Supporting Information

Oxidative C-C/C-X Coupling in Organometallic Nickel Complexes: Insights from DFT

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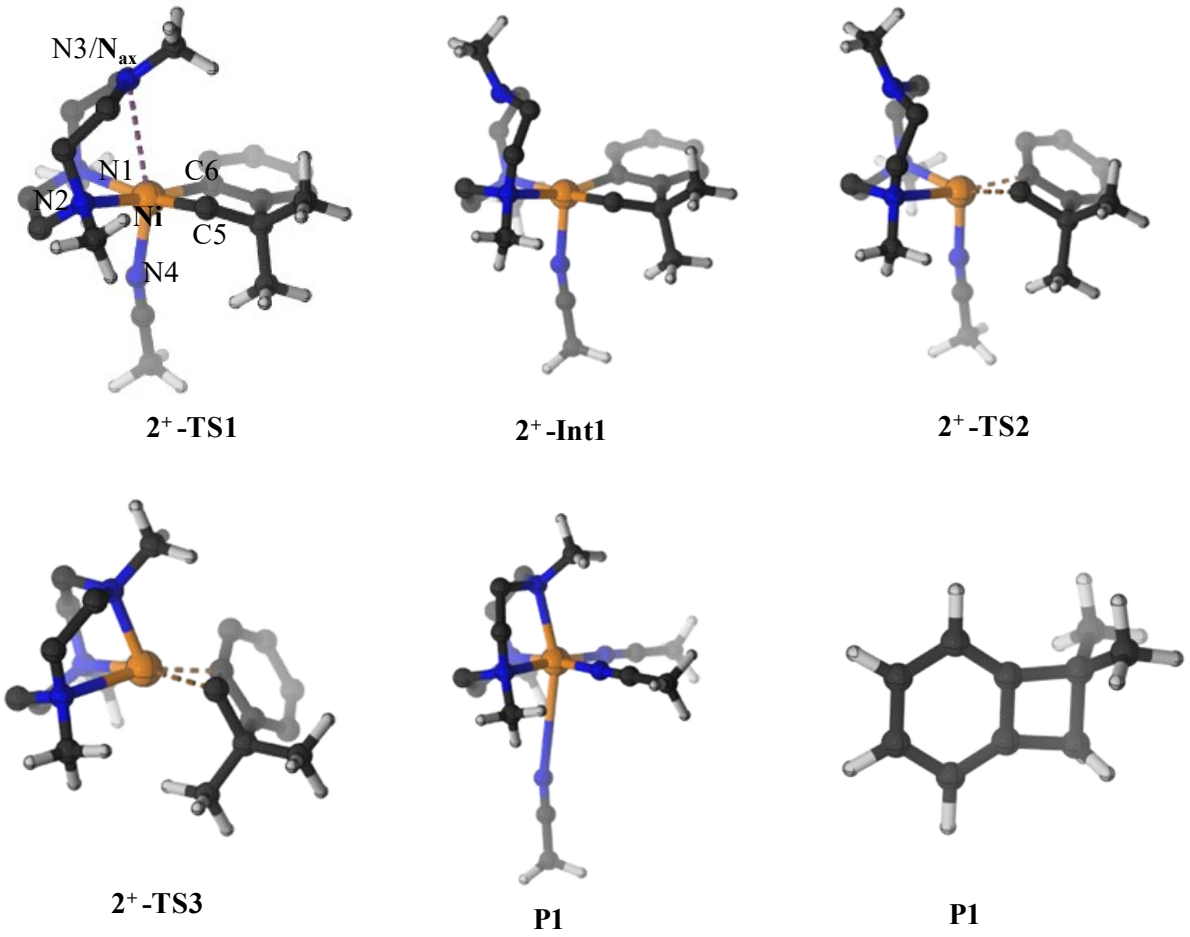

Fig. S1. Optimized geometries of **2**$^{+}$ complex intermediates, and transition states.

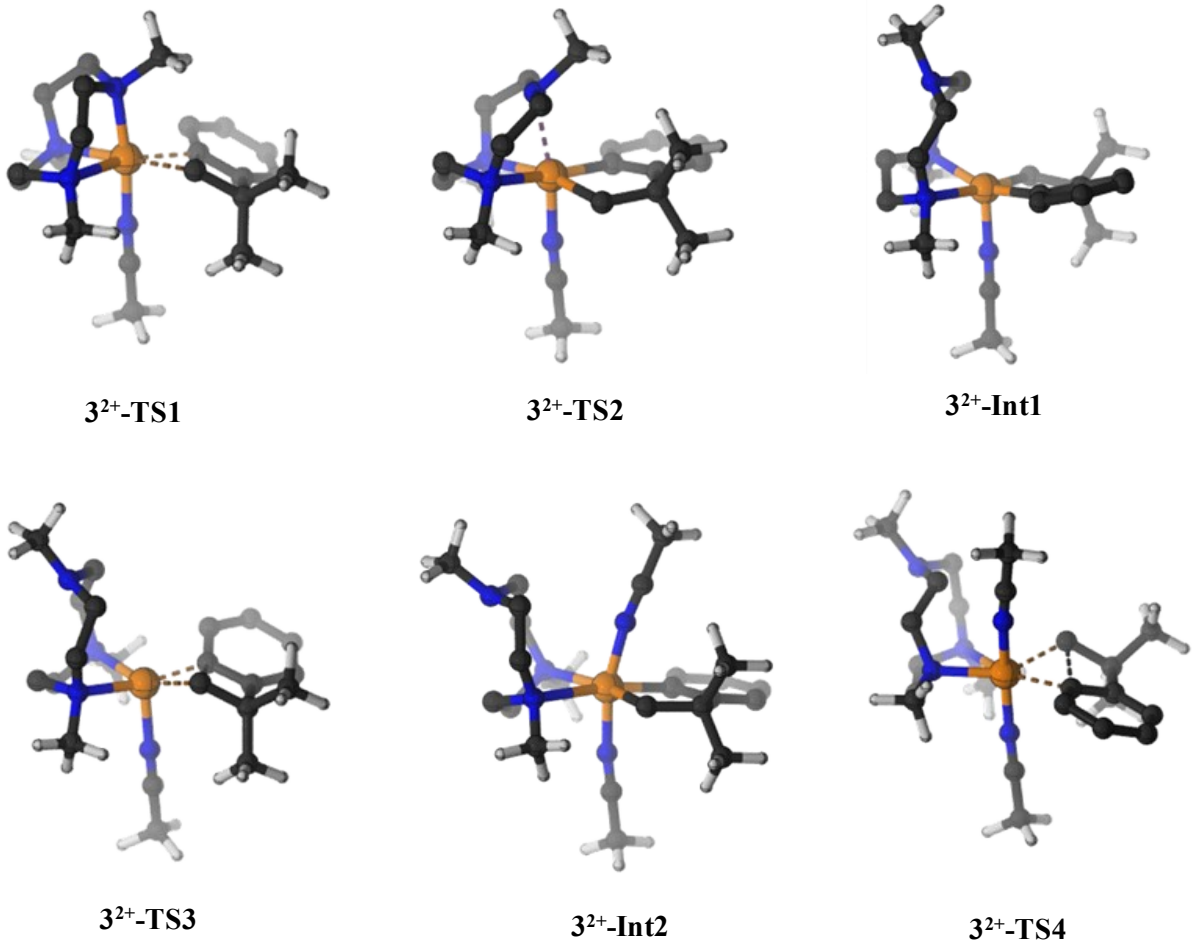

Fig. S2. Optimized geometries of $\mathbf{3}^{2+}$ complex intermediates, and transition states.

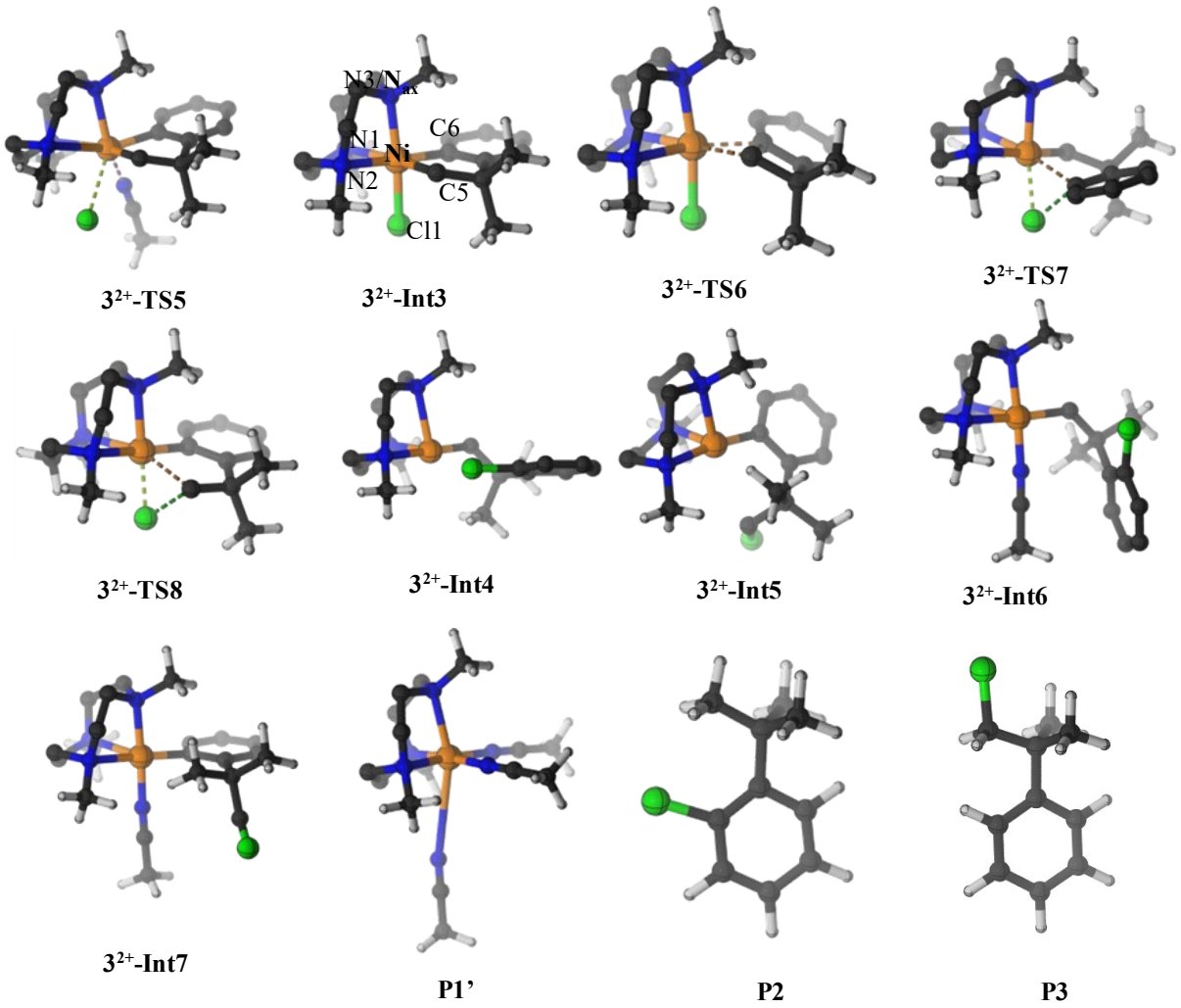

Fig. S3. Optimized geometries of $\mathbf{3}^{2+}$ complex intermediates, and transition states.

Table S1. NPA charges on selected atoms in the complexes and intermediates.

	Ni	N1	N2	N3	N4/Cl	C5	C6
1	0.332	-0.549	-0.544	-0.585	-	-0.658	-0.199
2^{+}	0.718	-0.558	-0.554	-0.546	-	-0.565	-0.200
2^{+}-Int1	0.686	-0.556	-0.558	-0.584	-0.382	-0.531	-0.264
2^{+}-TS2	0.598	-0.580	-0.569	-0.581	-0.400	-0.521	-0.143
2^{+}-TS3	0.789	-0.565	-0.568	-0.574	-	-0.588	-0.193
3^{2+}	0.481	-0.521	-0.524	-0.439	-0.351	-0.320	-0.200
3^{2+}-TS1	0.579	-0.545	-0.510	-0.472	-0.371	-0.588	-0.193
3^{2+}-TS2	0.511	-0.529	-0.522	-0.522	-0.354	-0.338	-0.041
3^{2+}-Int1	0.525	-0.534	-0.543	-0.519	-0.364	-0.332	0.008
3^{2+}-TS3	0.573	-0.526	-0.519	-0.519	-0.404	-0.291	-0.052
3^{2+}-Int2	0.451	-0.507	-0.507	-0.582	-0.371	-0.280	-0.052
3^{2+}-TS4	0.512	-0.471	-0.572	-0.571	-0.389	-0.238	-0.065
3^{2+}-TS5	0.494	-0.546	-0.538	-0.470	-0.358/ -0.570	-0.298	-0.002
3^{2+}-Int3	0.373	-0.528	-0.530	-0.479	-0.245	-0.359	-0.014
3^{2+}-TS6	0.467	-0.549	-0.519	-0.508	-0.327	-0.400	-0.073
3^{2+}-TS7	0.413	-0.545	-0.548	-0.524	-0.030	-0.497	-0.022
3^{2+}-TS8	0.388	-0.548	-0.554	-0.513	-0.132	-0.249	-0.118
3^{2+}-Int4	0.449	-0.569	-0.524	-0.565	-0.128	-0.624	-0.031
3^{2+}-Int5	0.566	-0.552	-0.571	-0.524	-0.045	-0.400	-0.184
3^{2+}-Int6	0.495	-0.557	-0.565	-0.529	-0.367	-0.594	-0.044
3^{2+}-Int7	0.466	-0.554	-0.559	-0.517	-0.357	-0.420	-0.152

For atom numbering see Fig. S1and S3

Table S2. Wiberg bond indices for selected bonds in nickel complexes at B3LYP/BS1

	Ni-N1	Ni-N2	Ni-N3	Ni-N4/Cl	Ni-C5	Ni-C6	C5/Cl-C6/Cl
1	0.221	0.233	0.015	-	0.675	0.662	0.159
2^{+}	0.218	0.224	0.227	-	0.565	0.552	0.270
2^{+}-TS1	0.229	0.233	0.011	0.289	0.557	0.559	0.266
2^{+}-Int1	0.231	0.233	0.014	0.300	0.569	0.544	0.270
2^{+}-TS2	0.194	0.172	0.016	0.305	0.288	0.286	0.702
2^{+}-TS3	0.190	0.148	0.181	-	0.268	0.291	0.733
3^{2+}	0.266	0.254	0.412	0.449	0.659	0.651	0.104
3^{2+}-TS1	0.213	0.320	0.453	0.467	0.332	0.339	0.587
3^{2+}-TS2	0.266	0.250	0.396	0.433	0.663	0.650	0.010
3^{2+}-Int1	0.257	0.272	0.089	0.422	0.668	0.752	0.055
3^{2+}-TS3	0.266	0.365	0.096	0.402	0.320	0.634	0.451
3^{2+}-Int2	0.248	0.255	0.006	0.439	0.674	0.661	0.064
3^{2+}-TS4	0.408	0.045	0.009	0.465	0.349	0.457	0.447
3^{2+}-TS5	0.087	0.247	0.325	0.367	0.572	0.680	0.011
3^{2+}-Int3	0.244	0.232	0.328	0.794	0.666	0.654	0.114
3^{2+}-TS6	0.185	0.294	0.360	0.842	0.317	0.305	0.638
3^{2+}-TS7	0.179	0.245	0.253	0.556	0.341	0.785	0.658
3^{2+}-TS8	0.255	0.151	0.300	0.632	0.741	0.309	0.521
3^{2+}-Int4	0.233	0.290	0.138	-	0.779	-	0.965
3^{2+}-Int5	0.252	0.276	0.187	-	-	0.771	1.011
3^{2+}-Int6	0.219	0.116	0.293	0.429	0.777	-	1.036
3^{2+}-Int7	0.246	0.112	0.324	0.420	-	0.743	0.990

For atom numbering see Fig. S1and S3