Electronic Supplementary Material (ESI) for RSC Advances

Platinum(II) and Palladium(II) Complexes derived from 1-Ferrocenylmethyl-3,5-diphenylpyrazole. Coordination, Cyclometallation or Transannulation?

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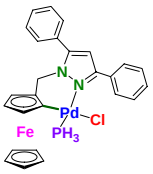
SUPPORTING INFORMATION

(25 pages)

Contents:

[‡] Letters **A**, **B** and **C** refer to the model complexes shown in the lower part of Table 5.

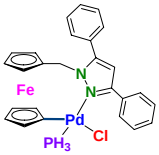
Table S5. a) Final atomic coordinates for the optimized geometry of



(**B**-type model complex with L = PH_3)

b) its calculated total energy (in vacuum, toluene and methanol).

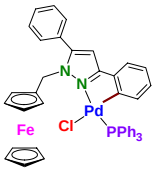
Table S6. a) Final atomic coordinates for the optimized geometry of



(**C**-type model complex with L = PH_3)

b) its calculated total energy (in vacuum, toluene and methanol).

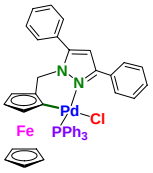
Table S7. a) Final atomic coordinates for the optimized geometry of



(**A**-type model complex with L = PPh_3)

b) its calculated total energy in vacuum, toluene and methanol.

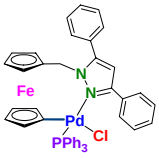
Table S8. a) Final atomic coordinates for the optimized geometry of



(**B**-type model complex with L = PPh_3)

b) its calculated total energy in vacuum, toluene and methanol.

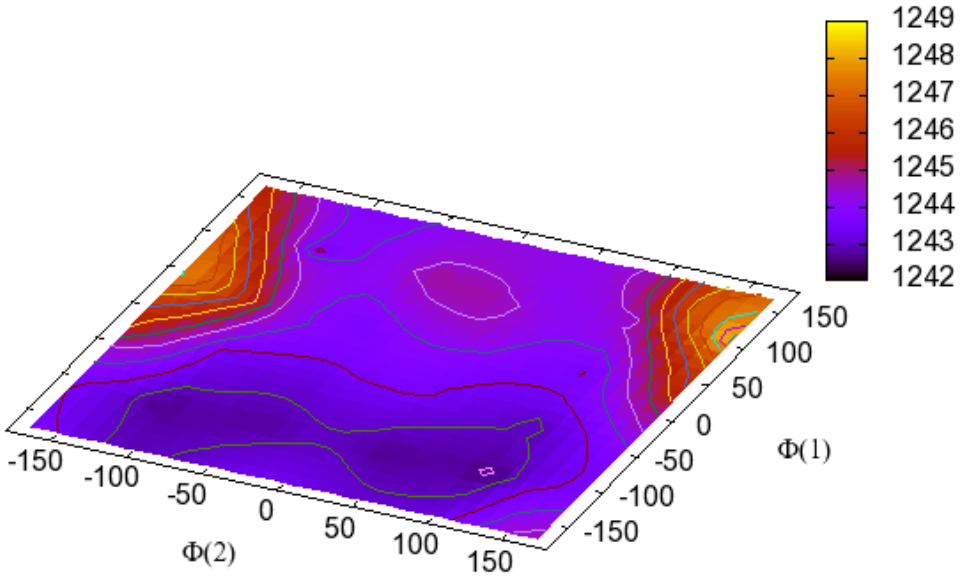
Table S9. a) Final atomic coordinates for the optimized geometry of



(**C**-type model complex with L = PPh_3)

b) its calculated total energy in vacuum, toluene and methanol.

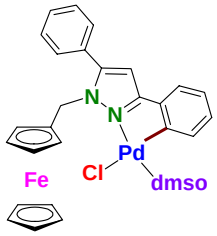
Figure S1. Conformational map showing the variation of the total energy of the ligand as a function of the torsion angles Φ(1) and Φ(2).[§]



[§] Total energy in Kcal /mol and the torsión angles Φ(1) and Φ(2) in degrees.

Supplementary Tables:[**]

Table S1. a) Final atomic coordinates for the optimized geometry of



(**A**-type model complex with L = dmso)

b) its calculated total energy in vacuum, toluene and methanol.

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	-3.264670	-1.900021	-0.709745
7	-0.518360	1.395871	0.532162
6	-2.903530	-3.533507	0.520802
1	-1.906503	-3.838705	0.809609
6	-3.710698	-2.574241	1.204599
1	-3.439315	-2.053225	2.113467
6	-4.916064	-2.395088	0.459626
1	-5.721232	-1.714605	0.704684
6	-4.855080	-3.244592	-0.686333
1	-5.604915	-3.319260	-1.463176
6	-3.612367	-3.947827	-0.647578
1	-3.253646	-4.643391	-1.395034
6	-3.276306	0.132178	-1.133113
1	-3.974907	0.841814	-0.709136
6	-3.459645	-0.612546	-2.335478
1	-4.328113	-0.575175	-2.980042
6	-2.319376	-1.455210	-2.510714
1	-2.176242	-2.169192	-3.311227
6	-1.432214	-1.235736	-1.417133
1	-0.504484	-1.754744	-1.219518
6	-2.022633	-0.256865	-0.553399
6	-1.432660	0.252409	0.732082
1	-2.219544	0.595894	1.404008
1	-0.853591	-0.525251	1.230925
6	-0.869980	2.703189	0.336320
6	0.242187	3.362370	-0.170186
1	0.314885	4.417635	-0.386554
6	1.249673	2.388780	-0.262314

[**] Letters **A**, **B** and **C** refer to the model complexes shown in the lower part of Table 5.

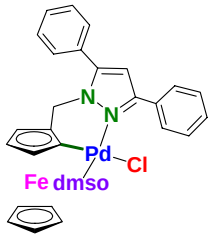
6	2.645036	2.414262	-0.670735
6	3.261470	3.551856	-1.205443
1	2.692565	4.471943	-1.317348
6	4.599217	3.502962	-1.594694
1	5.076954	4.385417	-2.011577
6	5.314491	2.315749	-1.444921
1	6.357594	2.267155	-1.748365
6	4.705208	1.172965	-0.904369
1	5.288784	0.264715	-0.791933
6	3.369520	1.209645	-0.515531
6	-2.200768	3.258927	0.650435
6	-2.894147	3.989648	-0.327402
1	-2.460639	4.095115	-1.317604
6	-4.134519	4.558716	-0.038325
1	-4.662178	5.117516	-0.806309
6	-4.698453	4.406013	1.230181
1	-5.665394	4.847891	1.454217
6	-4.011842	3.688263	2.212415
1	-4.438128	3.577994	3.205695
6	-2.769518	3.122087	1.927957
1	-2.224779	2.592024	2.704383
7	0.773486	1.202203	0.153699
46	2.279169	-0.300089	0.317921
17	0.923655	-2.103113	1.419507
16	4.044489	-1.879884	0.444639
6	4.186882	-2.419110	2.184403
1	4.569228	-1.558183	2.736814
1	4.910700	-3.238120	2.209027
1	3.199335	-2.708969	2.545589
6	3.465527	-3.416005	-0.358323
1	2.482684	-3.673095	0.038826
1	4.219307	-4.184428	-0.166986
1	3.413844	-3.194288	-1.426462
8	5.453883	-1.638878	-0.052600

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-1543.22982335	-1543.24340065	-1543.25496056

Table S2. a) Final atomic coordinates for the optimized geometry of



(**B**-type model complex with L =dmso)

b) its calculated total energy in vacuum, toluene and methanol.

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	-0.791271	-2.414980	1.015724
7	-1.444896	0.587259	-0.819888
6	-0.578821	-1.321511	2.785645
1	0.151484	-0.539751	2.943300
6	-1.893711	-1.143922	2.261224
1	-2.332662	-0.201333	1.963698
6	-2.515557	-2.427808	2.185919
1	-3.511499	-2.636488	1.816671
6	-1.582775	-3.398046	2.663869
1	-1.741275	-4.467904	2.701431
6	-0.385670	-2.713693	3.033676
1	0.522314	-3.173906	3.400580
6	-1.243460	-3.134995	-0.874273
1	-2.217921	-3.503861	-1.171572
6	-0.190193	-3.901284	-0.291518
1	-0.233715	-4.955431	-0.047754
6	0.907986	-3.022491	-0.027390
1	1.853045	-3.303002	0.413435
6	0.552656	-1.712080	-0.467209
6	-0.788182	-1.779472	-0.967067
6	-1.493549	-0.632974	-1.630459
1	-1.025937	-0.406263	-2.598261
1	-2.544491	-0.853837	-1.813769
6	-2.446863	1.458743	-0.511563
6	-1.860081	2.489480	0.210828
1	-2.373267	3.318515	0.674325
6	-0.492606	2.172585	0.321815
6	0.513890	2.907632	1.105478
6	0.475567	4.309603	1.138035
1	-0.248420	4.838713	0.524770
6	1.377818	5.024856	1.923300
1	1.344372	6.110909	1.927919

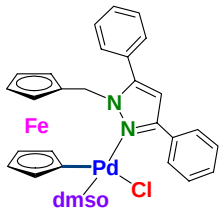
6	2.326186	4.349126	2.693978
1	3.028753	4.906749	3.307365
6	2.366671	2.953391	2.673303
1	3.096935	2.420670	3.276758
6	1.466749	2.236548	1.886896
1	1.494028	1.150960	1.877814
6	-3.867377	1.278252	-0.868487
6	-4.558078	2.336425	-1.480918
1	-4.021572	3.248058	-1.727592
6	-5.914004	2.215788	-1.783412
1	-6.434029	3.041514	-2.261066
6	-6.598809	1.037251	-1.479919
1	-7.654777	0.943270	-1.717424
6	-5.922347	-0.018345	-0.864702
1	-6.452631	-0.932670	-0.612907
6	-4.567520	0.100301	-0.555421
1	-4.054089	-0.711563	-0.047715
46	1.563288	0.009978	-0.725914
7	-0.256636	1.019911	-0.333800
17	2.671611	2.058700	-1.546366
16	3.602337	-1.098835	-1.050538
6	4.900320	-0.114546	-0.222607
1	5.865568	-0.543002	-0.506109
1	4.733732	-0.234532	0.849934
1	4.788027	0.929585	-0.520836
6	4.073623	-0.865643	-2.799711
1	5.090819	-1.246433	-2.925841
1	3.984124	0.196737	-3.036612
1	3.369713	-1.458564	-3.387586
8	3.833741	-2.546551	-0.687869

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-1543.21819539	-1543.23391011	-1543.24804485

Table S3. a) Final atomic coordinates for the optimized geometry of



(**C**-type model complex with L = dmso)

b) its calculated total energy (in vacuum, toluene and methanol).

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	0.248527	-2.408672	1.225600
7	1.589834	0.445073	-0.645775
6	-0.621792	-0.799138	2.194853
1	-0.106945	0.122396	2.424380
6	-1.341344	-1.086690	0.986453
6	-1.823074	-2.432048	1.097211
1	-2.406625	-2.960066	0.357977
6	-1.408939	-2.962868	2.356166
1	-1.596626	-3.967617	2.713598
6	-0.667996	-1.952649	3.037438
1	-0.194423	-2.052527	4.006211
6	1.014841	-3.299003	-0.477641
1	0.416969	-3.578713	-1.335784
6	1.293534	-4.119734	0.655866
1	0.936197	-5.129201	0.811105
6	2.074743	-3.353974	1.572180
1	2.415905	-3.680444	2.545880
6	2.286352	-2.062763	1.003926
1	2.819032	-1.244607	1.469583
6	1.622134	-2.018244	-0.264437
6	1.625651	-0.887169	-1.258958
1	2.532980	-0.917164	-1.867681
1	0.769198	-0.953531	-1.935147
6	2.646565	1.228800	-0.274199
6	2.124155	2.261129	0.490112
1	2.668516	3.103237	0.890524
6	0.730326	2.058583	0.528963
6	-0.272788	2.916876	1.187810
6	-0.022898	3.385916	2.487907
1	0.886726	3.083175	3.000116
6	-0.940158	4.217448	3.129159

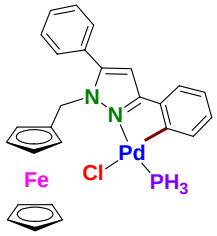
1	-0.738930	4.565154	4.138819
6	-2.114824	4.597560	2.476211
1	-2.829527	5.247062	2.974585
6	-2.361966	4.147181	1.177684
1	-3.263966	4.458020	0.656931
6	-1.449134	3.312875	0.530785
1	-1.624277	2.992462	-0.492023
6	4.046128	0.997140	-0.681807
6	5.054951	0.963339	0.293807
1	4.785455	1.064754	1.341363
6	6.389468	0.792279	-0.073656
1	7.159134	0.763144	0.692617
6	6.734194	0.653502	-1.419583
1	7.773612	0.517768	-1.705040
6	5.738792	0.696884	-2.398431
1	6.001883	0.605835	-3.448581
6	4.404050	0.872961	-2.034985
1	3.638210	0.944340	-2.802436
7	0.427928	0.941463	-0.152669
46	-1.458034	0.098983	-0.638743
16	-3.587690	-0.700114	-1.228013
6	-3.549413	-1.205820	-2.984504
1	-2.971981	-2.132281	-3.019399
1	-3.063698	-0.420190	-3.566082
1	-4.581367	-1.393477	-3.293673
6	-4.650112	0.782691	-1.336820
1	-4.758408	1.157581	-0.316962
1	-5.619416	0.468715	-1.733636
1	-4.149539	1.515913	-1.972891
8	-4.342376	-1.766565	-0.472147
17	-1.508306	1.487692	-2.706609

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-1543.22097937 H	-1386.43179221	-1386.44390268

Table S4. a) Final atomic coordinates for the optimized geometry of



(**A**-type model complex with L = PH_3)

b) its calculated total energy (in vacuum, toluene and methanol).

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	3.291246	-1.446110	0.668128
7	-0.082520	1.229450	-0.536661
6	3.294138	-3.160905	-0.503134
1	2.391885	-3.703287	-0.752224
6	3.834267	-2.063612	-1.239959
1	3.425162	-1.654774	-2.154513
6	4.980714	-1.578417	-0.539489
1	5.595302	-0.736397	-0.829960
6	5.151143	-2.377389	0.631703
1	5.912246	-2.242065	1.389105
6	4.109575	-3.354820	0.653093
1	3.944457	-4.088382	1.431401
6	2.877129	0.543042	1.092669
1	3.415402	1.383563	0.674290
6	3.205285	-0.148936	2.295256
1	4.041799	0.069855	2.946057
6	2.264631	-1.210915	2.464615
1	2.268728	-1.939517	3.264554
6	1.356697	-1.180639	1.366766
1	0.558057	-1.881536	1.163970
6	1.734646	-0.097569	0.507481
6	1.042091	0.298230	-0.766051
1	1.736645	0.796834	-1.442775
1	0.619393	-0.572633	-1.270579
6	-0.027131	2.575097	-0.297938
6	-1.270954	2.959540	0.189142
1	-1.576243	3.967088	0.428608
6	-2.044242	1.786932	0.224034
6	-3.425512	1.490463	0.586788
6	-4.283579	2.454210	1.129223
1	-3.927060	3.470519	1.279222
6	-5.589013	2.113755	1.481398

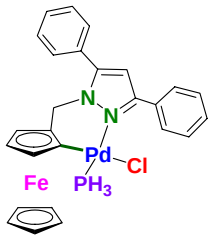
1	-6.252788	2.863044	1.903494
6	-6.030013	0.805592	1.290669
1	-7.043532	0.526003	1.568108
6	-5.174136	-0.160015	0.742066
1	-5.561839	-1.165504	0.614077
6	-3.864271	0.158198	0.378251
6	1.157705	3.416118	-0.554228
6	1.636310	4.262730	0.458588
1	1.153472	4.251696	1.431311
6	2.731639	5.094617	0.226979
1	3.093964	5.740553	1.021878
6	3.364384	5.092181	-1.018066
1	4.219208	5.738318	-1.196934
6	2.890070	4.259937	-2.034771
1	3.368089	4.263680	-3.010370
6	1.791889	3.430872	-1.807858
1	1.406637	2.810833	-2.612374
7	-1.306229	0.749730	-0.204473
46	-2.435468	-1.048042	-0.444891
17	-0.783948	-2.593516	-1.473136
15	-3.697619	-2.921772	-0.772375
1	-3.238908	-4.106957	-0.149759
1	-5.075277	-3.000015	-0.417945
1	-3.783816	-3.369798	-2.111496

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-1386.41837055	-1386.43179221	-1386.44390268

Table S5. a) Final atomic coordinates for the optimized geometry of



(**B**-type model complex with L = PH_3)

b) its calculated total energy (in vacuum, toluene and methanol).

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	-0.866310	-2.416596	0.881446
7	-1.058897	0.766918	-0.749089
6	-0.248141	-1.412952	2.604958
1	0.609991	-0.757566	2.654093
6	-1.578141	-1.022192	2.268502
1	-1.898978	-0.015903	2.035865
6	-2.398078	-2.191574	2.277489
1	-3.454425	-2.233756	2.045308
6	-1.573168	-3.305410	2.621895
1	-1.891724	-4.337962	2.681878
6	-0.244501	-2.823409	2.823516
1	0.620795	-3.427254	3.064000
6	-1.691634	-2.899879	-0.957492
1	-2.752836	-3.018284	-1.140782
6	-0.791026	-3.920321	-0.530944
1	-1.052291	-4.947995	-0.311890
6	0.504688	-3.326734	-0.382230
1	1.385836	-3.846278	-0.027115
6	0.425367	-1.942600	-0.735484
6	-0.943370	-1.682045	-1.067329
6	-1.435233	-0.366801	-1.600159
1	-1.015211	-0.185192	-2.598576
1	-2.521178	-0.350039	-1.688561
6	-1.828349	1.814107	-0.334067
6	-0.981896	2.672384	0.353533
1	-1.271564	3.570315	0.878175
6	0.295819	2.078657	0.329061
6	1.497550	2.568946	1.023689
6	1.710262	3.951645	1.137590
1	1.025975	4.640228	0.649729

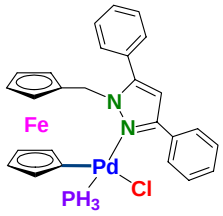
6	2.806027	4.445013	1.842897
1	2.963444	5.517987	1.911511
6	3.702508	3.563717	2.450928
1	4.557345	3.947861	3.000896
6	3.497037	2.186733	2.345919
1	4.190474	1.494648	2.815865
6	2.403012	1.691773	1.639287
1	2.246569	0.620353	1.560473
6	-3.277760	1.950599	-0.577667
6	-3.768660	3.151403	-1.115579
1	-3.068597	3.936867	-1.385083
6	-5.136794	3.330324	-1.317756
1	-5.500616	4.263201	-1.739422
6	-6.034320	2.312987	-0.987036
1	-7.099856	2.451861	-1.147313
6	-5.557160	1.117929	-0.444421
1	-6.251165	0.327606	-0.171678
6	-4.189962	0.937477	-0.235355
1	-3.828089	0.017982	0.216253
46	1.759559	-0.451212	-1.012538
7	0.233252	0.927933	-0.367930
17	3.401684	1.220890	-1.736565
15	3.393044	-1.825161	-1.787578
1	3.258873	-3.241711	-1.736443
1	4.674080	-1.687075	-1.202592
1	3.728276	-1.672986	-3.153555

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-1386.40766262	-1386.42284279	-1386.43697961

Table S6. a) Final atomic coordinates for the optimized geometry of



(**C**-type model complex with L = PH_3)

b) its calculated total energy (in vacuum, toluene and methanol).

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	0.087770	2.569302	0.902729
7	-1.347561	-0.528740	-0.568074
6	1.352338	1.187215	1.801058
1	1.027172	0.252588	2.236496
6	1.740583	1.380896	0.433893
6	2.050029	2.776699	0.292622
1	2.331498	3.277783	-0.625506
6	1.861085	3.426723	1.552734
1	1.983757	4.484244	1.750700
6	1.429541	2.439481	2.487130
1	1.169804	2.615529	3.523556
6	-1.136011	3.271690	-0.613059
1	0.777005	3.594086	-1.582333
6	-1.284509	4.094081	0.543936
1	-1.050356	5.148639	0.606978
6	-1.739872	3.268246	1.615207
1	-1.912009	3.585435	2.635343
6	-1.882766	1.938108	1.119008
1	-2.179776	1.072955	1.696192
6	-1.502353	1.932130	-0.261086
6	-1.554371	0.768559	-1.217285
1	-2.532823	0.717981	-1.701942
1	-0.798628	0.866784	-2.001437
6	-2.292423	-1.348931	-0.013644
6	-1.606379	-2.279178	0.751656
1	-2.032738	-3.122901	1.273476
6	-0.236585	-1.978815	0.603712
6	0.901222	-2.707841	1.196327
6	0.842827	-3.079883	2.549756
1	-0.023749	-2.801127	3.143830
6	1.893860	-3.783235	3.136744
1	1.839753	-4.057129	4.187001
6	3.013787	-4.129255	2.377004
1	3.833341	-4.678018	2.833425

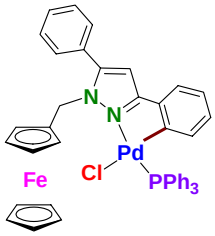
6	3.071591	-3.775163	1.027467
1	3.931476	-4.058593	0.426324
6	2.022958	-3.071207	0.433300
1	2.054648	-2.828686	-0.625038
6	-3.741292	-1.246891	-0.271794
6	-4.641132	-1.234118	0.805608
1	-4.255595	-1.254936	1.821063
6	-6.016299	-1.184284	0.578547
1	-6.700768	-1.170178	1.422208
6	-6.511330	-1.146326	-0.726534
1	-7.582634	-1.104942	-0.902426
6	-5.624518	-1.169737	-1.805301
1	-6.003163	-1.157664	-2.823541
6	-4.249246	-1.225668	-1.582057
1	-3.565146	-1.283612	-2.424203
7	-0.100336	-0.903132	-0.187720
46	1.675529	-0.014870	-1.024703
17	1.666706	-1.540075	-2.963128
15	3.612200	0.706547	-1.973118
1	4.393981	1.742357	-1.391847
1	4.612264	-0.281018	-2.139326
1	3.534201	1.188961	-3.302790

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-1386.41189326	-1386.42670869	-1386.44027157

Table S7. a) Final atomic coordinates for the optimized geometry of



(**A**-type model complex with L = PPh_3)

b) its calculated total energy in vacuum, toluene and methanol.

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	-4.237423	-2.30237	-0.700237
7	-2.116008	1.469444	0.403225
6	-3.357384	-3.856673	0.361359
1	-2.288222	-3.929383	0.510880
6	-4.269490	-3.146364	1.199728
1	-4.011919	-2.616237	2.107420
6	-5.568559	-3.223091	0.610492
1	-6.470244	-2.762735	0.993471
6	-5.460610	-3.982903	-0.593800
1	-6.264797	-4.195653	-1.286071
6	-4.095167	-4.374167	-0.746409
1	-3.683410	-4.930505	-1.578321
6	-4.754031	-0.309127	-0.967321
1	-5.525520	0.203177	-0.406798
6	-4.934184	-1.023008	-2.188618
1	-5.870370	-1.155734	-2.715091
6	-3.671433	-1.574367	-2.567127
1	-3.486485	-2.200482	-3.430318
6	-2.710892	-1.206657	-1.580532
1	-1.672564	-1.507034	-1.538182
6	-3.377676	-0.427371	-0.580462
6	-2.738226	0.152580	0.649685
1	-3.480496	0.294420	1.435763
1	-1.944416	-0.499728	1.017419
6	-2.735019	2.689762	0.371047
6	-1.868123	3.574617	-0.257187
1	-2.027432	4.633717	-0.395283
6	-0.729998	2.818288	-0.588647
6	0.530153	3.127662	-1.253889
6	0.718087	4.320117	-1.964559
1	-0.058421	5.081679	-1.953416
6	1.879258	4.517308	-2.709794
1	2.022302	5.441138	-3.263917

6	2.836683	3.505372	-2.758826
1	3.731767	3.629715	-3.363865
6	2.659775	2.321726	-2.028750
1	3.431201	1.564620	-2.093242
6	1.526201	2.117823	-1.239116
6	-4.069533	2.958690	0.939433
6	-5.035753	3.613006	0.158315
1	-4.800352	3.869249	-0.870528
6	-6.289808	3.915280	0.688879
1	-7.028543	4.417806	0.070476
6	-6.597908	3.567397	2.005909
1	-7.575880	3.800911	2.417685
6	-5.641263	2.922654	2.793540
1	-5.868784	2.660945	3.823295
6	-4.384624	2.624508	2.267533
1	-3.633067	2.152627	2.894369
7	-0.901900	1.543933	-0.199340
46	0.991610	0.459887	-0.167032
17	0.172538	-1.648203	0.846404
15	3.112089	-0.413508	0.292212
6	4.645759	0.512255	-0.202057
6	6.938974	1.989882	-0.867391
6	5.576493	0.003293	-1.117234
6	4.874945	1.772904	0.375106
6	6.014356	2.503379	0.047599
6	6.717142	0.742162	-1.448554
1	5.418020	-0.968666	-1.572434
1	4.156366	2.184952	1.078182
1	6.178213	3.476975	0.501332
1	7.431370	0.335234	-2.159442
1	7.826074	2.562303	-1.124966
6	3.445006	-0.623646	2.108777
6	4.000217	-0.900310	4.849379
6	2.416063	-0.520625	3.055135
6	4.759035	-0.858801	2.553541
6	5.031649	-1.004722	3.913530
6	2.696907	-0.655780	4.416593
1	1.396829	-0.364517	2.723757
1	5.574567	-0.918647	1.839668
1	6.051237	-1.191503	4.240041
1	1.888636	-0.572230	5.137995
1	4.213650	-1.006533	5.909784
6	3.322252	-2.068114	-0.505165
6	3.627735	-4.509273	-1.850258
6	3.930748	-3.155418	0.134407
6	2.857918	-2.217008	-1.821394
6	3.017795	-3.429024	-2.492392
6	4.078572	-4.371014	-0.536886

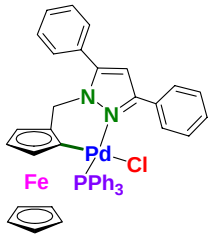
1	4.274492	-3.064578	1.159270
1	2.356277	-1.387530	-2.312833
1	2.653201	-3.532662	-3.510742
1	4.541966	-5.211745	-0.027592
1	3.742287	-5.457272	-2.369080

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-2079.56213985	-2079.57805683	-2079.59479313

Table S8. a) Final atomic coordinates for the optimized geometry of



(**B**-type model complex with L = PPh_3)

b) its calculated total energy in vacuum, toluene and methanol.

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	-1.626876	-2.121505	1.461128
7	-2.601561	0.315115	-0.932184
6	-2.039011	-0.659906	2.897105
1	-1.621290	0.336806	2.889950
6	-3.248644	-1.060802	2.256032
1	-3.910416	-0.413739	1.696334
6	-3.419097	-2.462502	2.471059
1	-4.230211	-3.072958	2.094967
6	-2.314045	-2.926604	3.248292
1	-2.134569	-3.950061	3.550931
6	-1.460966	-1.812034	3.510082
1	-0.517507	-1.844810	4.038746
6	-1.636308	-3.204875	-0.302682
1	-2.474043	-3.801513	-0.643760
6	-0.576735	-3.641193	0.545178
1	-0.474021	-4.627981	0.979332
6	0.288687	-2.523513	0.776235
1	1.155971	-2.543462	1.419545
6	-0.198949	-1.387656	0.052717
6	-1.411504	-1.817779	-0.589494
6	-2.214475	-0.964395	-1.531526
1	-1.632471	-0.742706	-2.436261
1	-3.132056	-1.463856	-1.841293
6	-3.820790	0.926707	-0.910879
6	-3.632147	2.143627	-0.270726
1	-4.401772	2.857749	-0.019309
6	-2.268706	2.202737	0.083045
6	-1.619251	3.259687	0.875610
6	-2.087890	4.579226	0.781627
1	-2.874250	4.818415	0.071333
6	-1.531725	5.588930	1.564838
1	-1.899231	6.607229	1.470159
6	-0.501093	5.295552	2.459856

1	-0.066323	6.082607	3.070095
6	-0.030020	3.985102	2.563062
1	0.773034	3.748461	3.256143
6	-0.584557	2.975203	1.779662
1	-0.214790	1.957738	1.860021
6	-5.068960	0.356347	-1.454271
6	-5.853201	1.134770	-2.321258
1	-5.500417	2.119673	-2.613133
6	-7.062827	0.646779	-2.814447
1	-7.655747	1.259941	-3.487542
6	-7.506995	-0.626210	-2.450760
1	-8.448496	-1.006939	-2.836911
6	-6.738076	-1.406026	-1.584292
1	-7.084140	-2.392018	-1.286119
6	-5.530428	-0.918872	-1.084236
1	-4.953544	-1.517566	-0.384964
46	0.431554	0.492232	-0.438966
7	-1.654701	1.084800	-0.346682
17	0.937943	2.631946	-1.463172
15	2.663008	-0.165055	-0.449010
6	3.104668	-1.430486	-1.729670
6	3.767708	-3.349863	-3.670384
6	4.443603	-1.628004	-2.110891
6	2.103400	-2.198787	-2.340863
6	2.435568	-3.152523	-3.305322
6	4.771433	-2.585370	-3.071081
1	5.228987	-1.023346	-1.668261
1	1.066709	-2.049957	-2.061663
1	1.648528	-3.737699	-3.773125
1	5.810415	-2.726395	-3.356681
1	4.023458	-4.090247	-4.423714
6	3.941081	1.145678	-0.735498
6	5.875795	3.108895	-1.261587
6	4.844537	1.536447	0.261693
6	4.009784	1.755647	-1.999584
6	4.976766	2.723890	-2.259548
6	5.805550	2.516535	-0.001632
1	4.808947	1.080893	1.245136
1	3.300405	1.485231	-2.772920
1	5.016943	3.189169	-3.240486
1	6.499559	2.809804	0.781600
1	6.624194	3.870036	-1.466131
6	3.172225	-0.890965	1.180979
6	3.897598	-1.868329	3.712328
6	2.676789	0.287098	2.347973
6	4.031803	-1.991983	1.296733
6	4.387270	-2.479526	2.556740
6	3.043697	-0.767536	3.605415

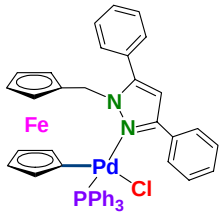
1	1.994018	0.554187	2.267832
1	4.415664	-2.480609	0.407304
1	5.047158	-3.339640	2.632370
1	2.656338	-0.287062	4.499855
1	4.176589	-2.249133	4.691083

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-2079.55290941	-2079.57138085	-2079.58956336

Table S9. a) Final atomic coordinates for the optimized geometry of



(**C**-type model complex with L = PPh_3)

b) its calculated total energy in vacuum, toluene and methanol.

a)

Atomic Number	Atomic Coordinates (Angstroms) X	Y	Z
26	-1.370972	-2.407046	-1.482653
7	-2.793162	0.384076	0.494864
6	-0.642078	-0.805696	-2.572880
1	-1.234093	0.065567	-2.818938
6	0.159911	-0.973884	-1.390584
6	0.691222	-2.307064	-1.460141
1	1.301334	-2.783183	-0.704372
6	0.246182	-2.933398	-2.666324
1	0.460548	-3.948993	-2.975306
6	-0.582102	-2.001276	-3.357739
1	-1.109688	-2.181584	-4.286164
6	-1.994330	-3.325476	0.263177
1	-1.329335	-3.580684	1.078414
6	-2.314328	-4.153870	-0.853750
1	-1.930030	-5.148874	-1.036286
6	-3.179152	-3.415080	-1.716610
1	-3.568293	-3.751896	-2.668646
6	-3.402761	-2.134512	-1.128953
1	-3.990492	-1.332576	-1.555373
6	-2.661971	-2.069193	0.093973
6	-2.643723	-0.944232	1.091487
1	-3.470028	-1.054136	1.798670
1	-1.713520	-0.936698	1.666567
6	-3.923996	1.143796	0.392596
6	-3.565714	2.287428	-0.301616
1	-4.218085	3.109306	-0.554997
6	-2.187086	2.168873	-0.576474
6	-1.332329	3.180052	-1.227226
6	-1.676315	4.537545	-1.109247
1	-2.539501	4.821126	-0.514542
6	-0.903836	5.526374	-1.715919
1	-1.184036	6.570388	-1.604174

6	0.230615	5.178862	-2.452206
1	0.834773	5.949313	-2.923701
6	0.583064	3.833492	-2.575667
1	1.460998	3.549512	-3.150172
6	-0.190693	2.842080	-1.971930
1	0.089391	1.801117	-2.081559
6	-5.240393	0.772232	0.951975
6	6.353584	0.670181	0.103316
1	-6.224371	0.826648	-0.963976
6	-7.612547	0.363988	0.620517
1	-8.464765	0.284143	-0.048775
6	-7.775642	0.155997	1.991492
1	-8.755859	-0.084739	2.393691
6	-6.675701	0.265052	2.845351
1	-6.798772	0.119069	3.914942
6	-5.416742	0.576251	2.332090
1	-4.570194	0.694072	3.003124
7	-1.740979	0.993184	-0.098860
46	0.306188	0.306515	0.184802
17	0.214479	1.452782	2.355334
15	2.566628	-0.122501	0.482752
6	3.689007	-0.287141	-0.990151
6	5.444795	-0.403852	-3.182116
6	5.073310	-0.442134	-0.792353
6	3.201322	-0.174087	-2.298605
6	4.076550	-0.231113	-3.386925
6	5.942088	-0.509042	-1.880245
1	5.477037	-0.495920	0.214260
1	2.138805	-0.050446	-2.468894
1	3.681331	-0.142161	-4.395235
1	7.008311	-0.632516	-1.710153
1	6.123264	-0.449904	-4.029888
6	3.443452	1.209609	1.422188
6	4.844824	3.286694	2.677540
6	3.249177	2.539335	1.019204
6	4.338155	0.930029	2.462451
6	5.034462	1.967705	3.087983
6	3.950958	3.569439	1.641157
1	2.535035	2.771649	0.234831
1	4.486763	-0.091484	2.797854
1	5.720884	1.740230	3.899385
1	3.786828	4.596334	1.326310
1	5.384263	4.093156	3.167195
6	2.797701	-1.659314	1.486242
6	2.967771	-3.976385	3.060572
6	2.149327	-1.719215	2.734052
6	3.521122	-2.771815	1.034049
6	3.602372	-3.925475	1.819528

6	2.243293	-2.870289	3.515367
1	1.569612	-0.866442	3.080091
1	4.019523	-2.745606	0.070700
1	4.164093	-4.782200	1.456731
1	1.744379	-2.903907	4.480255
1	3.033991	-4.873544	3.670401

b)

Calculated total energy (in Hartrees)

in vacuum	in toluene	in methanol
-2079.55795611	-2079.57564349	-2079.59266393