Supporting Information

Investigations into the Stability of Tethered Pd^{II} Pincer Complexes During Heck Catalysis

William J. Sommer[#], Kunquan Yu[§], John S. Sears[#], Yaying Ji[‡], Xiaolai Zheng[#], Robert J. Davis[‡], C. David Sherrill[#,], Christopher W. Jones[§,#,*] Marcus Weck[#,*]*

[#]School of Chemistry and Biochemistry and [§]School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA.

[‡]Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22904, USA.

X-ray Absorption Spectroscopy of Immobilized SCS Pd Pincer Compounds

Experimental Methods

X-ray absorption spectroscopy was conducted on beamlines X10C and X18B at the National Synchrotron Light Source, Brookhaven National Lab, Upton, NY. The Pd K edge spectra of catalysts and reference compounds were recorded at room temperature except those collected during the Heck reaction performed at 393 K. Spectra of samples in solvent or reaction medium were recorded in the fluorescence mode whereas other spectra were recorded in the transmission mode. For transmission measurements, ion-chambers were filled with Ar to have an absorbance of 10% in the first chamber and 80% in the second. A Pd foil (Goodfellow) was placed between the second and third ion chambers for energy calibration. At least four spectra were averaged for each sample studied in the transmission mode. For the samples examined during the Heck

reaction, an in-situ cell was constructed with Teflon as body material and Kapton as the window. The reaction slurry was continuously pumped from a heated, stirred reactor vessel to the in-situ cell. To improve the signal-to-noise ratio during the measurement, at least ten scans were averaged. Two data analysis methods were used in this work, specifically, fitting of a linear combination of the edge spectra and fitting of standard multi-shell EXAFS data. The data analysis was performed with the WinXAS 2.1 program. The pre-edge background was removed with a linear function and the post-edge background was subtracted with a cubic spline method. According to the Nyquist theorem,[1] the number of free parameters for EXAFS curve-fitting are determined by the available data range in *k* space and R space : Npts = $2\Delta k^*\Delta R/\pi + 2$. Typically, 16 parameters can be determined from the data.

Results and Discussion

Reference Compounds

The X-ray absorption near edge structure (XANES) associated with the Pd K edge of different reference materials is shown in Supplemental Figure 1. The zero valent Pd foil revealed a distinctly different edge shape compared to the other reference compounds having Pd in a higher oxidation state. The PdS and $PdCl_2$ samples have very similar XANES spectra, and the quick decay of oscillations above the peak at ~ 24360 eV in $Pd(NH_3)_4Cl_2$ was due to the presence of light N atoms as the nearest neighbor backscatterers. The Fourier transforms of the k^3 weighted EXAFS data are shown in Supplemental Figure 2. The large peak in each transform results from the first shell backscatterer atoms. The position of the peak is related to the first shell interatomic distance, not corrected for phase shift, whereas the intensity of the peak is

related to the number of nearest neighbor backscatterers, the atomic number of the backscatterer and the disorder in the sample.

We used the program FEFF 8.20 to calculate theoretical reference files containing the appropriate backscattering amplitudes and phase shifts for various absorber-backscatterer pairs.[2] We then used the EXAFS data from the reference spectra to calibrate the reference files calculated by FEFF. The known structural parameters for each standard compound listed in Table 1 were used in the calibration process. Curve-fitting of reference data with k^3- weighting was performed in R-space to produce a set of parameters for the calibration of theoretical FEFF reference files. Table 2 summarizes these parameters derived from curve fitting that were subsequently input to the revised theoretical FEFF reference files.[3] Since a reference compound having a Pd-C first shell was not available, we used the Pd-N reference file as a substitute.

Influence of immobilization

Supplemental Figure 3 shows the XANES of immobilized SCS pincer compounds on SBA and polymer support. Although the spectra are similar, with an obvious white line present at the absorption threshold, a subtle difference in the XANES can still be observed. The k^2 weighted Fourier transform of the EXAFS (Supplemental Figure 4) revealed that both samples have light backscatterers around Pd (at ~1.9 Å) associated with the pincer complex, but that a new peak was present at ~2.5 Å in the SBA-immobilized compound. It is reasonable to assume that this long distance may be due to the presence of some Pd in the first coordination shell, presumably from a small amount of Pd metal. Assuming the spectrum can be decomposed into contributions from the SCS pincer complex and metallic Pd, we performed a fitting analysis utilizing a linear combination of the edge spectra for SBA immobilized SCS pincer Pd. This method has been

used previously to study the local structure around an absorbing atom.[4,5] The XANES fitting analysis was performed in a region up to 150 eV above the edge. The fitting parameters in Table 3 indicated that 6.5% of the Pd in SBA immobilized SCS pincer complex was metallic in nature whereas 93.3% of the Pd was present in the SCS pincer complex. The estimated coordination number of the Pd-Pd shell was only about 0.8.

Curve-fitting of the EXAFS data with FEFF reference files utilizing k^2 weighting in R space was performed on the spectra of SBA and polymer-immobilized SCS pincer complex with a fixed S_0^2 value of 0.9. Since the number of free parameters in the fitting routine is so high (16), many are correlated, and the Nyquist theorem dictates only 16 can be independently fit, the coordination numbers and interatomic distances were fixed to a small region near the estimated values. In addition, the Debye-Waller factor was forced to be non-negative. Reasonable values of Debye-Waller factor and ΔE_0 as shown in Table 4 suggest that immobilization of the complex on the SBA support and the polymer did not cause a significant change in the atomic structure around Pd bound in the SCS pincer complex. However, curve-fitting for SBA immobilized SCS pincer Pd provided a coordination number of 1.4 and an interatomic distance of 2.71 Å for Pd-Pd shell as shown in Table 4. The Pd-Pd bond length is 0.04 Å shorter than that in bulk Pd, which suggests that the metallic particles must be nanometer size or less. Both fitting methods suggest that the new peak in Fourier transform of SBA-immobilized SCS pincer Pd can be assigned to the presence of small metallic Pd particles on the support, and most of Pd still remain bound in SCS pincer complex after immobilization on SBA support. It should be noted that if any O atoms were present on the Pd metal surface, they could not be distinguished from nearest neighbor C atoms associated with Pd in the pincer complex.

In-situ X-ray Absorption Spectroscopy during Heck Reaction

The influence of the solvent DMF on the structure of polymer-immobilized SCS pincer Pd was also investigated. As shown in Supplemental Figure 3, no change in XANES was observed between a sample in air and one dissolved in DMF. Likewise, the Fourier transform of the EXAFS region showed the same backscattering contribution in both samples (not shown). The linear combination of XANES analysis showed only the contribution from SCS pincer complex after stirring in DMF. Apparently, there is little change in the local environment around Pd with solvent addition.

To better understand the reaction mechanism of Heck catalysis, Evans *et al*. performed an *in-situ* X-ray absorption study of the Heck reaction with Pd acetate as catalyst.[6] We also performed an *in-situ* study during the Heck reaction catalyzed by polymer immobilized SCS Pd in DMF, with iodobenzene and butylacrylate as substrates and triethylamine as base. The Heck reaction was first carried out in flask at 393 K. Then the reacted solution was pumped into an *in-situ* cell from the reactor. A uniform solution (or suspension of catalyst in solution when the silica system was used) was achieved by recirculation between the cell and the reactor. Supplemental Figure 5 shows k^2-weighted Fourier transform of the EXAFS for a sample in air and a sample during Heck reaction. A new feature was observed at ~2.5 Å, which could arise from the backscattering contribution of a Pd-Pd or a Pd-I shell. In order to distinguish between them, we performed a fitting of the edge spectra involving SCS pincer complex on polymer, metallic Pd and PdI_2. The fitting results presented in Table 3 suggest that iodine was present in the first coordination shell of Pd. Although most of the Pd was associated with SCS pincer complex (85.5%), a Pd-I coordination number of ~ 0.6 was derived from the fitting procedure. Interestingly, no evidence for metallic Pd was found in the XANES, as shown in Supplemental Figure 6. To further support

this conclusion, a similar study was also performed with the SBA-immobilized SCS pincer complex, which was insoluble in DMF. In this case, the XANES fitting results also showed the presence of Pd-I in addition to a large amount of SCS pincer complex. A small amount of metallic Pd determined by the XANES fitting results may have been formed in the process of the immobilization, as discussed above. The observation of Pd-I compounds during Heck catalysis is in a good agreement with the results reported by Evans *et al*..[6]

The coordination number of Pd-I in Table 4 was about 1.2 as determined by EXAFS fitting in R space with k^2 weighting, the experimental data are compared to the fitted results with k^2-weighting in Supplemental Figure 7. The average Pd-I coordination number was slightly lower than those reported by Evans et al. (1.8 or 2.3) who studied Pd acetate as a catalyst for the Heck reaction.[6] The Pd in our study remained mostly bound in the SCS pincer complex, which may be related to its higher stability during Heck catalysis compared to Pd acetate. In order to achieve a good fitting for the Pd-I contribution, the interatomic distance of Pd-I shell need be lengthened to 2.67 Å, which is somewhat longer than the value in PdI_2. A long Pd-I bond was also observed by Evans et al. during their EXAFS study of $[Pd_2I_6][NEt_3H]_2$ dissolved in CH_3CN.[6]

Summary

The X-ray absorption spectroscopic studies have provided the following information on the Pd(II) SCS-O system in support of our previous results:[7]

- The Pd species are altered under reaction conditions, with a fraction of the pincer species supported on poly(norbornene) or silica decomposing to form new species.

- Heating the immobilized species in DMF did not result in any notable change in the Pd species as determined by spectroscopy. Previously, it was shown that base and one

of the reactants was required for generation of soluble catalytic species[7a]. Other characterization studies described in this work show that the addition of base is the key step that causes complex decomposition for both SCS and PCP complexes. No observation of decomposition in the presence of base and solvent alone in our previous work[7a] could be a consequence of several factors including:

(i) The presence of a silica support in our previous studies that could trap the Pd-pincer decomposition products in circumstances when aryl iodide or olefin are not present. In this work we show that the predominant mobile species may be a Pd-iodo species.

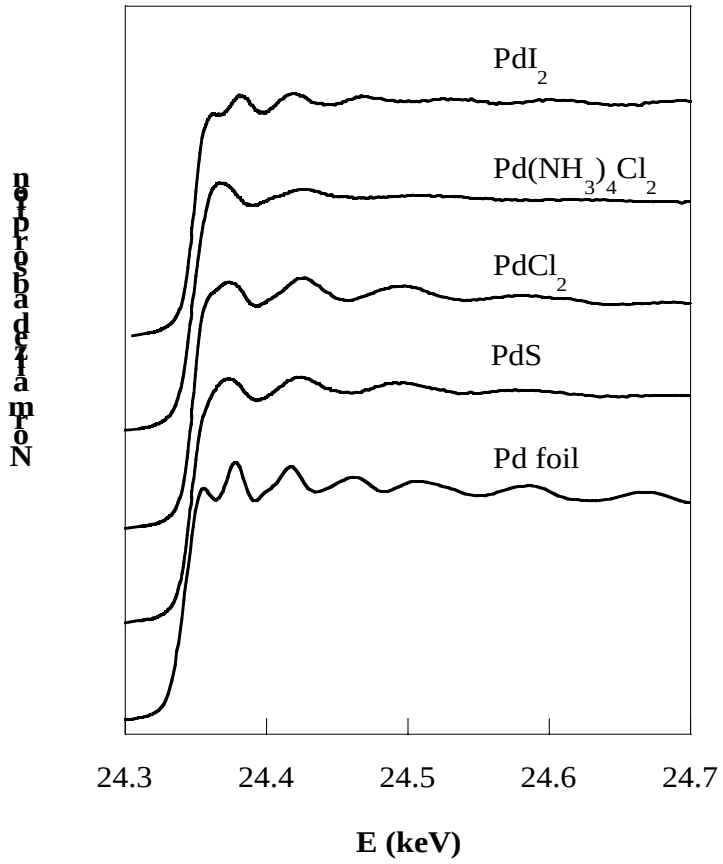
(ii) Variability in the water content in the reaction solution between our preliminary work[7a] and this work.

Furthermore, additional information obtained during this study:

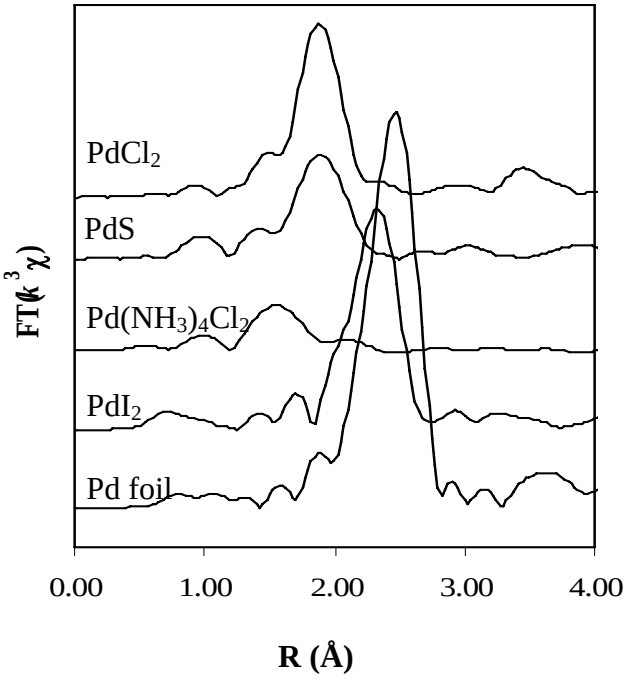
- Pd(II) SCS-O pincer species supported on silica have a small amount of Pd(0) that is formed during synthesis, most likely during the immobilization step. Pd(II) SCS-pincer species supported on poly(norbornene) look similar to the small molecule complex as determined by XAS.
- Palladium(II) iodo species are hypothesized to be the primary species formed under reaction conditions based on EXAFS and XANES analysis.[8] This is consistent with our works, which have found that Pd-iodo species are the primary resting state for Pd in the Heck reaction. This signal may also be enhanced in the EXAFS spectra by halide exchange under reaction conditions resulting from exchange of the HI formed in the reaction with the Pd-Cl bonds in the remaining unreacted pincer complexes (only a fraction decompose) to create Pd-I bonds and liberate HCl.

References.

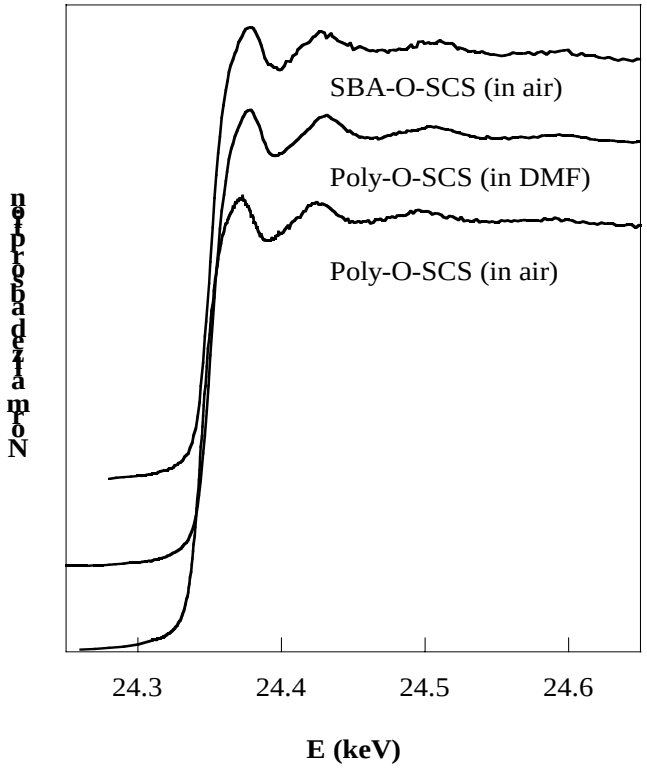
1. E. A. Stern, *Phys. Rev. B.* **1993**, *48*, 9825.
2. A. L. Ankudinov, B. Ravel, J. J. Rehr, S. D. Conradson, *Phys. Rev. B.* **1998**, *58*, 7565.
3. D. C. Koningsberger, B. L. Mojet, G. E. van Dorssen, D. E. Ramaker, *Top. Catal.* **2000**, *10*, 143-155.
4. J. W. Sobczak, E. Sobczak, A. Drelinkiewicz, M. Hasik, E. Wenda, *J. All. and Comp.* **2004**, *362*, 162-166.
5. T. Shido, A. Yamaguchi, Y. Inada, K. Asakura, M. Nomura, Y. Iwasawa, *Top. Catal.* **2002**, *18*, 53.
6. J. Evans, L. O'Neill, V. L. Kambhampati, G. Rayner, S. Turin, A. Genge, A. J. Dent and T. Neisius, *J. Chem. Soc., Dalton Trans.* **2002**, 2207-2212.
7. a) K. Yu, W. Sommer, M. Weck, C. W. Jones, *J. Catal.* **2004,** *226*, 101.; b) K. Yu, W. Sommer, M. Weck, C. W. Jones, *Adv. Synth. Catal.* **2005,** *347*, 161-171.
8. M. T. Reetz, J. G. de Vries *Chem. Commun.* **2004**, 1559-1563.



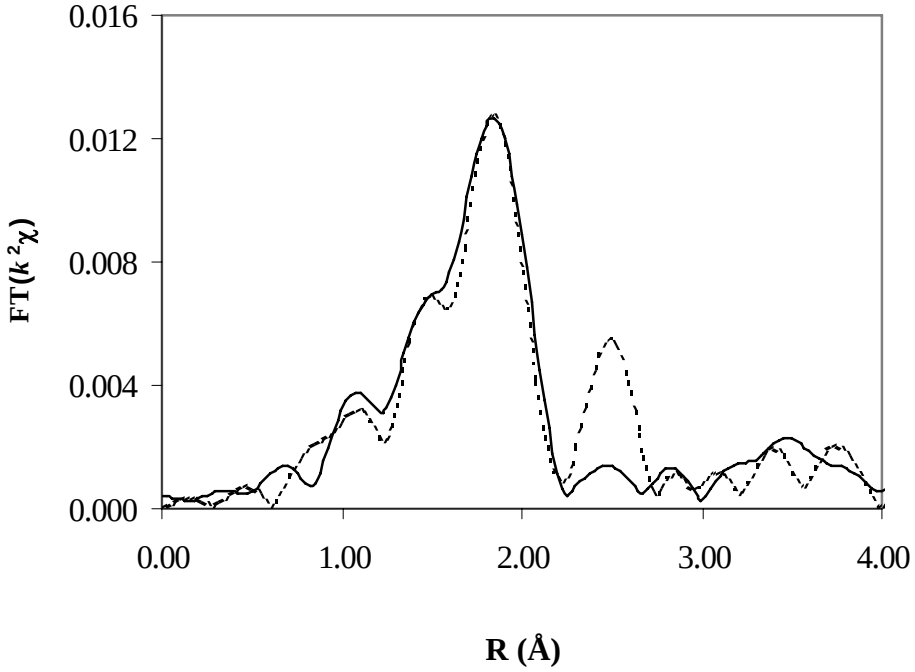
Supplemental Figure 1. Pd K edge spectra of standard compounds.



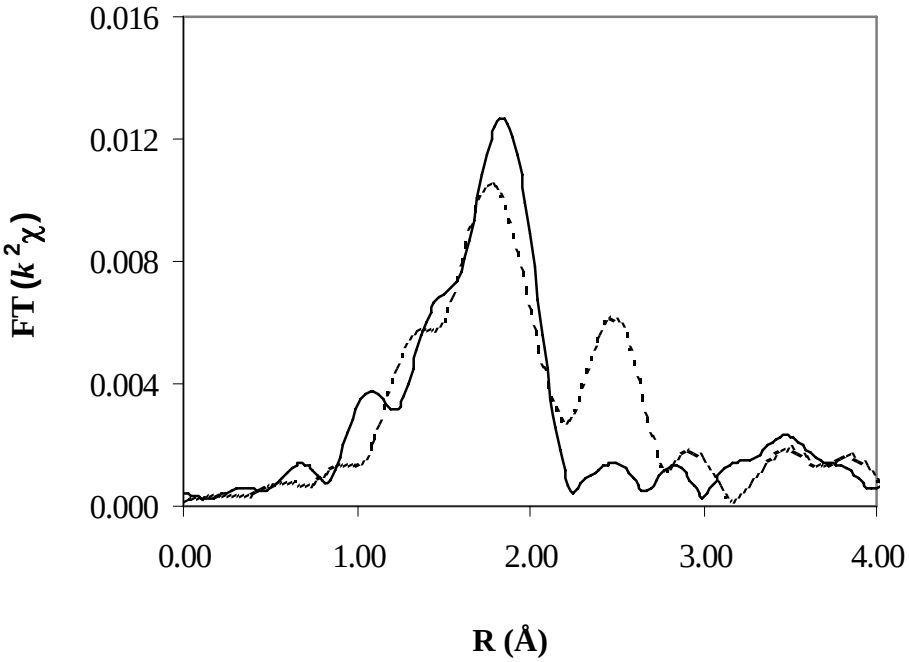
Supplemental Figure 2. k^3-weighted Fourier transform of EXAFS for standard compounds.



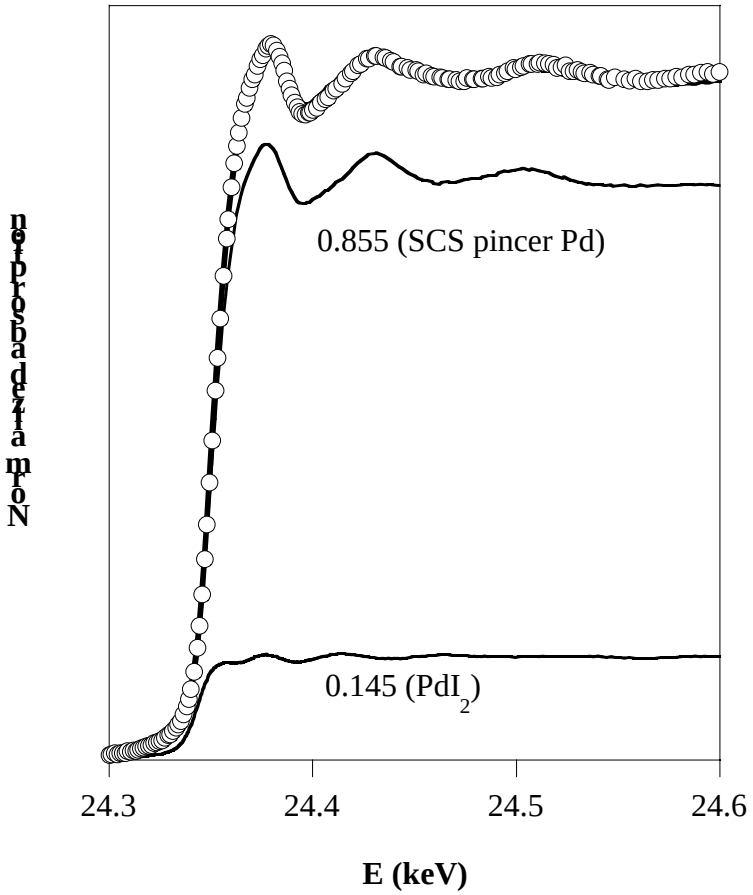
Supplemental Figure 3. Pd K edge spectra of SCS pincer compounds.



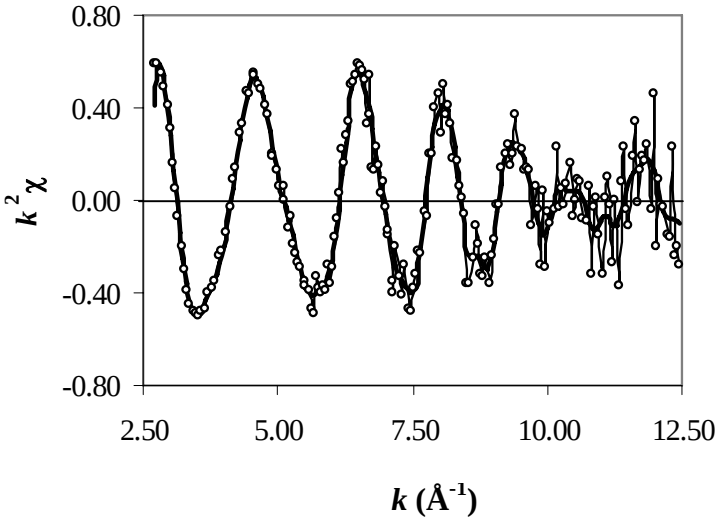
Supplemental Figure 4. k^2-weighted Fourier transform of EXAFS for immobilized SCS pincer Pd measured in air at RT (— : Poly-O-SCS; … : SBA-O-SCS).

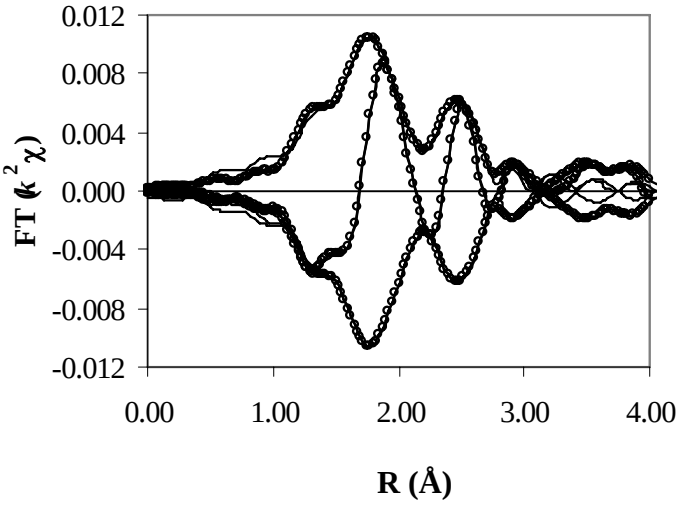


Supplemental Figure 5. k^2-weighted Fourier transform of EXAFS for polymer immobilized SCS pincer Pd compound (— : in air at RT; … : during Heck reaction at 120^{o}C).

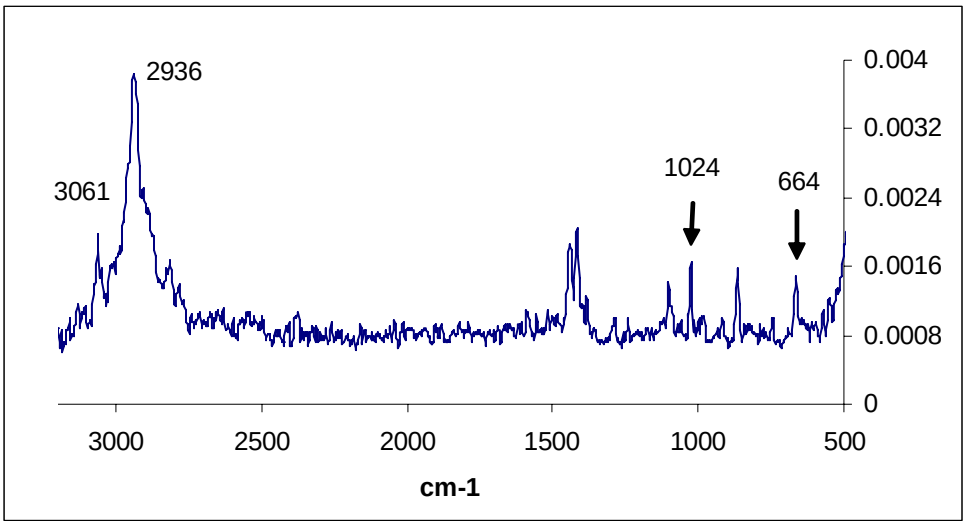


Supplemental Figure 6. Pd K edge spectrum of polymer immobilized SCS pincer compound during Heck reaction (circles), linear combination XANES (thick solid line) and single component XANES spectra (thin solid lines).





Supplemental Figure 7. Pd K edge k^2 -weighted EXAFS and Fourier transform (magnitude and imaginary part) for polymer immobilized -O-SCS pincer Pd during Heck reaction (squares experimental; — fitted).



Supplementary Figure 8. FT-Raman spectrum of SBA-15 immobilized Pd-Cl 1-[3-(3-Trimethoxysilane-propylsulfanyl)-propoxy]-3,5-bis-[(diphenylphosphanyl)-methyl]-benzene **(4).**

Supplementary Table 1. Structural parameters assigned to standard compounds.

Standard	Atom pair	CN	R(Å)
Pd foil	Pd-Pd	12	2.75
PdI_2	Pd-I	4	2.61
$PdCl_2$	Pd-Cl	4	2.31
PdS	Pd-S	4	2.33
$Pd(NH_3)_4Cl_2$	Pd-N	4	2.05

Supplementary Table 2. Parameters used for calibration of theoretical FEFF references derived from fits to standard compounds.

Atom pair	σ^2 (Å^2)	S_0^2	Vr (eV)	Vi (eV)	Δk (Å^{-1})	ΔR (Å)
Pd-Pd	0.00550	1.00	-5.5	3.0	3.0-15.0	1.5-3.2
Pd-I	0.00385	0.92	2.5	3.0	3.0-15.0	1.5-3.0
Pd-Cl	0.00303	0.90	2.7	3.0	2.5-14.0	1.5-2.8
Pd-S	0.00337	0.87	1.5	3.0	2.5-12.7	1.5-3.0
Pd-N	0.00008	0.90	0.8	3.0	2.5-12.8	1.0-2.5

Supplementary Table 3. Fitting results from linear combination of XANES (ΔE = 24.20-24.50 keV).

Pincer Compound	Measurement condition	SCS Pincer Pd (%)	Metallic Pd (%)	PdI_2 (%)	Residual factor (%)
Poly-O-SCS	In DMF at RT	100	0	---	0.31
SBA-O-SCS	In air at RT	93.3	6.5 (0.8)	---	0.36
Poly-O-SCS	During Heck reaction at 393 K	85.5	0	14.5 (0.6)	0.41
SBA-O-SCS	During Heck reaction at 393 K	81.7	2.4 (0.3)	15.7 (0.6)	0.44

***** The value in parentheses is the estimated coordination number for Pd-Pd or Pd-I.

Supplementary Table 4. Pd K edge EXAFS curve-fitting results for polymer and SBA immobilized SCS pincer compounds.

Catalyst	Measurement condition	Scatterer	CN	R (Å)	$\sigma^2(10^{-3}Å)$	ΔE_0 (eV)
SBA-O-SCS	In air at RT	S	2.1	2.29	1.4	-0.45
		Cl	1.0	2.37	5.0	4.53
		C	1.1	1.99	4.0	0.56
		Pd	1.4	2.71	5.4	-4.73
Poly-O-SCS	In air at RT	S	2.3	2.29	2.1	-3.17
		Cl	1.1	2.40	1.0	6.27
		C	1.2	1.99	3.7	1.73
Poly-O-SCS	During Heck reaction at 393 K	S	2.0	2.28	1.9	2.84
		Cl	1.1	2.39	4.0	6.99
		C	1.1	1.98	1.0	2.32
		I	1.2	2.67	3.6	-1.92

R-space fit, k^2 weighting, Δk = 2.5-12.0 $Å^{-1}$, ΔR = 0.8 – 3.2 Å

XYZ Coordinates in Ångstroms for Figures 9 and 10

Figure 9b:

C	0.2017977411	-1.1573849355	-1.4332789682
C	-0.5108596459	0.0717572842	-1.6060191868
C	-1.8711902409	0.0419084322	-2.0079445296
C	-2.5368629910	-1.1786151565	-2.2135787896
C	-1.8545718818	-2.3887247739	-2.0006727131
C	-0.4942304515	-2.3972864156	-1.5981262983
H	-2.4050750587	0.9890765083	-2.1501325646
H	-3.5855319571	-1.1867717953	-2.5298596558
H	-2.3752538562	-3.3439882114	-2.1375613669
C	0.1488155890	-3.7394000215	-1.2939136427
H	-0.1270260903	-4.0789570547	-0.2753199423
H	-0.1658811647	-4.5269871989	-2.0015389573
C	0.1137063438	1.4245553454	-1.3110678386
H	-0.1731082167	1.7707393682	-0.2978809801
H	-0.2054435557	2.2008909764	-2.0292646288
P	2.0475396975	-3.5400266442	-1.2908361936
P	2.0142650949	1.2498866032	-1.2927167913
C	3.7617815144	-6.8698692220	1.5610891966
C	4.3542771977	-5.5912442005	1.5218517926
C	3.8327373335	-4.5925957457	0.6719407424
C	2.7159474733	-4.8785091170	-0.1468726573
C	2.1232122924	-6.1641513845	-0.1110009029
C	2.6459362193	-7.1548234007	0.7451378577
H	4.1679195606	-7.6427168983	2.2227801443
H	5.2212980357	-5.3681741229	2.1529693912
H	4.2884821455	-3.5953457689	0.6353582242
H	1.2649622628	-6.4022152389	-0.7493592029
H	2.1849763194	-8.1481174710	0.7709807609
C	3.3856239081	-4.8565713726	-5.6188188363
C	2.3141583400	-3.9547285746	-5.4440028037
C	1.9200384239	-3.5655066616	-4.1483953485
C	2.5876163585	-4.0904365479	-3.0154865848
C	3.6657429156	-4.9868351338	-3.1928372452
C	4.0620587596	-5.3668908562	-4.4923341105
H	3.6938221995	-5.1538726127	-6.6268610649
H	1.7870925289	-3.5526653620	-6.3157747473
H	1.0970802468	-2.8528092994	-4.0236227082
H	4.1940378650	-5.3940116874	-2.3251574533
H	4.8974426089	-6.0637518928	-4.6201830186
C	3.6657467527	4.6084181088	1.5623767612
C	4.2685775435	3.3342794521	1.5389507751

C	3.7661478030	2.3264566638	0.6883268769
C	2.6576236826	2.5985013507	-0.1462291970
C	2.0550869717	3.8798652812	-0.1268778798
C	2.5587271399	4.8797597644	0.7298872636
H	4.0570791684	5.3884760068	2.2244504602
H	5.1291152995	3.1220067221	2.1825157455
H	4.2314457990	1.3333796176	0.6622275998
H	1.2035497227	4.1070972337	-0.7779224333
H	2.0897718809	5.8695766626	0.7431340372
C	3.3806219345	2.5591754869	-5.6132365605
C	2.3022646994	1.6647234086	-5.4436175446
C	1.8972723203	1.2816345503	-4.1496602255
C	2.5627575407	1.8016010455	-3.0136222554
C	3.6484797140	2.6898974220	-3.1855068511
C	4.0542189316	3.0658611402	-4.4832589141
H	3.6964475379	2.8536598317	-6.6196954759
H	1.7769586560	1.2643818772	-6.3174060575
H	1.0666337455	0.5779819354	-4.0277250258
H	4.1757649517	3.0932342731	-2.3154537501
H	4.8949582305	3.7569433036	-4.6071778783
Pd	2.1828812231	-1.1428082415	-0.9734934968
Cl	4.6257788325	-1.1234243379	-0.2505141229

Figure 9c:

C	0.1377908571	-0.9689989180	-1.7439967400
C	-0.4623285828	0.2251630874	-2.2165288019
C	-1.7272918808	0.1356338258	-2.8528403605
C	-2.3548000874	-1.1124872933	-3.0066562143
C	-1.7220915269	-2.2900526594	-2.5573263499
C	-0.4534299416	-2.2449756149	-1.9298120603
H	-2.2083763347	1.0481327370	-3.2234121793
H	-3.3365187080	-1.1748388907	-3.4872084467
H	-2.2167201149	-3.2550417239	-2.7087176685
C	0.3044513693	-3.5025599762	-1.4965911032
H	1.1270112771	-3.7316881178	-2.2029676889
H	0.7764680463	-3.3626740857	-0.5012717969
C	0.2276831362	1.5588624886	-2.0390644484
H	-0.2810691184	2.1835192063	-1.2799270766
H	0.2802900360	2.1427652660	-2.9753694088
P	-0.7873846702	-5.0869007193	-1.2227906909
P	1.9944435556	1.1887203859	-1.3902187363
C	-1.8067350580	-6.8999576490	-5.4773978526
C	-2.3224809018	-7.4533337883	-4.2859352990
C	-1.9833291389	-6.8877750397	-3.0417209412
C	-1.1169727144	-5.7670021223	-2.9694893914
C	-0.5959384216	-5.2251598657	-4.1664586907

C	-0.9457939308	-5.7862396392	-5.4143078141
H	-2.0792781415	-7.3311713830	-6.4465064379
H	-2.9948811804	-8.3172856469	-4.3255146976
H	-2.4035916528	-7.3137019715	-2.1221273352
H	0.0767805130	-4.3612707277	-4.1415652531
H	-0.5447506883	-5.3513045786	-6.3363075708
C	2.4902213889	-8.0680087572	0.4550162368
C	1.6216430541	-7.3753534074	1.3240078219
C	0.6546344442	-6.4919049700	0.8004873873
C	0.5551193501	-6.2871726887	-0.5970865936
C	1.4291569958	-6.9855825616	-1.4629825236
C	2.3914011930	-7.8731933512	-0.9389329535
H	3.2357743969	-8.7604423213	0.8604572392
H	1.6900254557	-7.5273590020	2.4069219298
H	-0.0307760156	-5.9727301352	1.4813397280
H	1.3493237100	-6.8502458645	-2.5469721896
H	3.0611672424	-8.4130695098	-1.6178811619
C	3.1546922241	4.5540706229	1.6775621181
C	3.7532202356	3.2797061551	1.7569872545
C	3.3893299597	2.2658573960	0.8483205860
C	2.4225552410	2.5324971616	-0.1490925879
C	1.8131809625	3.8085572683	-0.2262296561
C	2.1856137023	4.8163474616	0.6876941055
H	3.4400108522	5.3379635411	2.3868957441
H	4.5005274689	3.0703156596	2.5291914997
H	3.8386991206	1.2679564108	0.9234255257
H	1.0661802913	4.0352816876	-0.9939192665
H	1.7169478855	5.8036265135	0.6216968337
C	4.9285738450	1.7578826355	-5.0164673450
C	4.3642378745	0.4898597275	-4.7631539568
C	3.4982123981	0.3113587056	-3.6654436916
C	3.1993196001	1.4071740790	-2.8276042970
C	3.7623749978	2.6804697644	-3.0726920563
C	4.6272739620	2.8493335778	-4.1742751456
H	5.6073480243	1.8929990816	-5.8651134818
H	4.6057033488	-0.3599015312	-5.4100843279
H	3.0722126615	-0.6758603771	-3.4511031304
H	3.5385606674	3.5306913865	-2.4214527986
H	5.0693344399	3.8321184887	-4.3685291142
Pd	1.7671594418	-1.0385931362	-0.6392539700
Cl	3.7670029662	-1.3163225884	0.8864932841

Figure 9d:

C	0.3833021356	-0.9220123766	-0.2358184110
C	0.0072401933	0.3670955018	0.2333837565
C	-1.3211970749	0.5808702905	0.6764408645

C	-2.2626404458	-0.4616445110	0.5879090904
C	-1.9052418769	-1.6902720911	0.0000014241
C	-0.5801976880	-1.9439589209	-0.4415502142
H	-1.6136019958	1.5651064637	1.0612192064
H	-3.2903514242	-0.3029378695	0.9325060145
H	-2.6678041947	-2.4636923256	-0.1425330176
C	-0.2123485192	-3.1972088868	-1.2398031806
H	-0.2286627419	-2.9312358682	-2.3152544855
H	0.8171948522	-3.5242564913	-1.0134655581
C	1.0039441315	1.5059546004	0.1003580965
H	1.7475019753	1.5430240228	0.9188464776
H	0.5245341195	2.4980911058	0.0278779030
P	-1.4503339252	-4.6914761431	-1.0863957524
P	2.0222679966	1.0571206334	-1.4793355734
C	-0.7621466221	-7.2893551648	-4.9856443207
C	-1.7256961728	-7.6341953245	-4.0131732314
C	-1.8669472599	-6.8497912534	-2.8528754266
C	-1.0406595336	-5.7154287614	-2.6341790435
C	-0.0704006642	-5.3849440252	-3.6089693355
C	0.0619501406	-6.1653525853	-4.7796999820
H	-0.6612116994	-7.8890448051	-5.8967422815
H	-2.3751916607	-8.5034121386	-4.1645502422
H	-2.6367987380	-7.1115604455	-2.1160945901
H	0.5933978974	-4.5238876387	-3.4745787202
H	0.8130672907	-5.8900431767	-5.5286223081
C	0.2594913760	-7.3249585645	2.4685269584
C	-0.6308420067	-6.2573970664	2.7089842603
C	-1.1122653735	-5.4827353754	1.6330855656
C	-0.6970786283	-5.7567959067	0.3055966971
C	0.1950890664	-6.8298402512	0.0727813670
C	0.6679228307	-7.6110922481	1.1489643786
H	0.6244202462	-7.9354628478	3.3018925337
H	-0.9610327694	-6.0344892702	3.7298643125
H	-1.8274318728	-4.6741336728	1.8256333164
H	0.5151344098	-7.0619986530	-0.9480490647
H	1.3533876067	-8.4438827724	0.9543867463
C	5.6245651587	4.0942694428	-1.6379561693
C	5.7305877095	2.8931397127	-0.9072332253
C	4.6541547137	1.9828828022	-0.8768376005
C	3.4610190467	2.2779521065	-1.5756269599
C	3.3521372178	3.4865205819	-2.3035980332
C	4.4345904182	4.3892086600	-2.3353354493
H	6.4676012163	4.7926848350	-1.6713993338
H	6.6578025229	2.6539296098	-0.3758877432
H	4.7604318094	1.0206218566	-0.3657281740
H	2.4341456279	3.7218553877	-2.8504402407

H	4.3472107915	5.3194600274	-2.9069331414
C	-0.5882052723	2.1159118751	-5.2536808430
C	-1.1520106764	2.2469775378	-3.9689324924
C	-0.3890469318	1.9432625820	-2.8223664274
C	0.9473456673	1.5052515037	-2.9579222573
C	1.5090098587	1.3670254678	-4.2514821310
C	0.7441671411	1.6734300870	-5.3930156933
H	-1.1834253140	2.3524361766	-6.1417621298
H	-2.1866970298	2.5870688874	-3.8536575810
H	-0.8467594027	2.0442989769	-1.8347104310
H	2.5420396470	1.0211392416	-4.3706879058
H	1.1879606269	1.5653222083	-6.3883070445
Pd	2.3135035377	-1.2055791930	-0.5855761538
Cl	4.8419994745	-1.4716150077	-1.2015266858
N	2.6051711405	-2.6440585787	1.1832949323
C	3.6522099908	-1.9203728352	1.9848127100
H	4.5242828686	-1.7325809721	1.3427737321
H	3.2391845936	-0.9628578559	2.3409223435
H	3.9498700767	-2.5349433482	2.8621995618
C	3.1660911218	-3.9426530479	0.6809028525
H	4.0042396788	-3.7237060161	0.0026130677
H	3.5203404772	-4.5655843302	1.5299193078
H	2.3840562932	-4.4996630335	0.1420974754
C	1.4170927603	-2.8950579239	2.0564476800
H	1.7154437779	-3.5008663634	2.9384894234
H	1.0035583879	-1.9337986964	2.3971704086
H	0.6450646941	-3.4415785453	1.4985701130

Figure 9e:

C	-0.6584098148	-1.0120719894	-1.3910233240
C	-0.8882638310	0.3664149890	-1.1587298153
C	-2.2095937152	0.7545369493	-0.8106196279
C	-3.2401260846	-0.1954200577	-0.7080269563
C	-2.9743556117	-1.5525599513	-0.9525133457
C	-1.6656593708	-2.0047890499	-1.2905068746
H	-2.4215507548	1.8137001137	-0.6292614002
H	-4.2538896654	0.1248512535	-0.4458410577
H	-3.7831441308	-2.2892580179	-0.9028067361
C	-1.4662801069	-3.4761982341	-1.5994763980
H	-2.3761459172	-3.8831960492	-2.0771540291
H	-0.6226082428	-3.6277402363	-2.2984818106
C	0.2081128410	1.4168382528	-1.2976257415
H	0.0975766775	1.9925057079	-2.2379122897
H	1.2044338044	0.9386763846	-1.3411072779
P	-0.9636253241	-4.6817927729	-0.1101161930
P	0.2873323555	2.6566688988	0.2078104040

C	-4.5906397810	-5.0388081945	2.9169070345
C	-4.0895194871	-6.1936378726	2.2835524975
C	-3.0589349680	-6.0887554581	1.3265399184
C	-2.5091130079	-4.8266671204	0.9929149357
C	-3.0088391033	-3.6728553370	1.6477645469
C	-4.0477196507	-3.7787449752	2.5939573330
H	-5.3878395438	-5.1209290830	3.6629472902
H	-4.4973784555	-7.1794007195	2.5332506904
H	-2.6785261532	-6.9946540993	0.8466446409
H	-2.5823802145	-2.6877477948	1.4339038520
H	-4.4225397532	-2.8759170847	3.0884908032
C	-0.9379475769	-8.7540067350	-2.5412762249
C	0.2020787004	-8.3286789265	-1.8253326370
C	0.1642991639	-7.1149143996	-1.1011353556
C	-1.0116396043	-6.3173621186	-1.0851302248
C	-2.1528986943	-6.7536878853	-1.8046332033
C	-2.1162013937	-7.9657501890	-2.5280601866
H	-0.9110509019	-9.6948314144	-3.1054149431
H	1.1185762816	-8.9369085927	-1.8331479346
H	1.0509441210	-6.7920554303	-0.5410895869
H	-3.0780452184	-6.1587153832	-1.7914372977
H	-3.0050388409	-8.2947052343	-3.0804154052
C	-2.2117556692	6.4888497856	-1.0413762004
C	-1.5075821743	6.4208969094	0.1833487873
C	-0.7647971587	5.2681677106	0.5073900783
C	-0.7034339602	4.1697757375	-0.3926838236
C	-1.4109198836	4.2451748348	-1.6156431317
C	-2.1632271459	5.3992781976	-1.9365012868
H	-2.7972838031	7.3816752966	-1.2906056899
H	-1.5437801707	7.2612244601	0.8880342022
H	-0.2330116415	5.2217611013	1.4675106666
H	-1.3909139896	3.4132562561	-2.3308511192
H	-2.7078666447	5.4410234694	-2.8881254936
C	4.7580881659	4.2061679792	-0.1244144898
C	4.3766266203	3.2780388657	0.8660187677
C	3.0374274553	2.8369847840	0.9407413410
C	2.0712787479	3.3105819833	0.0193643880
C	2.4605285059	4.2483895426	-0.9644287776
C	3.7975743066	4.6934789985	-1.0361713968
H	5.7957403284	4.5551716688	-0.1807503316
H	5.1144410672	2.9070301446	1.5856566372
H	2.7381310644	2.1416420042	1.7343362352
H	1.7195026821	4.6390865503	-1.6698256710
H	4.0883667149	5.4213028295	-1.8021842013
Pd	1.0589469942	-1.4644147440	-2.1208730467
Cl	3.3246423468	-1.9409657604	-3.3132769568

N	1.9899801633	-1.7412125529	-0.1045009554
C	3.1503919807	-0.7834675724	-0.0613986831
H	3.7535182262	-0.9173327410	-0.9706829586
H	2.7809451193	0.2516739025	-0.0046673458
H	3.7640473749	-0.9921299819	0.8380152390
C	2.5194383994	-3.1541609635	-0.1274448842
H	3.1320155120	-3.2900059957	-1.0308580934
H	3.1388127604	-3.3249337610	0.7767308435
H	1.6727968369	-3.8559173276	-0.1208240745
C	1.1205633486	-1.5499797141	1.1039290578
H	1.7259709135	-1.7050963914	2.0217580633
H	0.7018869595	-0.5323159767	1.1135696446
H	0.3077557590	-2.2871793889	1.0815458608

Figure 9f:

C	0.0905360263	-1.0055609575	-1.6998211445
C	-0.4197644953	0.3123982371	-1.5519618439
C	-1.7919566936	0.5339508057	-1.8421641926
C	-2.6195320653	-0.5173669256	-2.2731042252
C	-2.0886841222	-1.8104504743	-2.4323512318
C	-0.7238842605	-2.0798654253	-2.1530227969
H	-2.1992935727	1.5455582853	-1.7360078043
H	-3.6762076100	-0.3297334959	-2.4928667848
H	-2.7310089115	-2.6249565687	-2.7867340071
C	-0.1845901199	-3.5048580715	-2.2529667344
H	0.9194633136	-3.5055826238	-2.2884502820
H	-0.4836408757	-4.0902204219	-1.3626742634
C	0.4592672302	1.4838736123	-1.1451827297
H	0.4080349827	2.3047204737	-1.8845759828
H	1.5109115247	1.1530126261	-1.0795382124
P	-0.8582128895	-4.5509536354	-3.7695183402
P	0.0893382619	2.2228022042	0.6290757702
C	2.8885378777	-4.9463167567	-6.6405884282
C	1.6810567819	-4.3731537495	-7.0884792817
C	0.5811595714	-4.2669580798	-6.2101350949
C	0.6837217714	-4.7235747813	-4.8742263791
C	1.9013570686	-5.2962181045	-4.4327126803
C	2.9967786694	-5.4118518065	-5.3123769353
H	3.7412656292	-5.0349348864	-7.3226388911
H	1.5911776627	-4.0126510158	-8.1192875881
H	-0.3605576662	-3.8321361087	-6.5648522110
H	1.9899284352	-5.6655828550	-3.4058351272
H	3.9314287584	-5.8643224476	-4.9631957790
C	-1.3913653135	-8.8502313692	-1.8187801955
C	-1.9201289432	-7.7012752278	-1.1937857162
C	-1.7159744267	-6.4277020383	-1.7626013554

C	-0.9672264787	-6.2785912888	-2.9581239726
C	-0.4507861265	-7.4390915494	-3.5836563016
C	-0.6614329606	-8.7145330364	-3.0175619693
H	-1.5516298829	-9.8404671011	-1.3785077718
H	-2.4959271959	-7.7930447626	-0.2653154895
H	-2.1631999005	-5.5540929929	-1.2724999984
H	0.1204356171	-7.3532491968	-4.5138261073
H	-0.2501309047	-9.6007760506	-3.5144339706
C	-3.5299971869	5.2253162613	0.0814756732
C	-3.3699582647	4.4722302998	1.2631123259
C	-2.2884382272	3.5741603598	1.3834986818
C	-1.3539033354	3.4274843428	0.3294483711
C	-1.5174173226	4.1943036986	-0.8497401964
C	-2.6045864982	5.0838665249	-0.9755770882
H	-4.3714245387	5.9203096710	-0.0155315149
H	-4.0841140310	4.5791134714	2.0883090003
H	-2.1710847354	2.9814316478	2.2993974767
H	-0.7977444907	4.1117866868	-1.6735317489
H	-2.7246946060	5.6696363317	-1.8945056620
C	3.7980223803	5.1595338047	1.1188993486
C	3.9864416398	3.7749964834	0.9269369673
C	2.8744075633	2.9256034276	0.7569869552
C	1.5558279465	3.4460607241	0.7612848653
C	1.3787190798	4.8367129599	0.9529845774
C	2.4909248255	5.6856282498	1.1358030269
H	4.6608245646	5.8191428510	1.2584490463
H	4.9981662780	3.3577746715	0.9120239034
H	3.0417845847	1.8501125491	0.6308554330
H	0.3715905717	5.2632260979	0.9614500317
H	2.3330013606	6.7590023854	1.2873684959
Pd	1.9459176804	-1.4028306370	-1.2389688252
Cl	4.4083955856	-2.1807308783	-0.7060149781
N	1.3347685505	-2.0617122459	0.8288820038
C	2.1928988402	-1.2532249388	1.7634569302
H	3.2448065635	-1.3785900312	1.4716024489
H	1.9007650779	-0.1933476860	1.6928796670
H	2.0410956358	-1.5970325600	2.8092576713
C	1.6991996514	-3.5144806641	0.9554011271
H	2.7533687584	-3.6385111440	0.6692276982
H	1.5434267015	-3.8547059224	2.0007626737
H	1.0620921905	-4.1115562050	0.2875529894
C	-0.1056528466	-1.8748300303	1.2154879761
H	-0.2619422063	-2.2278902003	2.2565711484
H	-0.3676730900	-0.8085295396	1.1477802731
H	-0.7533836184	-2.4489761358	0.5387007633
N	2.6186716811	-0.7142020942	-3.2625993430

C	3.6265531249	0.3723808466	-2.9845313479
H	4.3581920586	-0.0052237132	-2.2562729178
H	4.1458494568	0.6587218199	-3.9237461158
H	3.1077868122	1.2559064071	-2.5826267925
C	1.5915783543	-0.1948791731	-4.2254597120
H	1.0711771313	0.6700734860	-3.7923248787
H	2.0895059195	0.1154753087	-5.1681477290
H	0.8575546851	-0.9841108149	-4.4427324882
C	3.3154469763	-1.8889710931	-3.8918220541
H	3.8105045801	-1.5698286620	-4.8332990087
H	4.0632242928	-2.2754755275	-3.1867498239
H	2.5771597877	-2.6721340755	-4.1165475357

Figure 10b:

C	-3.8606025642	4.0655574811	3.1879171373
C	-3.0675179066	3.9954922288	2.0160572903
C	-3.2824915498	2.9937682740	1.0374039603
C	-4.2961814558	2.0339121061	1.2655711625
C	-5.0813187487	2.0826598048	2.4269844142
C	-4.8642081211	3.0871709020	3.3816416776
Pd	-1.5981291090	5.2644286651	1.7747363266
H	-4.4562803749	1.2430882165	0.5225617329
H	-5.8530452470	1.3239074580	2.5969405201
H	-5.4685413311	3.1200634533	4.2963150886
C	-3.6669576656	5.1428569405	4.2213093528
H	-4.1079667904	6.1094835718	3.9273454980
H	-4.0296280813	4.8546283569	5.2200211821
C	-2.4662762618	2.9250423651	-0.2260608732
H	-2.7709934850	3.6676435636	-0.9813824066
H	-2.4494893788	1.9199623605	-0.6751308188
S	-0.6683683269	3.3949997181	0.2937456792
S	-1.7613055159	5.4347115920	4.3244112819
C	-1.0264832529	9.3977369979	6.6438034210
C	-1.1542509488	9.4328458129	5.2430936890
C	-1.4106552995	8.2512538595	4.5228530765
C	-1.5409704039	7.0428549357	5.2266956393
C	-1.4032874382	6.9896243994	6.6268610337
C	-1.1496610003	8.1778756377	7.3342609514
H	-0.8171117630	10.3197867267	7.1982891737
H	-1.0432053545	10.3800913512	4.7031375707
H	-1.4629697150	8.2592974231	3.4296510339
H	-1.4750984941	6.0329987570	7.1568146545
H	-1.0375358363	8.1445083936	8.4241542000
C	1.7901634296	4.1172294803	-3.5884506907

Figure 10c:

C	-2.2087376257	9.0060827825	4.5171749623
C	-1.9683975861	8.0581899428	3.4866687611
C	-2.6503498636	8.1028170096	2.2524869930
C	-3.5934353791	9.1488935525	2.0838418150
C	-3.8382943644	10.1065350348	3.0709190444
C	-3.1400721217	10.0400750076	4.2825500760
Pd	-0.5617807627	6.7786516812	3.8124519870
H	-4.1205913527	9.2023803617	1.1235890151
H	-4.5637055767	10.9081778351	2.8923284597
H	-3.3045330909	10.7908390967	5.0655669567
C	-1.5372232029	8.9408420281	5.8562423632
H	-1.4992523025	9.9136254424	6.3708249405
H	-1.9954764201	8.1897256571	6.5211858249
C	-2.5068357361	7.0736440637	1.1476870487
H	-3.3761551716	6.3955855143	1.1301016944
H	-1.6079937075	6.4596409629	1.2684046321
S	-2.4231789327	7.8301868239	-0.6158066414
S	0.2678491647	8.3515782360	5.5738731883
C	1.1382478996	5.8709895182	9.4145168833
C	-0.0401882920	5.6194095056	8.6877008957
C	-0.3154405015	6.3462307025	7.5173684769
C	0.5911696832	7.3334864399	7.0952434250
C	1.7727388502	7.5961553963	7.8093976728
C	2.0428546611	6.8523375927	8.9728721367
H	1.3499709809	5.2996732574	10.3258587867
H	-0.7456526003	4.8509034142	9.0238526452
H	-1.2186821580	6.1294512243	6.9353655827
H	2.4655187925	8.3751822034	7.4726460825
H	2.9601412754	7.0516017103	9.5389973678
C	-5.8128465998	5.8061181569	-3.0910797165
C	-4.5015781639	5.8935035899	-3.5912449239
C	-3.4814751454	6.4676388015	-2.8120236777
C	-3.7798198651	6.9658394996	-1.5293919023
C	-5.0939756630	6.8963945073	-1.0285822642
C	-6.1032514462	6.3040467754	-1.8075921551
H	-6.6058063746	5.3540361466	-3.6982612423
H	-4.2626623919	5.5043039643	-4.5885401773
H	-2.4552629235	6.5162544180	-3.1940994563
H	-5.3403664682	7.3058045078	-0.0418553767
H	-7.1253792712	6.2509463545	-1.4130499149
Cl	-1.4155396936	4.6250678966	2.9485765001

Figure 10d:

C	-2.7288883663	7.5999481450	4.8107769736
C	-2.1371416982	7.1585849399	3.6017553457
C	-2.2380595906	7.9196914079	2.4166794951

C	-3.0007813044	9.1073810764	2.4582459124
C	-3.6196004326	9.5428535037	3.6380175792
C	-3.4699536295	8.8018190743	4.8167784281
Pd	-1.0191089219	5.5540362786	3.6848582278
H	-3.0910772300	9.7013126628	1.5406158372
H	-4.2004373994	10.4728803843	3.6403194807
H	-3.9171537253	9.1526700110	5.7560523826
C	-2.5384723179	6.8340688864	6.0867296384
H	-2.6874887029	7.4400190956	6.9949687829
H	-3.1644768012	5.9260127195	6.1572504862
C	-1.5551278114	7.4498948772	1.1380329672
H	-2.0041018972	6.5094770209	0.7780449167
H	-0.4857353681	7.2372554989	1.3188310940
S	-1.4866232608	8.6590212919	-0.3133280210
S	-0.7572538191	6.0932923590	6.1466116228
C	2.0704725236	9.6337290008	7.1756528456
C	1.6526050089	9.4575596729	5.8444051200
C	0.7791566305	8.4078250966	5.5114742944
C	0.3264020704	7.5475542319	6.5253300466
C	0.7415604034	7.7085235568	7.8595123619
C	1.6157307071	8.7614792555	8.1804717881
H	2.7588433172	10.4487559749	7.4288530340
H	2.0117877917	10.1330766955	5.0587999253
H	0.4544017266	8.2541020555	4.4769428289
H	0.3887752653	7.0204029450	8.6358883802
H	1.9442723849	8.8939732778	9.2181780678
C	-5.5435671288	8.5290855790	-2.5919002536
C	-4.4138731620	9.1790737409	-3.1221312070
C	-3.2032563518	9.1912696207	-2.4123508636
C	-3.1196157740	8.5459038115	-1.1604637928
C	-4.2419011057	7.8922426853	-0.6229072065
C	-5.4504591334	7.8901140786	-1.3447802578
H	-6.4884611336	8.5217426449	-3.1477170767
H	-4.4698381656	9.6792746951	-4.0968650306
H	-2.3248424254	9.6944042996	-2.8355637412
H	-4.1887827491	7.3922437501	0.3494046539
H	-6.3254715596	7.3829594870	-0.9205743743
Cl	-2.4233333632	4.3941410859	1.9702254651
N	0.4314200326	3.7074019517	3.7605467086
C	1.5775272358	3.9275276542	4.6699890038
H	1.2159839330	4.0313183170	5.7062687212
H	2.1109990013	4.8495090659	4.3815492018
H	2.2943861954	3.0771192967	4.6301607680
C	0.9342728909	3.5194153335	2.3805393518
H	0.0797428836	3.3726885170	1.7014932129
H	1.6154540102	2.6416528322	2.3159963569

H	1.4906526471	4.4205812675	2.0681012564
C	-0.3303063134	2.5126671911	4.1878292557
H	-0.6951770944	2.6590847593	5.2192025871
H	0.3000709646	1.5961276628	4.1603725621
H	-1.1949976578	2.3831297594	3.5175221037

Figure 10e:

C	-1.3037735766	9.1540532907	2.1401083953
C	-2.0346001994	7.9724604322	2.3803185366
C	-3.4374090523	7.8911892261	2.2453970568
C	-4.1023999702	9.0260863691	1.7214475666
C	-3.4012257414	10.1944689565	1.3932299839
C	-2.0206100961	10.2611594133	1.6214203361
Pd	-1.0999686483	6.3985859409	2.9256272998
H	-5.1909890743	8.9797383441	1.5834340248
H	-3.9352689536	11.0616263101	0.9871968875
H	-1.4686505518	11.1866051845	1.4119873400
C	0.1602022694	9.3345736078	2.4696912901
H	0.3237101121	10.3032551329	2.9710436117
H	0.5382662920	8.5196868769	3.1036473622
C	-4.2510468768	6.7059179698	2.6921716519
H	-3.7082871687	5.7549956293	2.5967695244
H	-5.2121069136	6.6400450000	2.1573407802
S	-4.7059189530	6.8384283085	4.5767781281
S	1.2088513642	9.4078962460	0.8628152275
C	5.0367931546	11.8594990607	1.8808282002
C	4.5224062051	11.8058495083	0.5737404873
C	3.3519661629	11.0797418194	0.2998954298
C	2.6979570862	10.3861928110	1.3383168834
C	3.2124135937	10.4253430855	2.6466247164
C	4.3763916599	11.1720571353	2.9116930538
H	5.9464744102	12.4337009834	2.0930334268
H	5.0256144644	12.3418093322	-0.2388072145
H	2.9424687403	11.0605457524	-0.7160685920
H	2.7291494569	9.8738051228	3.4588386489
H	4.7701981050	11.2044554079	3.9335510459
C	-9.2845840362	6.1606736217	5.0606886835
C	-8.3586201704	5.3575504801	5.7465644063
C	-6.9800494234	5.5329230993	5.5358006559
C	-6.5253735605	6.5332136218	4.6539004648
C	-7.4488009652	7.3482293686	3.9732182662
C	-8.8260416863	7.1489944289	4.1684130798
H	-10.3594646885	6.0231773871	5.2253925105
H	-8.7051436652	4.5855737472	6.4455193613
H	-6.2570751782	4.9005403119	6.0624825769
H	-7.0992612843	8.1495139427	3.3113206720

H	-9.5421535610	7.7868206716	3.6385798852
N	-0.9454409221	5.3876352876	0.9695506078
C	-2.0972958992	4.4879011714	0.7058213089
H	-2.2747245665	3.8423858490	1.5818140727
H	-1.8915098357	3.8434192317	-0.1753600883
H	-2.9964446651	5.0893954520	0.4994653973
C	0.2694688134	4.5736229533	1.2460740633
H	1.1357848405	5.2387143728	1.3860598548
H	0.4824692901	3.8788399518	0.4064049374
H	0.1168136978	3.9727364765	2.1601052065
C	-0.7148389703	6.2591598987	-0.2103875843
H	0.1594399340	6.9026406775	-0.0275247347
H	-1.6028030889	6.8896756078	-0.3759603562
H	-0.5285244066	5.6449578158	-1.1186519449
Cl	-0.9533809750	7.2443293723	5.1969766779

Figure 10f:

C	9.0071685921	3.6139669067	3.6853289169
C	8.3293833954	4.8072617420	3.9712222362
C	6.9571230818	4.9579142224	3.6611977479
C	6.2778167357	3.8663940503	3.0705021469
C	6.9554250284	2.6712827225	2.7317068171
C	8.3274760565	2.5602471368	3.0586103566
H	10.0706681450	3.5133189739	3.9322356563
H	8.8630012581	5.6464058506	4.4364724607
H	8.8595557472	1.6335185015	2.8066599242
Pd	4.4013620451	4.0426971606	2.6221381423
Cl	1.8417555661	4.2955026169	1.9944199788
N	3.8145677873	3.2314439144	4.6194205452
C	2.9627183851	4.2809827060	5.2527507298
H	2.5071482436	3.8849923457	6.1858710780
H	3.5936248448	5.1500591164	5.5026665815
H	2.1731320833	4.5720982248	4.5446829569
C	2.9839692429	2.0249342054	4.3305971269
H	3.6324833959	1.2381201799	3.9103368769
H	2.5240354158	1.6491505417	5.2698417355
H	2.1968978081	2.2984876142	3.6125731600
C	4.8775352845	2.8465673199	5.5887734259
H	5.4922541301	3.7240653188	5.8393702474
H	4.4078485495	2.4580169214	6.5177712129
H	5.5159320066	2.0621054293	5.1553359115
N	4.9708210536	4.8230341036	0.5972497597
C	4.3430989130	6.1733135795	0.4893158626
H	4.4563523141	6.5635626986	-0.5444057686
H	3.2766379732	6.0886460469	0.7456638609
H	4.8424254723	6.8650376771	1.1869507280

C	4.3242835217	3.9040699976	-0.3859462498
H	4.8100633049	2.9163949981	-0.3344272655
H	3.2576886112	3.8084740261	-0.1345674858
H	4.4390164113	4.3059112675	-1.4152600509
C	6.4122645432	4.9478806581	0.2431621211
H	6.9128078414	5.6337780192	0.9429459893
H	6.8987321172	3.9626878381	0.2976988998
H	6.5103408358	5.3444466376	-0.7888329330
C	6.2855537613	1.5493403259	1.9718163918
H	5.2469047470	1.8010818277	1.7077210884
H	6.8517988128	1.2641989682	1.0697100455
S	6.2100362841	-0.0588755734	3.0521144139
C	4.7559210535	-3.4042947894	0.1541622690
C	6.1285178440	-3.2394627055	0.4111557077
C	6.5705843890	-2.2040953868	1.2543506073
C	5.6309312026	-1.3377202862	1.8439813346
C	4.2555397190	-1.4999703474	1.5918915153
C	3.8214439897	-2.5330469960	0.7424537541
H	4.4130153264	-4.2149252508	-0.4998250509
H	6.8595721876	-3.9204145996	-0.0406133300
H	7.6384591705	-2.0762300228	1.4643644320
H	3.5257756261	-0.8345812968	2.0662048645
H	2.7493100846	-2.6621250306	0.5508613502
C	6.2912153861	6.2909574981	3.9168694088
H	6.8686435576	7.1306830864	3.4965214778
H	5.2584774814	6.3063095461	3.5356195767
S	6.2072314891	6.6336297950	5.8251050838
C	4.5747254675	10.9768251113	6.2637304378
C	3.8055510177	10.0103324201	5.5907540281
C	4.2935848173	8.7024399856	5.4265164719
C	5.5659853732	8.3657758601	5.9262821993
C	6.3453746360	9.3326360284	6.5898474543
C	5.8421116962	10.6342900249	6.7661438122
H	4.1829565777	11.9919417435	6.3989190177
H	2.8123227359	10.2689729771	5.2046258853
H	3.6794815685	7.9442038528	4.9286455087
H	7.3364349551	9.0649229058	6.9735934521
H	6.4487194185	11.3813366185	7.2921567516