000
H	4.446973000	0.520630000	-0.396754000
C	3.239812000	-3.656448000	-2.124859000
H	3.365640000	-3.053994000	-3.039094000
H	4.241676000	-3.767969000	-1.674265000
H	2.884785000	-4.660118000	-2.415212000

O	1.458623000	-0.141571000	-1.131062000
H	1.878072000	0.436034000	-1.779454000

TS2

Atom	X	Y	Z
Pd	0.956052000	0.119620000	-0.238217000
N	-0.665758000	2.693148000	-0.766810000
N	1.107620000	3.050531000	0.386195000
C	0.394922000	2.067307000	-0.210999000
C	-0.621217000	4.052461000	-0.518026000
H	-1.386132000	4.733052000	-0.880311000
C	0.499506000	4.278284000	0.206719000
H	0.917010000	5.197106000	0.608264000
C	-0.739535000	-0.391897000	0.666214000
C	-1.017977000	-0.093470000	2.017878000
C	-1.695366000	-1.107694000	-0.058143000
C	-2.236430000	-0.492690000	2.582536000
C	-2.913731000	-1.497959000	0.516675000
H	-1.505642000	-1.377227000	-1.098208000
C	-3.192168000	-1.183830000	1.849913000
H	-2.440997000	-0.253995000	3.629140000
C	-3.877222000	-2.207003000	-0.276536000
H	-4.138477000	-1.480906000	2.304156000
C	1.575842000	-1.984895000	-0.264536000
C	1.023514000	-2.697600000	-1.347295000
C	1.600508000	-2.651673000	0.972667000
C	0.508197000	-3.982584000	-1.204806000
H	0.997829000	-2.229447000	-2.336475000
C	1.091358000	-3.939287000	1.135632000
H	2.031872000	-2.138587000	1.836852000
C	0.537643000	-4.606027000	0.044168000
H	0.080645000	-4.503527000	-2.065269000
H	1.122352000	-4.423848000	2.114783000
H	0.133661000	-5.614415000	0.163438000
O	2.891068000	0.367765000	-1.143017000
B	3.277187000	-0.943368000	-0.658334000
O	3.837411000	-1.717553000	-1.689434000
H	3.888673000	-2.652125000	-1.462673000
O	3.905788000	-0.818751000	0.593067000
H	4.236187000	-1.663245000	0.915990000
H	2.837839000	0.366495000	-2.107861000
C	-0.025210000	0.652864000	2.868344000
H	0.972484000	0.194532000	2.799562000
H	0.078488000	1.692968000	2.524148000
H	-0.328214000	0.673025000	3.924209000
N	-4.652547000	-2.765619000	-0.927569000
C	2.378170000	2.873163000	1.084619000
H	2.326442000	3.452775000	2.017578000
H	2.450850000	1.812293000	1.353146000
C	3.567758000	3.294228000	0.239547000
H	3.636201000	2.655668000	-0.650828000
H	3.486572000	4.346974000	-0.069248000
H	4.494293000	3.179303000	0.820568000
C	-1.752247000	2.050044000	-1.494646000
H	-1.920398000	2.616176000	-2.422978000
H	-1.404354000	1.049229000	-1.775605000

TS2′

Atom	X	Y	Z
Pd	-0.071064000	0.333517000	0.098116000
C	1.414099000	-0.116453000	-1.132150000
C	1.335327000	0.116432000	-2.521286000
C	-0.632184000	-1.751931000	0.166329000
C	-0.100529000	-2.316298000	1.343363000
Si	-2.747502000	-0.788708000	0.408965000
C	-0.573932000	-2.549207000	-0.990973000
C	0.463202000	-3.589677000	1.368620000
C	-0.027156000	-3.829572000	-0.983774000
H	-0.000463000	-4.423980000	-1.900755000
C	0.498644000	-4.350151000	0.199301000
H	0.936532000	-5.351634000	0.210466000
C	2.537228000	-0.776895000	-0.632819000
C	3.581931000	-1.184821000	-1.476070000
C	4.720668000	-1.854793000	-0.914403000
C	2.382842000	-0.299633000	-3.353292000
C	3.507338000	-0.941685000	-2.851025000
H	4.313686000	-1.257454000	-3.514525000
H	0.873847000	-3.994211000	2.297395000
H	-0.135833000	-1.741809000	2.274883000
H	-0.973136000	-2.141595000	-1.922931000
H	2.610933000	-1.004000000	0.432035000
H	2.311162000	-0.118510000	-4.428747000
O	-2.707886000	-0.501712000	-1.243363000
O	-4.287912000	-0.136464000	0.755529000
O	-3.088583000	-2.303614000	0.999310000
C	-3.738994000	-0.880016000	-2.121719000
H	-4.738765000	-0.737189000	-1.679033000
H	-3.671578000	-0.267992000	-3.034335000
H	-3.640726000	-1.940745000	-2.412816000
C	-4.727000000	1.139614000	0.403014000
H	-4.353881000	1.461213000	-0.586779000
H	-5.828901000	1.159047000	0.364962000
H	-4.419789000	1.909495000	1.137618000
C	-4.314790000	-2.730148000	1.547772000
H	-4.605712000	-2.132199000	2.425651000
H	-5.138292000	-2.667126000	0.818469000
H	-4.201238000	-3.780247000	1.858559000
O	-1.854799000	0.353031000	1.332914000
H	-2.358637000	1.090566000	1.700957000
C	0.133423000	0.797784000	-3.118214000
H	-0.797685000	0.365454000	-2.720898000
H	0.128448000	1.865652000	-2.850296000
H	0.127784000	0.725725000	-4.214807000
N	5.634155000	-2.388243000	-0.447294000
N	-0.161139000	3.325444000	-0.392354000
N	1.676681000	2.821631000	0.593996000
C	0.540320000	2.277765000	0.099726000
C	0.527293000	4.510709000	-0.211560000
H	0.135938000	5.469305000	-0.538834000
C	1.685610000	4.191614000	0.411032000

C	-3.034135000	1.964351000	-0.678192000
H	-3.362628000	2.980599000	-0.402372000
H	-2.819006000	1.432868000	0.261745000
C	-4.148884000	1.250463000	-1.433167000
H	-3.791737000	0.255750000	-1.747299000
H	-4.373820000	1.800785000	-2.362696000
C	-5.415617000	1.095112000	-0.602532000
H	-5.815046000	2.075714000	-0.299124000
H	-6.202462000	0.567564000	-1.161462000
H	-5.212228000	0.520685000	0.314637000
H	2.514479000	4.814196000	0.734961000
C	2.781880000	2.084042000	1.203554000
H	3.538039000	2.826376000	1.491998000
H	3.231856000	1.441297000	0.435251000
C	2.373144000	1.253213000	2.409462000
H	1.915374000	1.909443000	3.168526000
H	1.592525000	0.538977000	2.100200000
C	3.548951000	0.491835000	3.010531000
H	4.306540000	1.207334000	3.372900000
H	4.043914000	-0.097041000	2.219131000
C	-1.488860000	3.252571000	-0.996216000
H	-1.434445000	3.706839000	-1.996558000
H	-1.723279000	2.189023000	-1.130670000
C	-2.541789000	3.946911000	-0.149641000
H	-2.324845000	5.018603000	-0.034592000
H	-3.528204000	3.849300000	-0.623288000
H	-2.593768000	3.500215000	0.853531000
C	3.123844000	-0.435104000	4.142083000
H	3.983096000	-0.972459000	4.569641000
H	2.639545000	0.127767000	4.955555000
H	2.401922000	-1.185870000	3.782896000

Int6

Atom	X	Y	Z
Pd	0.374715000	0.510536000	-0.415255000
N	1.626435000	-2.238415000	0.404612000
N	2.925874000	-1.168620000	-0.918471000
C	1.713078000	-1.100088000	-0.323086000
C	2.772268000	-3.000584000	0.274297000
H	2.896054000	-3.955029000	0.777831000
C	3.595152000	-2.324352000	-0.561937000
H	4.586590000	-2.564009000	-0.935470000
C	-1.080750000	-0.586198000	-1.197020000
C	-1.074969000	-1.018765000	-2.541876000
C	-2.137995000	-0.995832000	-0.382278000
C	-2.108682000	-1.837746000	-3.014145000
C	-3.160167000	-1.829143000	-0.862170000
H	-2.181039000	-0.678788000	0.660870000
C	-3.149483000	-2.253908000	-2.193664000
H	-2.093952000	-2.163137000	-4.057387000
C	-4.207998000	-2.242663000	0.027904000
H	-3.941768000	-2.897799000	-2.577998000
C	-0.860404000	2.134928000	-0.411318000
C	-1.885861000	2.308255000	0.538146000
C	-0.572655000	3.248809000	-1.224562000
C	-2.567108000	3.519093000	0.684921000
H	-2.170697000	1.475189000	1.188489000
C	-1.255351000	4.461368000	-1.093180000
H	0.208555000	3.175463000	-1.988923000
C	-2.254385000	4.604012000	-0.132970000
H	-3.350594000	3.613738000	1.441719000
H	-1.002088000	5.301139000	-1.746093000
H	-2.786619000	5.551681000	-0.023248000
O	2.522515000	0.834313000	2.552516000
B	1.615986000	1.652162000	1.965891000
O	0.544211000	2.123164000	2.651252000
H	-0.143669000	2.530974000	2.102714000

Int6′

Atom	X	Y	Z
Pd	-0.123319000	0.071861000	0.225209000
N	-1.504659000	2.797910000	-0.494298000
N	0.145994000	3.104427000	0.833541000
C	-0.542192000	2.133796000	0.188926000
C	-1.418030000	4.160770000	-0.280563000
H	-2.106181000	4.865964000	-0.737627000
C	-0.374555000	4.355729000	0.559997000
H	0.036102000	5.266420000	0.986082000
C	-1.886089000	-0.369288000	1.016597000
C	-2.195788000	-0.107804000	2.370153000
C	-2.880096000	-0.943696000	0.218735000
C	-3.470555000	-0.411218000	2.866351000
C	-4.157407000	-1.231552000	0.723396000
H	-2.672114000	-1.177174000	-0.827159000
C	-4.458653000	-0.964265000	2.062442000
H	-3.695878000	-0.203630000	3.915533000
C	-5.148854000	-1.799188000	-0.146250000
H	-5.447462000	-1.188582000	2.464991000
C	0.270742000	-1.933814000	0.245777000
C	0.642040000	-2.568874000	-0.956058000
C	0.268156000	-2.742359000	1.398718000
C	0.983145000	-3.920305000	-1.007277000
H	0.673854000	-1.990842000	-1.885058000
C	0.631291000	-4.092231000	1.362907000
H	-0.037469000	-2.311233000	2.357151000
C	0.987003000	-4.689601000	0.156196000
H	1.259520000	-4.375877000	-1.962201000
H	0.625869000	-4.681685000	2.283940000
H	1.264092000	-5.745857000	0.120813000
C	-1.176881000	0.515723000	3.286439000
H	-0.962364000	1.549052000	2.972990000
H	-1.522908000	0.538252000	4.329188000
H	-0.220718000	-0.026890000	3.244324000

O	1.858374000	1.958240000	0.627797000	N	-5.941018000	-2.248343000	-0.859044000
H	1.411575000	2.766302000	0.331517000	C	1.301909000	2.882588000	1.696486000
H	2.266453000	0.584526000	3.449281000	H	1.086789000	3.336438000	2.675593000
C	0.042503000	-0.628878000	-3.471099000	H	1.379889000	1.798593000	1.844405000
H	0.991427000	-1.074568000	-3.134627000	C	2.584589000	3.445114000	1.110013000
H	-0.146597000	-0.960973000	-4.501381000	H	2.825843000	2.954185000	0.158967000
H	0.190578000	0.461396000	-3.475520000	H	2.508983000	4.530423000	0.948022000
N	-5.040619000	-2.574080000	0.758771000	H	3.420152000	3.259541000	1.799167000
C	3.495613000	-0.139143000	-1.781533000	C	-2.522370000	2.168869000	-1.331776000
H	3.947654000	-0.642193000	-2.648811000	H	-3.119666000	1.496001000	-0.702051000
H	2.658428000	0.466638000	-2.150686000	H	-3.188572000	2.967926000	-1.684452000
C	4.513822000	0.727615000	-1.060024000	C	-1.944748000	1.402035000	-2.511017000
H	4.034866000	1.256977000	-0.225690000	H	-1.267219000	0.622646000	-2.123780000
H	5.345609000	0.121593000	-0.671163000	H	-1.328650000	2.081501000	-3.123802000
H	4.930563000	1.470916000	-1.755191000	C	-3.026706000	0.756779000	-3.368355000
C	0.476402000	-2.632747000	1.214342000	H	-3.670962000	0.129701000	-2.728392000
H	-0.397600000	-2.719982000	0.554945000	H	-3.683651000	1.539664000	-3.784206000
H	0.690140000	-3.634781000	1.610230000	C	-2.449427000	-0.089418000	-4.495611000
C	0.178932000	-1.667363000	2.350378000	H	-1.823917000	-0.903090000	-4.095021000
H	-0.029278000	-0.674435000	1.920895000	H	-3.242133000	-0.545009000	-5.107183000
H	1.078028000	-1.554770000	2.977259000	H	-1.816220000	0.517093000	-5.162279000
C	-1.007239000	-2.105502000	3.199648000	Si	3.290548000	-0.245235000	-0.128899000
H	-1.883411000	-2.264070000	2.547577000	O	3.797586000	-1.358872000	-1.215063000
H	-0.792334000	-3.084482000	3.660874000	O	4.415273000	0.935914000	0.000037000
C	-1.350104000	-1.085489000	4.277990000	O	1.917192000	0.509287000	-0.711585000
H	-1.587637000	-0.106981000	3.831275000	O	2.942726000	-0.875521000	1.340527000
H	-2.215413000	-1.403184000	4.878076000	H	2.158230000	-1.453191000	1.361465000
H	-0.501008000	-0.934829000	4.963389000	C	4.181138000	-2.699691000	-0.994535000
				H	5.279324000	-2.781662000	-0.956498000
				H	3.762927000	-3.095210000	-0.056376000
				H	3.809199000	-3.321737000	-1.820645000
				C	5.813463000	0.771251000	-0.111516000
				H	6.258189000	1.726328000	-0.425739000
				H	6.255611000	0.483792000	0.856293000
				H	6.070688000	0.001994000	-0.857760000
				C	1.912073000	1.145281000	-1.986639000
				H	1.587130000	0.437375000	-2.763757000
				H	1.210301000	1.988264000	-1.951924000
				H	2.914769000	1.526009000	-2.231953000

Int7

Atom	X	Y	Z
Pd	-0.918752000	-0.560617000	-0.376328000
N	1.863115000	-2.014677000	-0.593874000
N	0.596117000	-3.019520000	0.806066000
C	0.642669000	-1.941847000	-0.012609000
C	2.565658000	-3.119315000	-0.150304000
H	3.566815000	-3.355148000	-0.499132000
C	1.760942000	-3.757584000	0.732595000
H	1.914652000	-4.664367000	1.310714000
C	-0.225172000	0.834651000	0.827527000
C	-0.774641000	1.087962000	2.104434000
C	0.857180000	1.608175000	0.405389000
C	-0.202372000	2.076378000	2.915676000
C	1.414049000	2.599592000	1.228885000
H	1.291784000	1.459206000	-0.582845000
C	0.884768000	2.833833000	2.500392000

H	-0.629032000	2.260771000	3.904572000
C	2.536612000	3.360906000	0.759426000
H	1.314246000	3.598503000	3.148976000
C	-2.496681000	0.625070000	-0.837619000
C	-3.547543000	-0.088776000	-1.445202000
C	-2.678612000	2.011596000	-0.701055000
C	-4.710513000	0.539421000	-1.896304000
H	-3.467452000	-1.175876000	-1.575088000
C	-3.836322000	2.649986000	-1.148688000
H	-1.898501000	2.614595000	-0.229392000
C	-4.859923000	1.917220000	-1.748546000
H	-5.504655000	-0.050762000	-2.362157000
H	-3.941122000	3.732053000	-1.027790000
H	-5.767406000	2.416129000	-2.097387000
C	-1.979650000	0.340013000	2.603513000
H	-2.830339000	0.501294000	1.924976000
H	-1.795481000	-0.743555000	2.623282000
H	-2.266201000	0.658728000	3.615124000
N	3.447201000	3.961874000	0.376106000
C	-0.570392000	-3.410677000	1.589539000
H	-0.214525000	-4.028924000	2.424693000
H	-1.002878000	-2.497926000	2.016223000
C	-1.603138000	-4.155904000	0.761168000
H	-1.970195000	-3.520631000	-0.058697000
H	-1.176032000	-5.072016000	0.327326000
H	-2.460335000	-4.437394000	1.389493000
C	2.390317000	-1.062240000	-1.561837000
H	2.666829000	-1.612063000	-2.474468000
H	1.563153000	-0.390401000	-1.826434000
C	3.585986000	-0.279413000	-1.036434000
H	4.402797000	-0.977770000	-0.789558000
H	3.305747000	0.217881000	-0.093559000
C	4.085273000	0.749309000	-2.044812000
H	4.309123000	0.240645000	-2.998044000
H	3.274158000	1.464469000	-2.266670000
C	5.315788000	1.506072000	-1.562058000
H	6.142809000	0.814010000	-1.337417000
H	5.671099000	2.217502000	-2.322402000
H	5.092791000	2.079137000	-0.649788000

TS3

Atom	**X**	**Y**	**Z**
N	2.606572000	1.267399000	-0.802608000
N	3.501895000	-0.669723000	-0.670004000
C	2.303217000	-0.040086000	-0.625783000
C	3.969382000	1.455582000	-0.934909000
H	4.410408000	2.436259000	-1.089355000
C	4.536871000	0.228016000	-0.851790000
H	5.575155000	-0.084118000	-0.919750000
C	3.681891000	-2.104222000	-0.474542000
H	2.866434000	-2.616829000	-1.003245000
H	4.621078000	-2.389870000	-0.967929000
C	3.698601000	-2.493185000	0.994464000
H	2.744077000	-2.225864000	1.471781000
H	3.845922000	-3.577933000	1.097284000
H	4.512501000	-1.981140000	1.528704000
C	1.630933000	2.347969000	-0.772068000

H	1.997314000	3.153242000	-1.425250000
H	0.697222000	1.962911000	-1.202827000
C	1.379626000	2.867162000	0.635727000
H	2.331971000	3.210869000	1.074204000
H	1.026327000	2.027302000	1.255407000
C	0.355535000	3.994597000	0.661341000
H	-0.576754000	3.642064000	0.190827000
H	0.718000000	4.832672000	0.041578000
C	0.057531000	4.486188000	2.071245000
H	-0.688563000	5.294748000	2.068751000
H	-0.337190000	3.669307000	2.695347000
H	0.967222000	4.868256000	2.560964000
C	-1.313240000	-1.917696000	0.101609000
C	-1.970202000	-2.471385000	-1.014152000
C	-1.356824000	-2.647706000	1.304059000
C	-2.619628000	-3.699549000	-0.938997000
H	-1.980121000	-1.934866000	-1.964560000
C	-2.014442000	-3.875734000	1.380784000
H	-0.860627000	-2.268267000	2.194956000
C	-2.651384000	-4.407449000	0.262903000
H	-3.110116000	-4.105340000	-1.827155000
H	-2.023397000	-4.421326000	2.327630000
C	-1.352263000	0.052459000	0.159306000
C	-2.016469000	0.592275000	-0.956192000
C	-1.548580000	0.693901000	1.409939000
C	-2.847295000	1.710952000	-0.855100000
H	-1.889040000	0.134356000	-1.936719000
C	-2.407218000	1.797350000	1.492661000
C	-3.063134000	2.316907000	0.387903000
C	-3.479759000	2.233707000	-2.034086000
H	-2.547135000	2.278037000	2.463822000
H	-3.170409000	-5.366349000	0.325611000
H	-3.718385000	3.183689000	0.479660000
Pd	0.413347000	-0.895324000	-0.254359000
C	-0.850168000	0.256963000	2.669487000
H	-1.474236000	-0.442473000	3.248306000
H	0.102791000	-0.241747000	2.447377000
H	-0.645626000	1.120293000	3.318474000
N	-3.986561000	2.654460000	-2.983991000

Int8

Atom	X	Y	Z
Pd	4.118553000	0.342156000	-0.145830000
N	1.243880000	0.257500000	-1.004770000
N	2.016966000	-1.724341000	-0.722053000
C	2.382958000	-0.412789000	-0.670272000
C	0.197643000	-0.613114000	-1.241522000
H	-0.793748000	-0.268313000	-1.515555000
C	0.684020000	-1.863375000	-1.062151000
H	0.202491000	-2.832766000	-1.153054000
C	1.116637000	1.706866000	-1.032801000
H	0.347177000	1.966382000	-1.774873000
H	2.076674000	2.109938000	-1.384262000
C	0.769914000	2.298366000	0.326555000
H	1.509540000	1.929975000	1.057297000
H	-0.218746000	1.929309000	0.648059000
C	0.775292000	3.822266000	0.312453000

H	1.752134000	4.176379000	-0.060032000
H	0.022543000	4.181070000	-0.409073000
C	0.502372000	4.426644000	1.683388000
H	-0.477108000	4.103805000	2.066788000
H	0.504532000	5.526438000	1.648650000
H	1.265403000	4.111650000	2.412744000
C	2.890136000	-2.843789000	-0.393627000
H	2.564347000	-3.705852000	-0.993353000
H	3.902229000	-2.569554000	-0.720458000
C	2.880669000	-3.178885000	1.088815000
H	1.872508000	-3.452935000	1.432238000
H	3.554984000	-4.024888000	1.288343000
H	3.228912000	-2.312761000	1.671265000
C	-2.895686000	1.645260000	-1.042606000
C	-3.097738000	0.900749000	0.126040000
C	-3.146002000	1.575709000	1.351267000
C	-3.008739000	2.960334000	1.405907000
C	-2.808052000	3.690559000	0.236804000
C	-2.747690000	3.028446000	-0.987536000
C	-3.206859000	-0.584209000	0.084355000
C	-2.311100000	-1.329092000	0.851799000
C	-2.331507000	-2.726025000	0.829705000
C	-3.274154000	-3.395034000	0.042334000
C	-4.178965000	-2.653359000	-0.702616000
C	-4.166761000	-1.253286000	-0.703997000
H	-1.562406000	-0.811235000	1.452386000
C	-5.180792000	-0.509885000	-1.530265000
H	-3.297688000	-4.485261000	0.017841000
H	-3.302708000	1.007197000	2.270497000
H	-2.841214000	1.136469000	-2.007007000
C	-1.359662000	-3.460588000	1.588733000
H	-4.926020000	-3.175714000	-1.303758000
H	-2.579520000	3.591724000	-1.907767000
H	-2.690162000	4.775075000	0.280728000
H	-3.056421000	3.471406000	2.369740000
H	-6.057365000	-1.140587000	-1.729837000
H	-5.514027000	0.410172000	-1.031874000
H	-4.760170000	-0.214655000	-2.503814000
N	-0.560162000	-4.042053000	2.187070000