Supporting Information for the Paper Entitled "Structural, Spectroscopic ad Theoretical Elucidation of a Redox Active Pincer-Type Ancillary Applied in Catalysis"

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Cartesian coordinates of the simplified computational model for [(PNP)NiCl] (**1**)

Ni	0.00000	0.00000	0.00000
Cl	0.04041	-2.15820	-0.27194
P	-2.19431	0.18884	0.06577
C	-2.96230	0.06017	1.73518
H	-3.99026	0.42084	1.76718
H	-2.33789	0.58051	2.46138
H	-2.93529	-0.83113	1.96947
C	-3.27673	-0.75409	-1.08656
H	-4.10284	-0.30737	-1.11377
H	-3.46318	-1.76791	-0.73259
H	-2.83711	-0.74245	-2.08401
C	-2.32845	1.91324	-0.43263
C	-3.45659	2.52719	-0.96362
H	-4.27449	2.02332	-1.05190
C	-3.43776	3.83092	-1.44037
H	-4.32222	4.28444	-1.88718
C	-2.22972	4.51080	-1.33372
H	-2.16597	5.31879	-1.71819
C	-1.07997	3.93436	-0.80907
H	-0.30212	4.39865	-0.87987
C	-1.09946	2.61307	-0.33162
N	0.01004	1.89912	0.13733
C	1.15637	2.55469	0.60544
C	1.18170	3.83101	1.17856
H	0.39815	4.33450	1.28496
C	2.36934	4.39575	1.62283
H	2.33307	5.21375	2.05956
C	3.58661	3.72711	1.51930
H	4.51625	4.20908	1.82190
C	3.56221	2.44063	1.00470
H	4.34001	1.93648	0.98865
C	2.37860	1.85269	0.56281
P	2.18137	0.15852	-0.02306
C	3.21323	-0.87173	1.10625
H	3.99417	-0.40540	1.18684
H	2.72298	-0.90529	2.07921
H	3.41064	-1.87149	0.71962
C	2.90857	0.06595	-1.70697
H	3.96941	0.31088	-1.75847
H	2.32224	0.68939	-2.38145
H	2.75966	-0.79349	-1.97713

Cartesian coordinates of the simplified computational model for [(PNP)NiCl][OTf] (**[1][OTf]**)

Ni	0.00000	0.00000	0.00000
Cl	0.09087	-2.13658	0.21033
P	-2.18530	0.14777	0.31055
C	-3.03085	-0.83257	1.59967
H	-3.81441	-0.35733	1.81178
H	-2.40437	-0.87883	2.49026
H	-3.31097	-1.82796	1.25522
C	-3.23177	0.14095	-1.20383
H	-4.25970	0.44051	-1.00116
H	-3.21042	-0.71475	-1.50421
H	-2.77542	0.75995	-1.97588
C	-2.19096	1.87015	0.86955
C	-3.16130	2.49988	1.63054
H	-3.89891	2.07486	1.92577
C	-3.03893	3.85080	1.96709
H	-3.80197	4.33130	2.57860
C	-1.91972	4.54688	1.51282
H	-1.83095	5.42091	1.74135
C	-0.93800	3.94528	0.74884
H	-0.17778	4.40826	0.56123
C	-1.06340	2.58572	0.42471
N	-0.09343	1.83643	-0.24380
C	0.83302	2.43196	-1.11848
C	0.53186	3.52222	-1.94643
H	-0.30064	3.88899	-1.90096
C	1.47794	3.96736	-2.85048
H	1.26071	4.65970	-3.40718
C	2.74593	3.38623	-2.93217
H	3.47885	3.74716	-3.65308
C	3.03249	2.29976	-2.10101
H	3.85065	1.89684	-2.12939
C	2.08382	1.79707	-1.21742
P	2.19167	0.29004	-0.21829
C	3.04004	0.70103	1.36121
H	4.04889	1.07983	1.19875
H	3.07440	-0.14157	1.75871
H	2.43102	1.39098	1.94450
C	3.28348	-0.86406	-1.13620
H	4.06247	-0.27069	-1.38025
H	2.78104	-1.21584	-2.03694
H	3.61842	-1.69545	-0.51578