Supported Information

Aminated Chlorinated Polyvinylchloride Nanofiber Mat-Supported Palladium Heterogeneous Catalysts: Preparation, Characterization and their Applications

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Supporting information

1. Experimental

1.1 Materials

Chlorinated polyvinylchloride (CPVC, M_n= 85,000) was purchased from Hangzhou Qianjing Chemical Co., Ltd. Ethylenediamine, 1,3-propylenediamine, diethylenetriamine and tetraethylenepentamine were purchased from Aladdin Chemical Co. Ltd. Palladium chloride ($PdCl_2$) was purchased from Zhejiang Metallurgical Research Institute (Zhejiang, China). All other solvents and chemicals were analytical grade or the best grade available and used without further treatment.

1.2 Preparation of chlorinated polyvinylchloride (CPVC) nanofiber mat

A homogeneous solution was obtained from the dissolution of 2.0 gram of CPVC into *N,N*-dimethylacetamide (8.0 g). The resultant CPVC solution was then loaded into the syringe (20 mL) with a capillary (0.8 mm inner diameter) as spinneret, which was connected to a high voltage power supply (GDW-a, Tianjin Dongwen High-voltage Power Supply Plant, China). A ground aluminum foil was placed at 15 cm away from the syringe tip as a collector. The applied electric voltage was 24 kV between the CPVC solution and the syringe tip. The feeding rate of the polymer solution was set at 2.5 mL/h, which was monitored by a micro-infusion pump (WZ-502C, Zhejiang Smiths Medical Instruments Co., Ltd. China). The final nanofiber mats were dried under vacuum to remove the residual solvent at room temperature.

1.3 Amination of the chlorinated polyvinylchloride nanofiber mat (CPVC-NH_2)

The nanofiber mat was collected by filtration after a mixture of 100 mg CPVC nanofiber mat, 0.04 mol 1,3-propylenediamine and 3.72 g ethylene glycol was stirred at 50 ^{o}C for 6 hours. The resultant nanofiber mat (CPVC-NH_2) was washed with water for three times and then with ethanol for three times, and finally dried under a reduced pressure for 12 hours. The same protocol has been repeated for the amination of the CPVC nanofiber mat with other amines (ethylenediamine, diethylenetriamine and tetraethylenepentamine).

1.4 Preparation of the CPVC-NH_2 nanofiber mat supported palladium (CPVC-NH_2-Pd) heterogeneous catalyst

To an aqueous solution (10 mL) containing 5.0 mg $PdCl_2$ and 4.0 mg NaCl, 100 mg CPVC-NH_2 nanofiber mat was added and stirred magnetically for 12 hours, followed by addition of 20 mg hydrazine to reduce the oxidative Pd^{2+} into the reductive Pd^0 species. The nanofiber mat was collected from the solution by filtration, washed with water for three times and then with ethanol for three times. The resultant aminated CPVC-NH_2-Pd heterogeneous catalysts were dried under a reduced pressure for 12 hour at room temperature. The ICP-AES analysis showed that the palladium content of the CPVC-NH_2-Pd catalyst is 3.0 wt %.

1.5 General procedure for the CPVC-NH_2-Pd catalyzed Heck cross-coupling reactions in DMSO solution

To a 20 mL round bottom flask containing 3.0 ml DMSO and a magnetic stir bar, aromatic iodide (0.70 mmol), *n*-butyl acrylate (1.4 mmol), CPVC-NH_2-Pd (50 mg, Pd content: 0.014 mmol) and CH_3CO_2K (5.2 mmol) were added. The resultant solution was allowed to stir at 110 ^{0}C for 3 hours. The reaction mixture was cooled down to room temperature, and then quenched with 10 mL of water and extracted with ethyl acetate for three times (3×20 mL). The combined organic layer was washed with water, saturated brine, and then dried over anhydrous Na_2SO_4. Solvent was removed under a reduced pressure. The residue was purified to afford the cross-coupling product by silica gel chromatography with a mixture of petroleum ether and ethyl acetate. All of the cross-coupling products were confirmed by ^{1}H NMR spectroscopic and mass spectroscopic analysis.

1.6 General procedure for the CPVC-NH_2-Pd catalyzed Heck cross-couplings in the aqueous solution

To a 20 ml reaction flask containing 5.0 ml water and a magnetic stir bar, aromatic iodide (0.70 mmol), *n*-butyl acrylate (1.4 mmol), CPVC-NH_2-Pd (50 mg, Pd content: 0.014 mmol), CH_3CO_2K (5.2 mmol) and cetyltrimethylammonium bromide (0.070 mmol) were added. The resulting mixture was allowed to stir in an oil bath (~105 ^{0}C) for 20 hours. The work-up procedure for the reactions in the aqueous solution was similar to those from the DMSO solution.

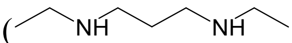
1.7 General procedure for the recovery and reuse of the CPVC-NH_2-Pd heterogeneous catalysts

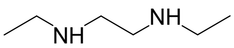
The CPVC-NH_2-Pd heterogeneous catalyst was collected from the reaction mixture by filtration, and then washed with DMSO, water, and ethanol. The recovered CPVC-NH_2-Pd catalyst was dried at 30 ^{0}C for 12 hours under a reduced pressure before the next application.

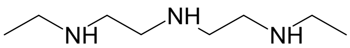
1.8 Characterizations of the CPVC nanofiber mats

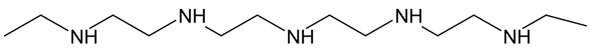
The morphology of the electrospun nanofiber mats was characterized with a scanning electron microscope (SEM) (Jeol, Jsm-6360lv, Japan). The nanofiber samples were analyzed by Fourier transform infrared spectrometer (FT-IR) with the accessories of attenuated total reflection (Nicolet, Nexus-470, USA). Proton NMR spectra were recorded in $CDCl_3$ (Bruker, AVANCE III 400 MHz, Switzerland) and the proton chemical shifts are reported in ppm relative to TMS as the internal reference. Multiplicities are reported as: singlet (s), doublet (d), and multiplet (m). The elemental analysis was performed on the EuroEA 3000 from Leeman, USA. Phase composition of the prepared samples was determined by means of X-ray powder diffraction (XRD) (Rigaku D, max-3BX, Japan). The mechanical tensile strength of the nanofiber mats was measured by the universal testing machine (Laizhouhuaying, China). Each sample was tested at least for five times. The quantitative analysis of the reaction products was performed on the Agilent 6890/5975 GC/MS instrument with a programmable split/splitless injector. The injector-port temperature was set at 270 ^{o}C. The oven-temperature program was initially set at 80 ^{o}C and ramped to 220 ^{o}C at 5.0 ^{o}C/min, and maintained at 220 ^{o}C for 2.0 min at each step. Inductively coupled plasma-atomic emission spectroscopic (ICP-AES) analysis was performed on a Leeman ICP-AES Prodigy XP (Leeman Labs, USA).

2. Density functional theory (DFT) calculations

All the calculations were performed with the Gaussian 03 programs at the B3LYP/6-31G(d)-SDD level. Each optimized structure was confirmed by the frequency calculation. In order to minimize the calculation time, the ligands for the 1,3-propanediamine, ethylenediamine, diethylenetriamine, tetraethylenepentamine modified CPVC and CPVC-NH_2-Pd catalysts were simply represented by *N^1^,N^3^*-diethyl-1,3-propanediamine (

), *N^1^,N^2^*-diethyl-ethylenediamine (

), *N^1^*-ethyl-*N^2^*-(2-(ethylamino)ethyl)ethane-1,2-diamine (

), *N^1^*-ethyl-*N^2^*-(2-(2-(2-(ethylamino)ethylamino)ethylamino)ethyl)ethane-1,2-diamine (

), respectively.

3. Characterization data of the fiber mats

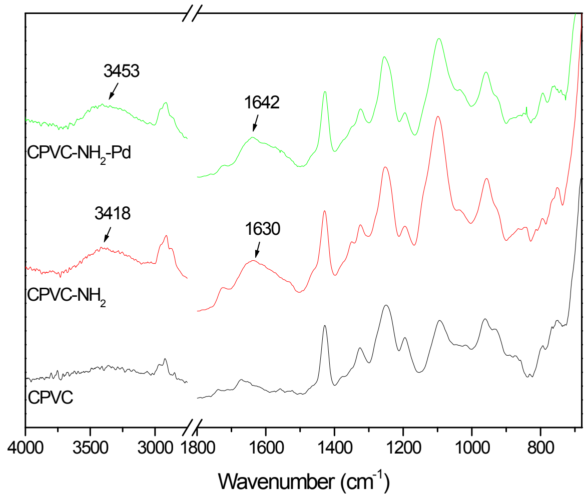


Figure 1S. FT-IR spectra of CPVC, $CPVC-NH_2$ and $CPVC-NH_2-Pd$ fiber mats.

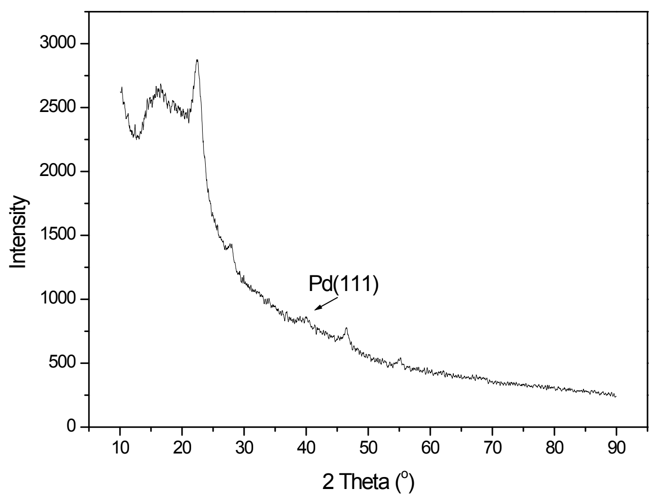
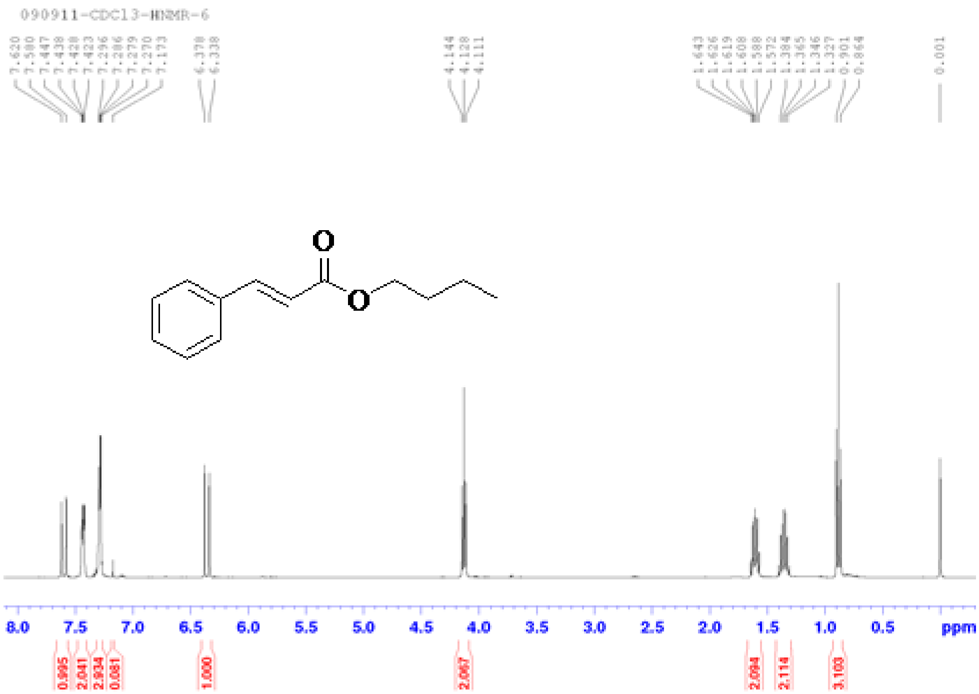


Figure 2S. XRD pattern of the $CPVC-NH_2-Pd$ heterogeneous catalyst.

4.Characterization data of the cross-coupling products

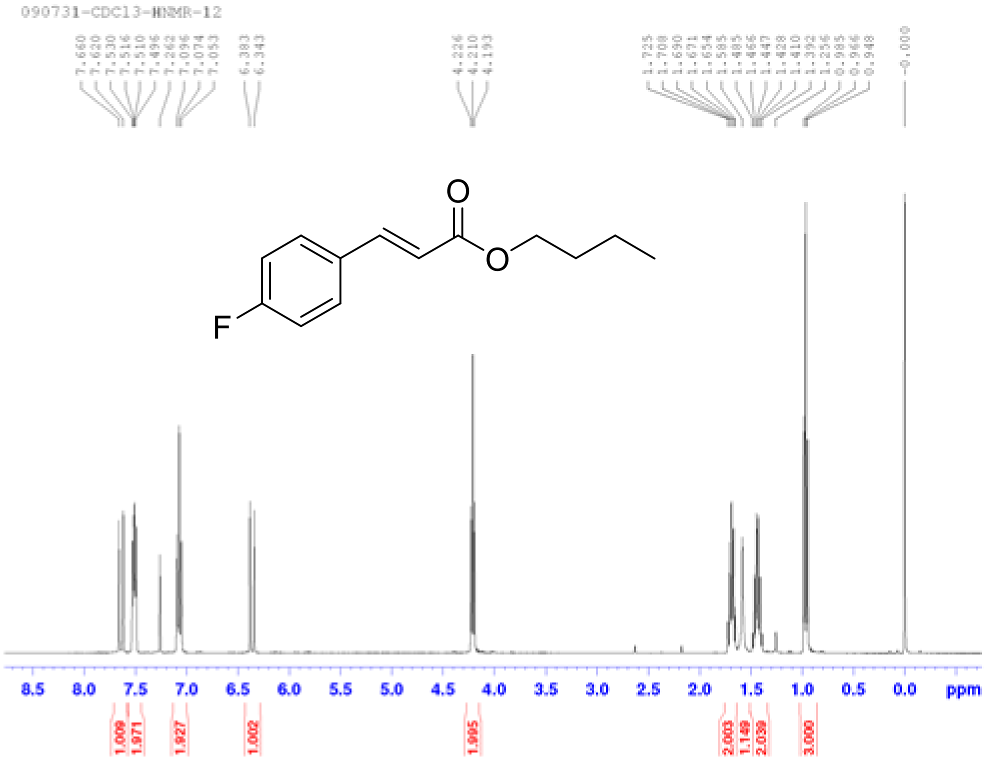
4.1. (*E*)-*n*-butyl cinnamate

^{1}H NMR (400Hz, $CDCl_3$, TMS): δ = 7.60 (d, 1H, J = 16.0 Hz), 7.44 (d, 1H, J = 3.6 Hz), 7.42 (d, 1H, J = 2.0 Hz), 7.28 (dd, 3H, J = 6.4, 4.0 Hz), 6.35 (d, 1H, J = 16.0 Hz), 4.12 (dd, 2H, J = 13.2, 6.4 Hz), 1.64-1.57 (m, 2H), 1.35 (dd, 2H, J = 15.2, 7.6 Hz), 0.88 (d, 3H, J = 14.8 Hz); MS m/z (%) 131 (99.9), 148 (71.5), 147 (59.2), 103 (13.3), 149 (11.7).



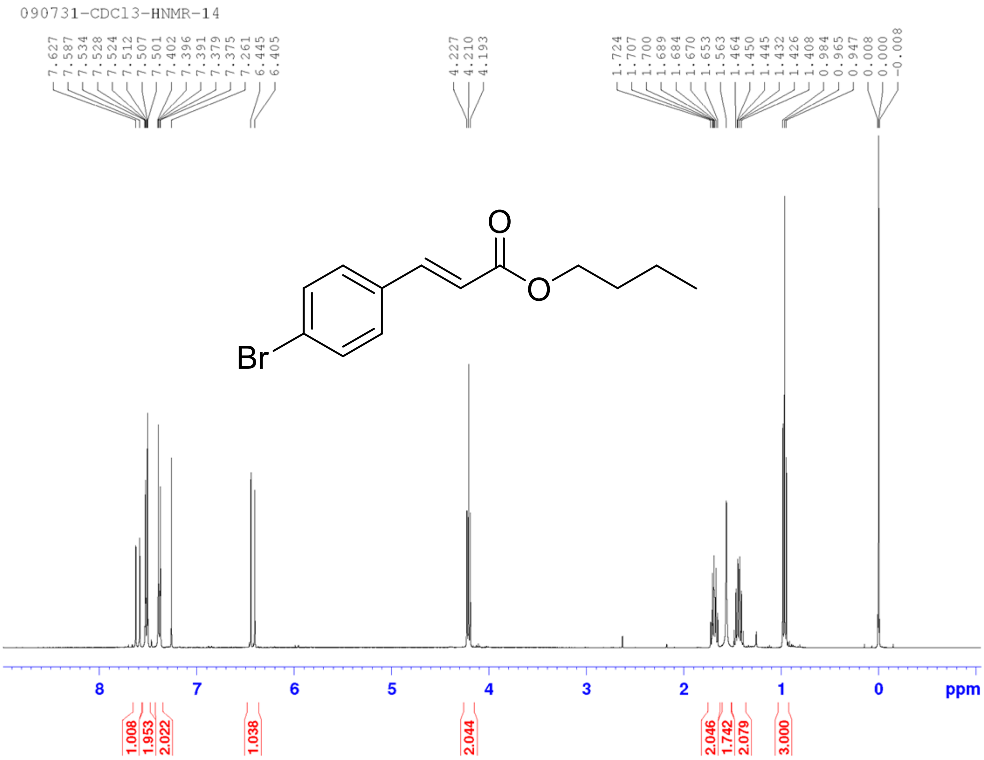
4.2. (*E*)-*n*-butyl 3-(*p*-fluorophenyl)acrylate

^{1}H NMR (400Hz,$CDCl_3$,TMS): δ = 7.64 (d, 1H, J = 16.0 Hz), 7.51 (dd, 2H, J = 8.0, 5.6 Hz), 7.06 (t, 2H, J = 8.6 Hz), 6.36 (d, 1H, J = 16.0 Hz), 4.20 (t, 2H, J = 6.6 Hz), 1.72-1.65 (m, 2H), 1.44 (sext, 2H, J = 7.6 Hz), 0.95 (t, 3H, J = 7.6 Hz); MS m/z (%) 149 (99.9), 166 (93.0), 121 (35.4), 101 (35.17), 165 (27.8), 222 (19.7).



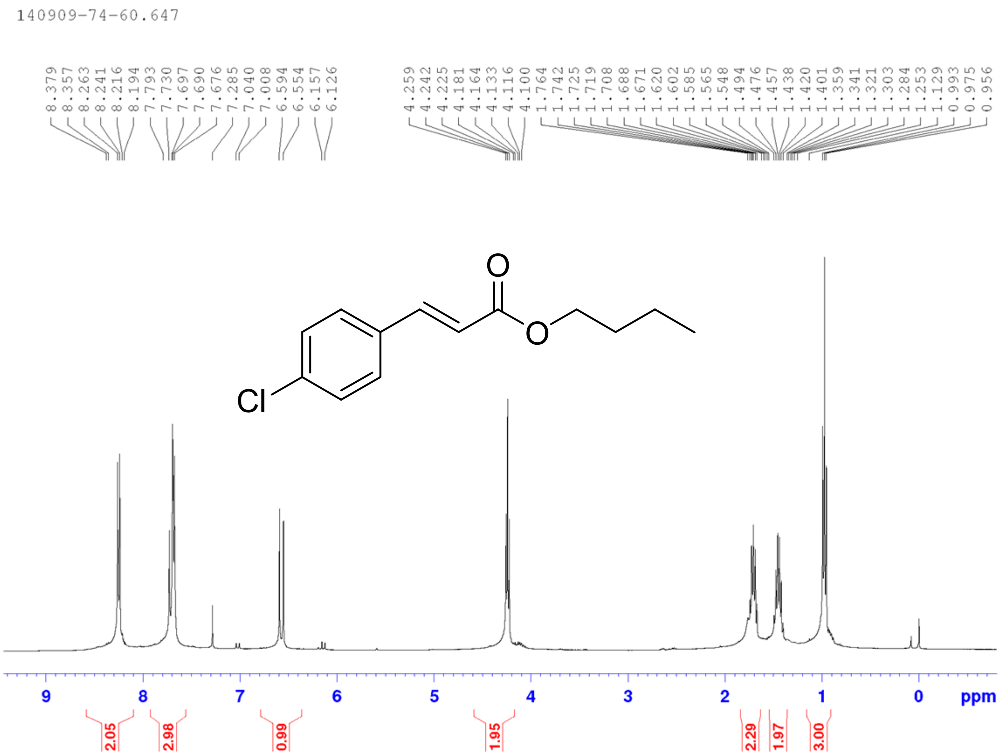
4.3. (*E*)-*n*-butyl 3-(*p*-bromophenyl)acrylate

^{1}H NMR (400Hz, $CDCl_3$, TMS): δ = 7.61 (d, 1H, J = 16.0 Hz), 7.53-7.50 (m, 2H), 7.40-7.37 (m, 2H), 6.42 (d, 1H, J = 16.0 Hz), 4.21 (t, 2H, J = 6.8 Hz), 1.72-1.65 (m, 2H), 1.46-1.40 (m, 2H), 0.96 (t, 3H, J = 7.4Hz); MS m/z (%) 226 (99.9), 228 (97.9), 102 (77.7), 209 (71.5), 211 (70.5), 282 (24.0).



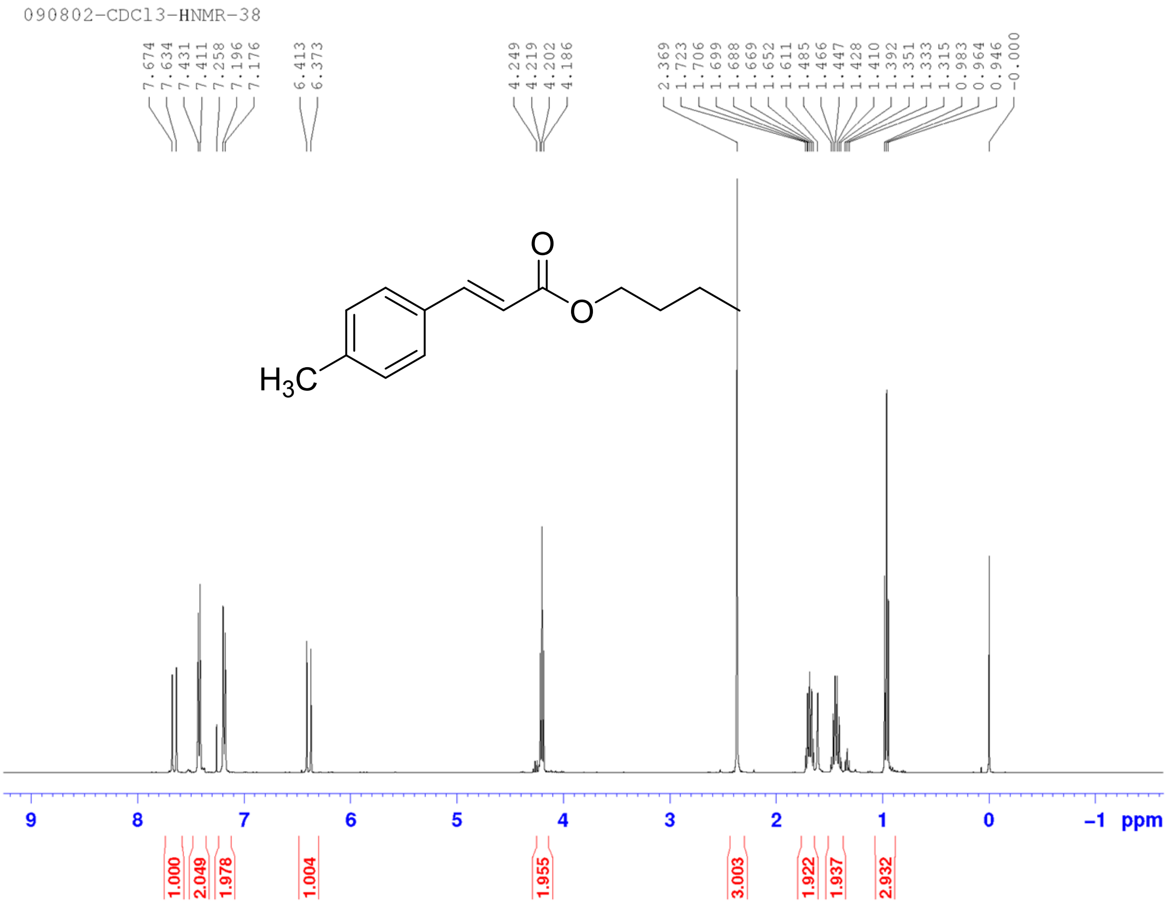
4.4. (*E*)-*n*-butyl 3-(*p*-chlorophenyl)acrylate

[1]H NMR (400Hz, $CDCl_3$, TMS): δ = 7.64 (d, 1H, J = 16.0 Hz), 7.48 (dd, 2H, J = 6.8, 2.0 Hz), 6.91-6.86 (m, 2H), 6.31 (d, 1H, J = 15.6 Hz), 4.19 (t, 1H, J = 6.8 Hz), 4.12 (t, 1H, J = 4.4 Hz), 1.68 (dd, 2H, J = 14.8, 6.8 Hz), 1.46-1.41 (m, 2H), 0.98-0.91 (m, 3H); MS m/z (%) 182 (99.9), 181 (25.3), 165 (87.7), 184 (33.1), 102 (30.6), 167 (29.4).



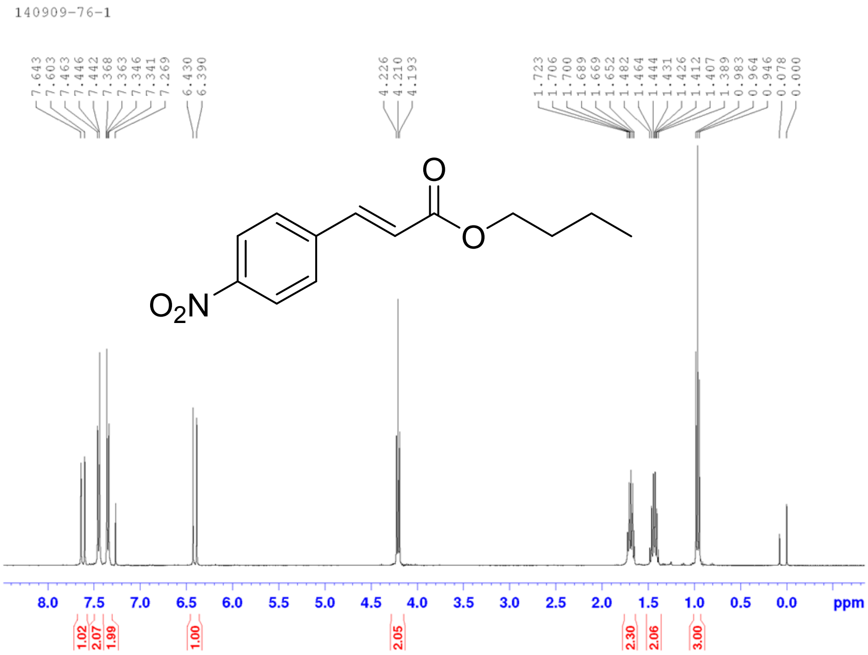
4.5. (*E*)-*n*-butyl 3-(*p*-tolyl)acrylate

^{1}H NMR (400Hz, $CDCl_3$, TMS): δ = 7.65 (d, 1H, J = 16.0 Hz), 7.42 (d, 2H, J = 8.6 Hz), 7.19 (d, 2H, J = 16.0 Hz), 6.39 (d, 1H, J = 16.0 Hz), 4.23 (d, 1H, J = 12.0 Hz), 4.19 (d, 1H, J = 6.4 Hz), 2.36 (s,3H), 1.72-1.16 (m, 2H), 1.48-1.31 (m, 2H), 0.95 (dd, 3H, J = 7.6 Hz); MS m/z (%) 145 (99.9), 162 (95.6), 115 (46.5), 218 (34.9), 117 (28.8), 161 (26.17), 147 (22.3).



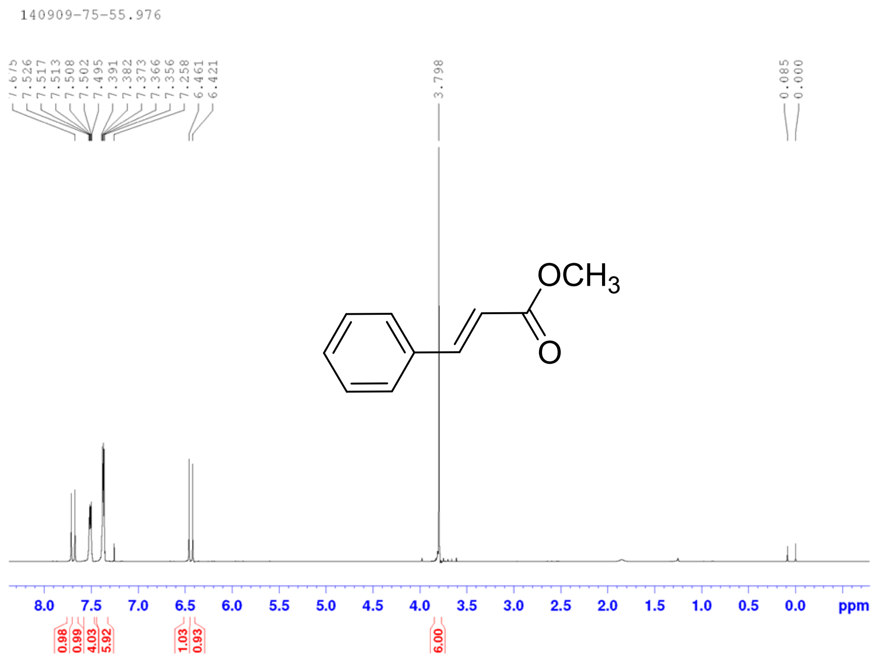
4.6. (*E*)-*n*-butyl 3-(*p*-nitrophenyl)acrylate

^{1}H NMR (400Hz, $CDCl_3$, TMS): δ = 8.23 (dd, 2H, J = 18.0, 8.8 Hz), 7.70 (d, 3H, J = 15.6 Hz), 6.56 (d, 1H ,J = 16.4 Hz), 4.23 (t, 2H, J = 6.4 Hz), 1.74-1.67 (m, 2H), 1.45 (sext, 2H, J = 7.2 Hz), 0.96 (t, 2H, J = 7.6 Hz), 0.89 (t, 1H, J = 7.2 Hz); MS m/z (%) 176 (99.9), 194 (54.5), 193 (43.7), 102 (38.1), 56 (33.4), 130 (31.6), 177 (19.2).



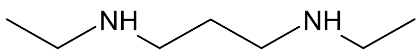
4.7. (*E*)-methyl cinnamate

[1]H NMR (400Hz, $CDCl_3$, TMS): δ = 7.71 (dd, 1H, J = 25.2, 16.0 Hz), 7.53 (d, 2H, J= 20.8 Hz), 7.39 (d, 3H, J= 22.4 Hz), 6.45 (dd, 1H, J = 25.2, 16.6 Hz), 3.84-3.71 (m, 3H); MS m/z (%) 131 (99.9), 103 (59.8), 162 (55.0), 77 (32.2), 161 (27.0), 102 (15.4), 51 (14.5), 132 (10.1).



5. Cartesian coordinates for the optimized structures

5.1. *N*[1],*N*[3]-diethylpropane-1,3-diamine



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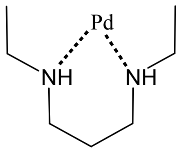
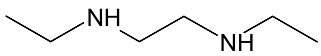
H	1.192685	0.941372	-1.255753
C	-0.288377	-0.045821	0.000006
H	-1.013628	0.786838	0.000271
H	-0.869928	-0.975207	-0.000260
C	0.560831	0.025851	1.281912
H	1.193569	0.940075	1.255745
H	1.249797	-0.831538	1.311451
C	0.430509	0.009824	3.772175
H	1.066089	0.916142	3.869813
H	1.110105	-0.853976	3.808862
C	-0.548977	-0.058093	4.954972
H	-1.149310	-0.973703	4.898880
H	-0.009219	-0.048381	5.910652
H	-1.235863	0.800681	4.949421
C	0.430510	0.009958	-3.772162
H	1.110383	-0.853629	-3.808795
H	1.065798	0.916478	-3.869834
N	-0.289698	-0.034280	2.485422
H	-1.044192	0.654129	2.450612
N	-0.289714	-0.034297	-2.485419
H	-1.044619	0.653668	-2.450793
C	-0.548927	-0.058352	-4.954972
H	-1.236432	0.799927	-4.949196
H	-0.009175	-0.047996	-5.910646
H	-1.148602	-0.974412	-4.899142

5.2. Complex of N^1,N^3-diethylpropane-1,3-diamine with palladium (Pd)



C	1.767343	-0.104650	1.141261
C	1.345012	0.740370	-1.346282
C	1.950664	-0.323849	-0.385820
H	1.750821	0.969735	1.353333
H	2.649070	-0.527619	1.665156
H	1.989489	0.793161	-2.242492
H	1.390453	1.722642	-0.858952
H	1.583975	-1.322537	-0.662379
H	3.037714	-0.328675	-0.572736
Pd	-1.024009	-0.064320	0.208950
N	-0.086006	0.518568	-1.755875
N	0.514903	-0.700398	1.717827
C	-0.278271	-0.447940	-2.883866
H	0.239504	-1.376731	-2.618067
H	-1.346367	-0.686026	-2.926528
C	0.197919	0.061494	-4.263719
H	0.005669	-0.698091	-5.033299
H	1.272416	0.283583	-4.277275
H	-0.343758	0.973182	-4.552589
C	0.363368	-0.462752	3.187688
C	-0.084816	0.970283	3.515021
H	1.309909	-0.689792	3.717484
H	-0.397663	-1.167158	3.545239
H	0.682382	1.711029	3.256648
H	-0.294119	1.065150	4.589138
H	-0.993434	1.205494	2.947584
H	-0.512597	1.415768	-2.000247
H	0.511342	-1.709315	1.538901

5.3. N^1,N^2-diethylethane-1,2-diamine



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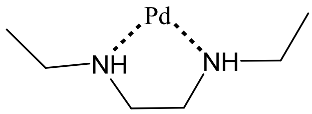
C	1.322780	0.157318	0.614657
H	2.086433	0.878781	0.970004
H	1.731762	-0.852466	0.748207
C	-0.185125	-0.621200	-2.822659
H	0.740016	-0.576703	-3.416464
H	-0.674274	-1.571313	-3.079861
C	0.142459	-0.185730	2.792170
H	0.908526	0.383582	3.359269
H	0.457613	-1.238420	2.806656
C	-1.219197	-0.045842	3.491815
H	-1.978708	-0.640555	2.970578
H	-1.159216	-0.387577	4.533051
H	-1.553664	1.001705	3.502111
C	-1.114395	0.550953	-3.240281
H	-0.648343	1.524593	-3.040406
H	-1.342178	0.501277	-4.314523
H	-2.064342	0.509081	-2.689483
N	0.189168	-0.677054	-1.401743
H	-0.590789	-0.846629	-0.766340
N	0.059217	0.241424	1.380189
H	-0.367237	1.167548	1.295859

5.4. Complex of N^1,N^2-diethylethane-1,2-diamine with palladium (Pd)



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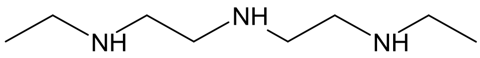
H	1.420748	1.204140	-1.461056
C	1.902843	-0.332434	-0.017168
H	2.927255	-0.013290	0.247219
H	1.854506	-1.424349	0.042726
C	0.155858	-0.396956	-3.449720
H	1.058165	-0.553184	-4.060500
H	-0.571193	-1.156893	-3.766569
C	1.367707	-0.137401	2.398164
H	2.446066	0.073999	2.520729
H	1.225934	-1.217837	2.504135
C	0.566169	0.614517	3.467827
H	-0.505136	0.411770	3.348312
H	0.880970	0.294768	4.469502
H	0.720918	1.700442	3.396176
C	-0.425763	1.011314	-3.744226
H	0.293290	1.805389	-3.503786
H	-0.687046	1.106307	-4.807507
H	-1.334010	1.185287	-3.151333
N	0.501711	-0.676761	-2.043887
H	-0.316660	-0.694067	-1.415819
N	0.946302	0.235394	1.001664
H	0.971702	1.259697	0.921379
Pd	-1.173942	-0.130726	0.671644

5.5. *N*[1]-ethyl-*N*[2]-(2-(ethylamino)ethyl)ethane-1,2-diamine



C	-2.028468	0.010724	1.110192
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H	-1.877993	0.437922	3.235357
H	-1.012570	1.579513	2.178586
C	-1.892146	-0.237310	-1.357259
H	-2.858906	0.260035	-1.531564
C	0.976288	0.332429	3.467802
H	0.527130	0.387567	4.482115
H	1.220586	1.363406	3.175461
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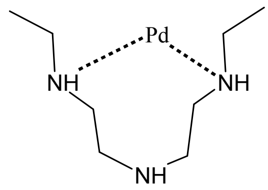
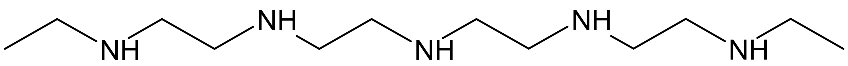
H	-0.304991	0.037169	-0.046770
N	0.037187	-0.210474	2.466684
H	-0.112053	-1.213965	2.595052
H	-2.107617	-1.330675	-1.301348
C	-0.973206	0.027237	-2.560396
H	-1.509750	-0.231641	-3.496705
H	-0.751518	1.099982	-2.592257
N	0.298155	-0.712587	-2.416874
H	0.131509	-1.717956	-2.349707
C	1.360208	-0.394468	-3.396500
H	2.110424	-1.195243	-3.342644
H	0.975021	-0.384047	-4.437327
C	2.049021	0.951656	-3.100340
H	1.347267	1.791079	-3.179584
H	2.458442	0.947979	-2.083576
H	2.866175	1.129643	-3.812862

5.6. Complex of N^1-ethyl-N^2-(2-(ethylamino)ethyl)ethane-1,2-diamine with palladium (Pd)



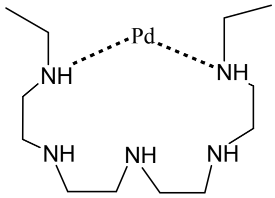
C	2.572343	0.171976	0.121737
H	3.642615	-0.070312	0.042578
H	2.506377	1.285499	0.157801
C	2.061452	-0.398140	1.458008
H	2.820387	-0.212466	2.238999
H	1.929651	-1.480676	1.357865
C	2.086632	0.248003	-2.327468
H	3.026114	-0.109585	-2.776041
C	0.379874	-0.325404	3.283520
H	1.245234	-0.211100	3.962605
H	0.172161	-1.395996	3.185138
C	-0.839124	0.402650	3.863579
H	-1.698080	0.289067	3.191670
H	-1.094979	-0.011823	4.847228
H	-0.641006	1.476559	3.990985
N	1.854361	-0.395206	-1.026121
H	0.838307	-0.405313	-0.828371
N	0.744110	0.185485	1.915759
H	0.854876	1.205594	1.974718
Pd	-0.878849	-0.009863	0.480245
H	2.173380	1.354589	-2.236032
C	0.911461	-0.069709	-3.282988
H	1.164177	0.306408	-4.292496
H	0.807838	-1.160425	-3.355769
N	-0.342264	0.473414	-2.754125
H	-0.374125	1.482179	-2.649441
C	-1.639489	-0.193326	-2.860904
H	-2.287835	0.268849	-3.628914
H	-1.466876	-1.229680	-3.179980
C	-2.399334	-0.191943	-1.509851
H	-1.931492	-0.951072	-0.817362
H	-2.411449	0.824829	-1.077656
H	-3.444544	-0.511899	-1.621175

5.7. *N*[1]-ethyl-*N*[2]-(2-(2-(2-(ethylamino)ethylamino)ethylamino)ethyl)ethane-1,2-diamine



C	-2.759397	-0.252952	-0.725692
H	-3.637483	0.164991	-1.240429
H	-2.872876	-1.355614	-0.719886
C	-2.759191	0.252866	0.726964
H	-3.637108	-0.165109	1.241974
H	-2.872659	1.355526	0.721223
C	-1.592929	0.027548	-2.908414
H	-2.329377	0.728640	-3.328027
C	-1.592028	-0.027436	2.909288
H	-2.328309	-0.728515	3.329226
H	-1.907642	0.993551	3.224706
C	-0.209355	-0.326976	3.510874
H	-0.281871	-0.337596	4.617411
H	0.096253	-1.329398	3.189722
N	-1.549721	0.181699	-1.446567
H	-0.704138	-0.266069	-1.087859
N	-1.549266	-0.181791	1.447446
H	-0.703833	0.265994	1.088389
H	-1.908582	-0.993413	-3.223926
C	-0.210439	0.327251	-3.510373
H	-0.283338	0.338233	-4.616887
H	0.095304	1.329551	-3.188988
N	0.786684	-0.647695	-3.018167
H	0.534179	-1.599584	-3.288592
C	2.206296	-0.349327	-3.310700
H	2.777776	-1.274201	-3.153200
H	2.358098	-0.054466	-4.369376
C	2.777180	0.749205	-2.393341
H	2.258380	1.705103	-2.536105
H	2.664649	0.457503	-1.342413
H	3.843018	0.911179	-2.605190
N	0.787675	0.647730	3.017990
H	0.535578	1.599701	3.288484
C	2.207414	0.349002	3.309608
H	2.778956	1.273876	3.152333
H	2.359701	0.053545	4.368041
C	2.777609	-0.749134	2.391352
H	2.258449	-1.704906	2.533659
H	2.664849	-0.456717	1.340648
H	3.843452	-0.911678	2.602753

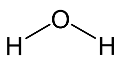
5.8. Complex of N^1-ethyl-N^2-(2-(2-(2-(ethylamino)ethylamino)ethylamino)ethyl)ethane-1,2-diamine with palladium (Pd)



C	3.389889	0.237629	-0.736606
H	4.335181	-0.057194	-1.214702
H	3.350410	1.346444	-0.743020
C	3.392770	-0.233741	0.728997
H	4.339172	0.062480	1.203963
H	3.354718	-1.342514	0.735348
C	1.758944	0.406028	-2.629761
H	2.416898	0.231745	-3.494426
C	1.763773	-0.410156	2.622550
H	2.424222	-0.242056	3.486513
H	1.769697	-1.509131	2.436027
C	0.339347	0.016166	3.015463
H	0.130556	-0.328641	4.043633
H	0.273648	1.107442	3.000005
N	2.246751	-0.347960	-1.467900
H	1.457958	-0.569798	-0.842776
N	2.250749	0.350056	1.464208
H	1.462313	0.573396	0.839280
H	1.766931	1.506115	-2.449796
C	0.332799	-0.020598	-3.016210
H	0.120378	0.321607	-4.044494
H	0.266449	-1.111785	-2.997531
N	-0.719466	0.542058	-2.090792
H	-0.531675	1.548290	-1.996092
C	-2.105746	0.397502	-2.668272
H	-2.774955	0.984475	-2.030053
H	-2.125941	0.834060	-3.684351
C	-2.592193	-1.057796	-2.720223
H	-1.995162	-1.668170	-3.408464
H	-2.531594	-1.501723	-1.719854
H	-3.634776	-1.088636	-3.063835
N	-0.716864	-0.543323	2.092755
H	-0.532150	-1.550077	1.997422
C	-2.101199	-0.394934	2.673922

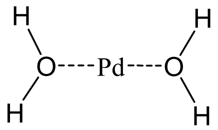
H	-2.773595	-0.980732	2.037969
H	-2.119657	-0.830744	3.690348
C	-2.584023	1.061573	2.726143
H	-1.983648	1.671072	3.412245
H	-2.525105	1.504597	1.725271
H	-3.625576	1.095175	3.072609
Pd	-0.680631	-0.000468	0.000975

5.9. H_2O



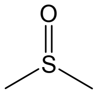
O	0.000000	0.112009	0.000000
H	0.800381	-0.448036	0.000000
H	-0.800381	-0.448036	0.000000

5.10. Complex of H_2O with palladium (Pd)



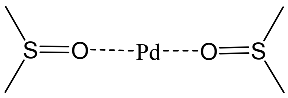
Pd	-0.016352	-0.000021	-0.000001
O	-0.016050	0.064206	-2.127846
O	-0.016018	-0.064115	2.127830
H	-0.342862	0.762396	2.529557
H	0.847066	-0.335543	2.491800
H	0.847106	0.335792	-2.491542
H	-0.342585	-0.762393	-2.529649

5.11. DMSO



O	1.591897	0.414463	-0.000059
S	0.188627	-0.515848	-0.000040
C	-0.822882	0.229868	1.432694
H	-0.817595	1.312805	1.292545
H	-1.834756	-0.183360	1.432969
H	-0.286357	-0.039884	2.343866
C	-0.822980	0.229908	-1.432567
H	-1.835344	-0.182167	-1.431859
H	-0.816414	1.312926	-1.293145
H	-0.287570	-0.041111	-2.344026

5.12. Complex of DMSO with palladium (Pd)



Pd	-0.045505	-0.361285	0.117256
O	-0.934514	-0.716656	1.900820
O	0.824846	-0.350770	-1.705400
S	-0.336131	0.050736	3.406058
S	0.043159	0.723508	-2.911505
C	1.046426	0.198327	-4.428379
H	0.518108	0.486420	-5.340801
H	2.006967	0.709517	-4.352079
H	1.178938	-0.882669	-4.347801
C	-1.550221	-0.227773	-3.263386
H	-2.100137	0.263899	-4.070581
H	-1.271698	-1.253320	-3.514571
H	-2.101837	-0.208025	-2.322065
C	1.495628	-0.387372	3.314545
H	1.759703	-0.289640	2.253301
H	2.071359	0.282262	3.959096
H	1.583354	-1.425322	3.639298
C	-0.218091	1.853335	2.868805
H	0.507581	2.382699	3.491918
H	0.080816	1.806841	1.811397
H	-1.217485	2.278843	2.973384

5.13. Palladium (Pd)

Pd	0.000000	0.000000	0.000000