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Supplementary Information

Kinetic C−H Oxidative Addition *vs.* Thermodynamic C−X Oxidative Addition of Chlorobenzene by a Neutral Ir(I) System. A Density Functional Theory Study

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Table S2 – S3

Table S1. Energetic and Thermodynamic Data.

Molecule	*E*	*ZPVE*	*TE*	*S*	E_0	E_{298}	H_{298}	G_{298}	*NIM*
1a	-488.158933	152.75	163.51	131.13	-487.915517	-487.898361	-487.897417	-487.959721	0
1b	-488.114219	151.55	162.40	131.64	-487.872705	-487.855415	-487.854471	-487.917017	0
TS(1a,1b)	-488.114089	151.30	161.76	128.94	-487.872975	-487.856313	-487.855368	-487.916633	1
H_2	-1.175482	6.36	7.84	31.13	-1.165343	-1.162983	-1.162038	-1.176831	0
2	-272.724047	96.11	99.38	73.01	-272.570887	-272.565669	-272.564725	-272.599414	0
3a	-760.900731	251.18	265.44	154.57	-760.500445	-760.477724	-760.476780	-760.550220	0
3b	-760.898452	251.14	265.44	156.31	-760.498229	-760.475453	-760.474509	-760.548777	0
3c	-760.894640	251.09	265.21	153.87	-760.494502	-760.472006	-760.471062	-760.544168	0
4a	-760.899360	251.47	266.35	163.71	-760.498621	-760.474912	-760.473968	-760.551752	0
4b	-760.896143	251.79	266.59	162.62	-760.494897	-760.471303	-760.470359	-760.547626	0
4c	-760.895778	252.57	267.06	158.11	-760.493286	-760.470191	-760.469247	-760.544369	0
4d	-760.895575	252.61	267.17	158.88	-760.493012	-760.469817	-760.468873	-760.544362	0
TS(3a,4a)	-760.869765	249.54	263.66	154.33	-760.472105	-760.449599	-760.448655	-760.521981	1
TS(3c,4a)	-760.877108	249.51	263.66	155.67	-760.479482	-760.456936	-760.455992	-760.529955	1
TS1	-760.876932	251.63	266.11	160.11	-760.475934	-760.452857	-760.451913	-760.527988	1
IM1	-760.887515	253.66	268.44	164.16	-760.483281	-760.459726	-760.458782	-760.536780	0
5	-759.693839	239.87	254.01	157.13	-759.311584	-759.289047	-759.288103	-759.362761	0
6	-273.965151	111.35	114.86	74.85	-273.787707	-273.782113	-273.781169	-273.816732	0
7	-486.908276	142.23	152.61	129.74	-486.681615	-486.665076	-486.664132	-486.725775	0
8	-246.584904	57.04	60.51	75.05	-246.494010	-246.488468	-246.487524	-246.523183	0
9a	-733.558689	198.09	212.83	162.19	-733.243005	-733.219528	-733.218584	-733.295644	0
9b	-733.548550	197.76	212.62	164.92	-733.233396	-733.209727	-733.208783	-733.287140	0
TS(9a,9b)	-733.529391	198.37	212.51	155.05	-733.213270	-733.190740	-733.189796	-733.263464	1
9c	-733.547009	197.64	212.57	166.99	-733.232056	-733.208261	-733.207317	-733.286660	0

9d	-733.547040	197.65	212.56	166.66	-733.232069	-733.208311	-733.207367	-733.286549	0
TS(9c,9d)	-733.542512	198.05	212.25	156.31	-733.226902	-733.204272	-733.203328	-733.277598	1
9e	-733.545485	197.59	212.54	166.95	-733.230606	-733.206782	-733.205838	-733.285163	0
10	-733.597674	200.33	215.16	163.58	-733.278431	-733.254802	-733.253858	-733.331580	0
11a	-733.537888	200.07	214.58	160.67	-733.219060	-733.195929	-733.194985	-733.271325	0
11b	-733.536871	200.05	214.55	160.32	-733.218064	-733.194961	-733.194017	-733.270190	0
11c	-733.535211	200.12	214.62	159.95	-733.216305	-733.193190	-733.192246	-733.268244	0
TS2-a	-733.508999	199.21	213.59	161.43	-733.191546	-733.168622	-733.167677	-733.244379	1
TS2-b	-733.509002	199.21	213.60	161.42	-733.191541	-733.168616	-733.167672	-733.244367	1
TS2-c	-733.509943	199.18	213.60	162.02	-733.192521	-733.169547	-733.168603	-733.245583	1
TS2-d	-733.509982	199.16	213.62	162.52	-733.192593	-733.169559	-733.168615	-733.245834	1
TS2-e	-733.510388	199.18	213.61	162.09	-733.192981	-733.169976	-733.169032	-733.246047	1
IM3	-733.516559	199.86	214.79	167.70	-733.198062	-733.174275	-733.173331	-733.253010	0
TS3	-733.497565	199.45	213.95	162.25	-733.179720	-733.156620	-733.155676	-733.232767	1
TS4	-733.520001	197.34	211.94	160.91	-733.205527	-733.182261	-733.181317	-733.257768	1
IM4	-733.547954	198.25	213.07	162.08	-733.232021	-733.208402	-733.207458	-733.284469	0
TS5	-733.536390	196.84	211.45	159.56	-733.222712	-733.199416	-733.198471	-733.274283	1