Supporting Information

Diboron-Controlled Product Selectivity Switch in Copper-Catalyzed

Decarboxylative Substitutions of Alkynyl Cyclic Carbonates

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Section 1. Optimization with D3 dispersion correction

$$\mathbf{B_2pin_2} \quad \begin{matrix} \textbf{4-TS}_{\textbf{B1}} \\ \textbf{4-TS}_{\textbf{B1}}\textbf{-D3} \end{matrix} \quad \xrightarrow[\Delta G = -2.0]{\Delta G = -3.6} \quad \begin{matrix} \textbf{9-TS}_{\textbf{B1}} \\ \textbf{9-TS}_{\textbf{B1}}\textbf{-D3} \end{matrix}$$

x = 1 or 2

$$\mathbf{B_2neop_2} \quad \begin{matrix} \textbf{4-TS}_{\textbf{B2}} \\ \textbf{4-TS}_{\textbf{B2}}\textbf{-D3} \end{matrix} \quad \xrightarrow[\Delta G = 5.9]{\Delta G = 4.9} \quad \begin{matrix} \textbf{9-TS}_{\textbf{B2}} \\ \textbf{9-TS}_{\textbf{B2}}\textbf{-D3} \end{matrix}$$

Fig. S1 Calculated free-energy difference for key species using the M06/BS2//B3LYP/BS1 and M06/BS2//B3LYP-D3/BS1 levels. Values shown are relative free energies in kcal/mol.

Section 2. Optimization with M06 and BPW91 methods

$$\mathbf{B_2pin_2} \quad \begin{matrix} \textbf{4-TS}_{\textbf{B1}}\textbf{-B3LYP} \\ \textbf{4-TS}_{\textbf{B1}}\textbf{-BPW91} \\ \textbf{4-TS}_{\textbf{B1}}\textbf{-M06} \end{matrix} \quad \begin{matrix} \Delta G = -3.6 \\ \Delta G = -3.9 \\ \Delta G = -3.0 \end{matrix} \quad \begin{matrix} \textbf{9-TS}_{\textbf{B1}}\textbf{-B3LYP} \\ \textbf{9-TS}_{\textbf{B1}}\textbf{-BPW91} \\ \textbf{9-TS}_{\textbf{B1}}\textbf{-M06} \end{matrix}$$

x = 1 or 2

$$\mathbf{B_2neop_2} \quad \begin{matrix} \textbf{4-TS}_{\textbf{B2}}\textbf{-B3LYP} \\ \textbf{4-TS}_{\textbf{B2}}\textbf{-BPW91} \\ \textbf{4-TS}_{\textbf{B2}}\textbf{-M06} \end{matrix} \quad \begin{matrix} \Delta G = 4.9 \\ \Delta G = 4.2 \\ \Delta G = 11.0 \end{matrix} \quad \begin{matrix} \textbf{9-TS}_{\textbf{B2}}\textbf{-B3LYP} \\ \textbf{9-TS}_{\textbf{B2}}\textbf{-B3LYP} \\ \textbf{9-TS}_{\textbf{B2}}\textbf{-M06} \end{matrix}$$
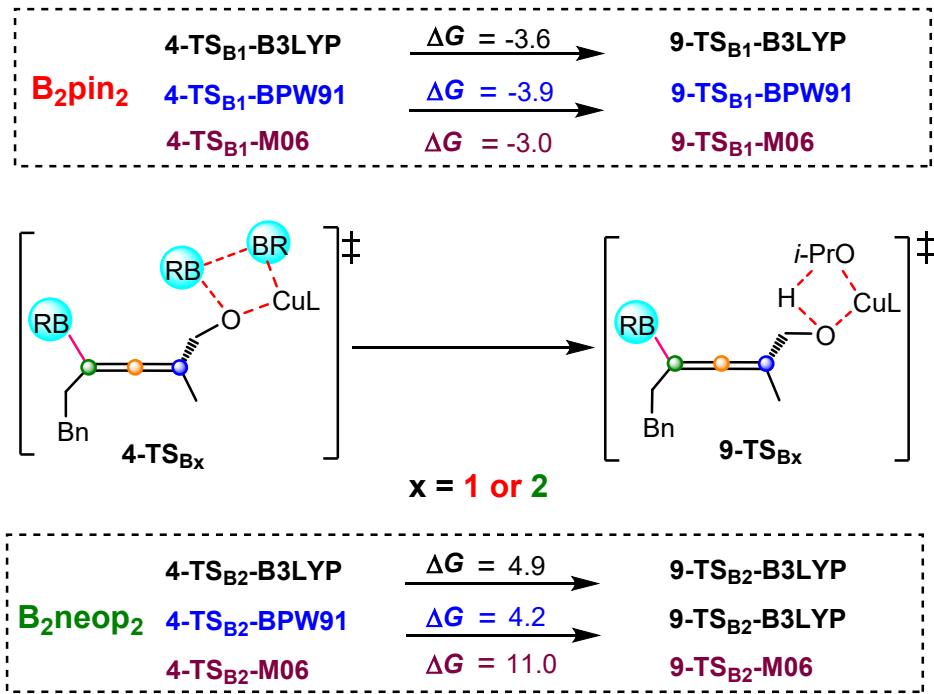
Fig. S2 Calculated free-energy difference for key species using the

M06/BS2//M06/BS1 and M06/BS2//BPW91/BS1 levels. Values shown are relative

free energies in kcal/mol.

## Section 3. Other possible pathways to afford *E*-P1, *E*-P1' and P2
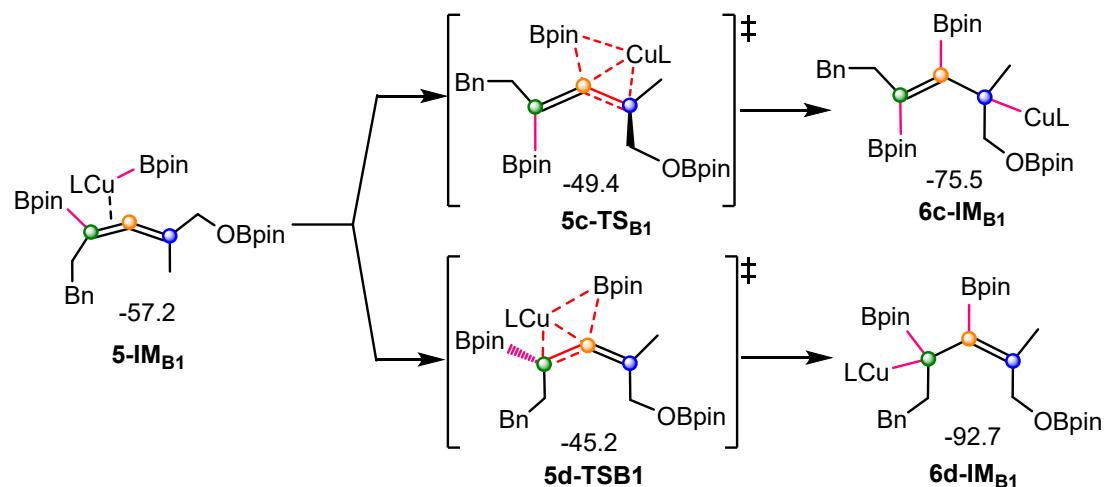
Fig. S3 Other possible pathways from intermediate **5-IM$_{B1}$**. Values shown are relative

free energies in kcal/mol.
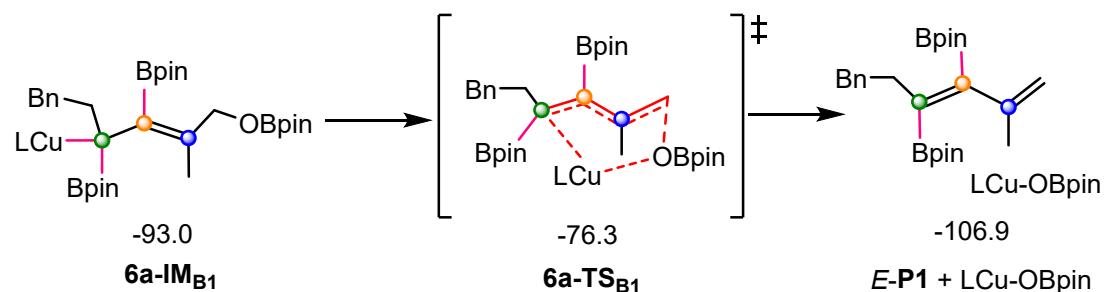
Fig. S4 Other possible pathways from intermediate **6a-IM$_{B1}$**. Values shown are

relative free energies in kcal/mol.
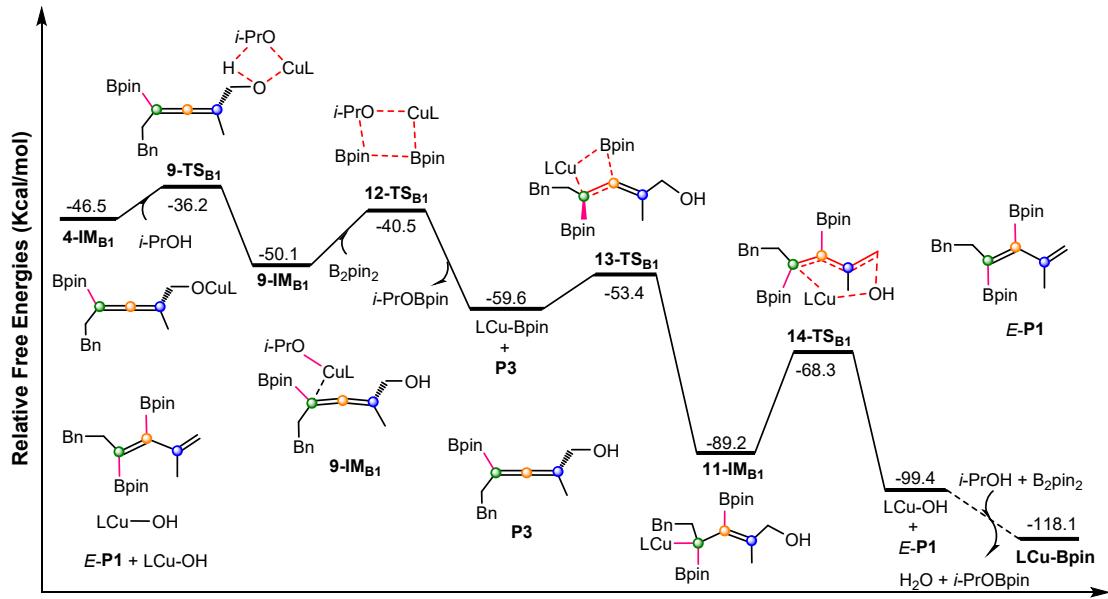
Fig. S5 Calculated free-energy profiles for other possible mechanism of process **4-IM$_{B1}$** → *E*-**P1** with B$_2$pin$_2$ substrate. Values shown are relative free energies in kcal/mol.
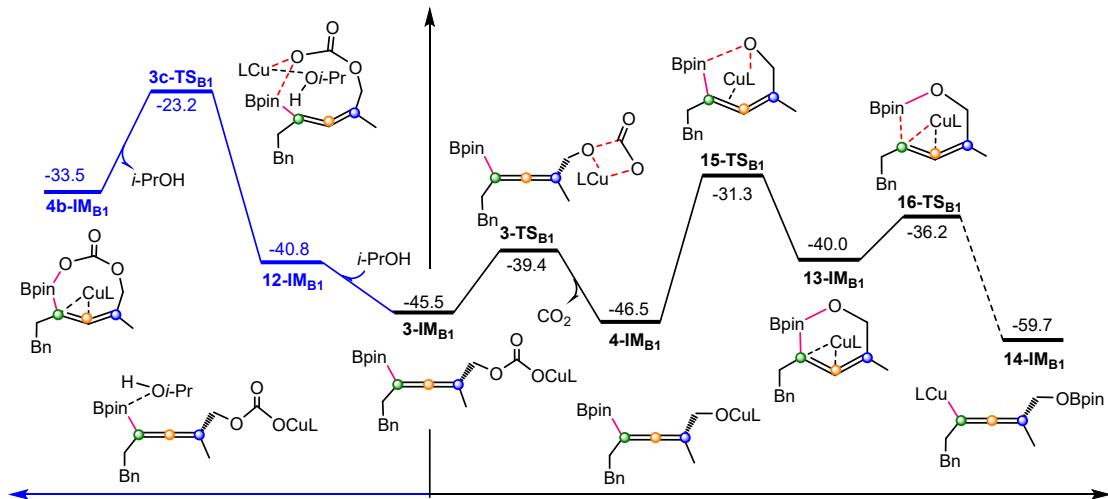
Fig. S6 Calculated free-energy profiles for other possible pathways from **3-IM$_{B1}$** with B$_2$pin$_2$ substrate. Experiment-based mechanism is given in blue. Values shown are relative free energies in kcal/mol.
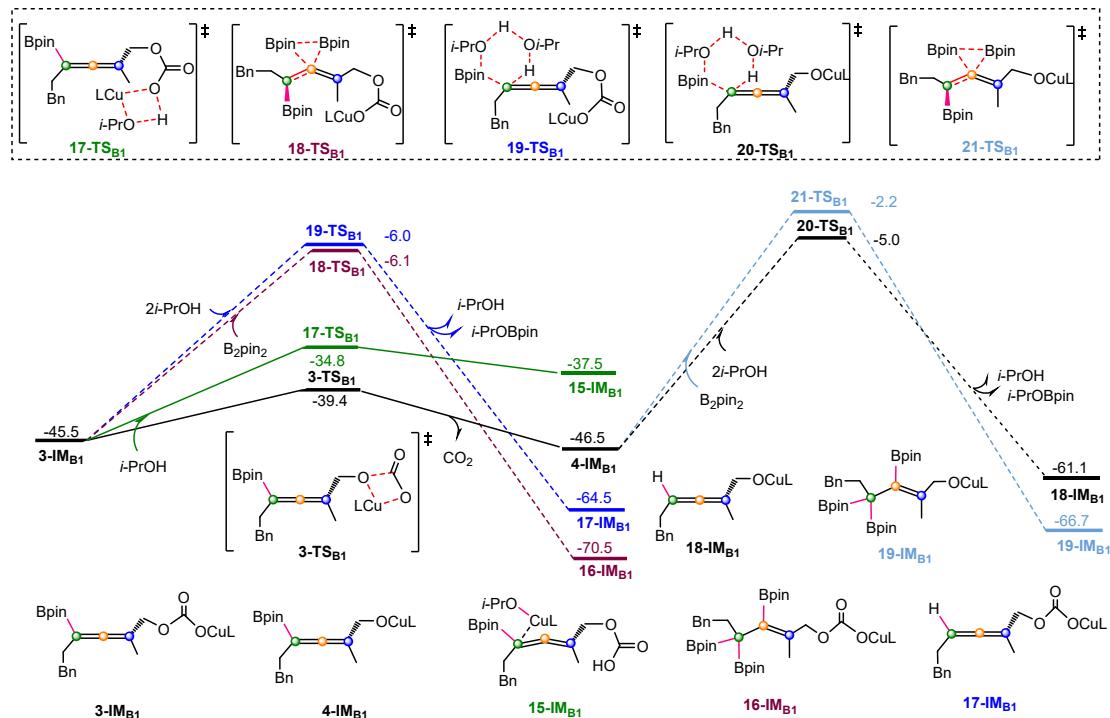
Fig. S7 Calculated free-energy profiles for other possible pathways from **3-IM$_{B1}$** with

B$_2$pin$_2$ substrate. Values shown are relative free energies in kcal/mol.
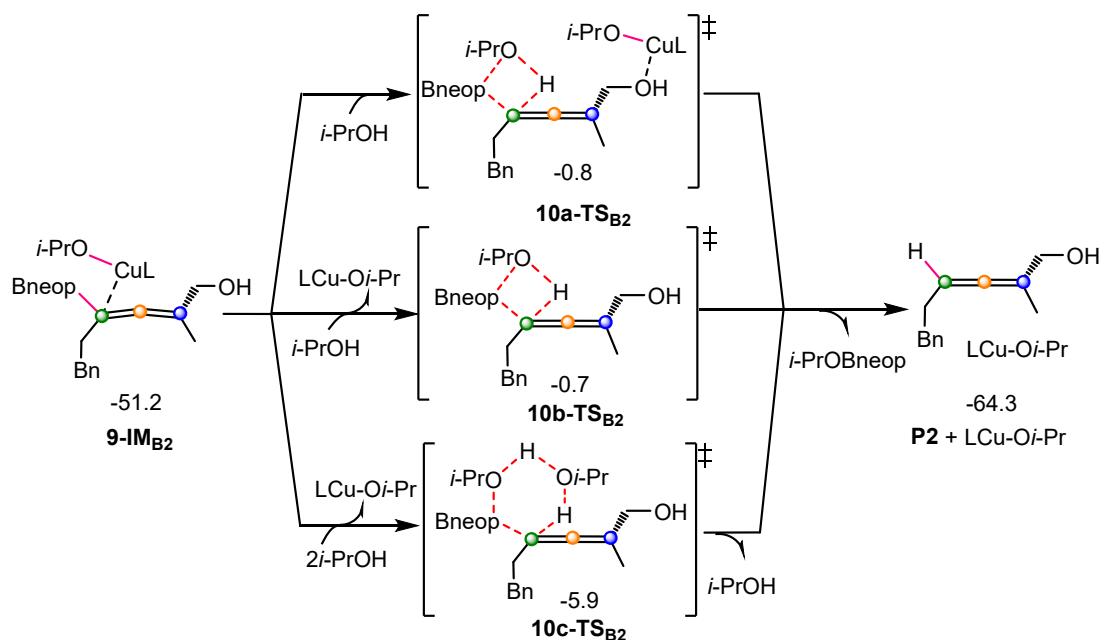
Fig. S8 Other possible pathways from intermediate **9-IM$_{B2}$**. Values shown are relative

free energies in kcal/mol.
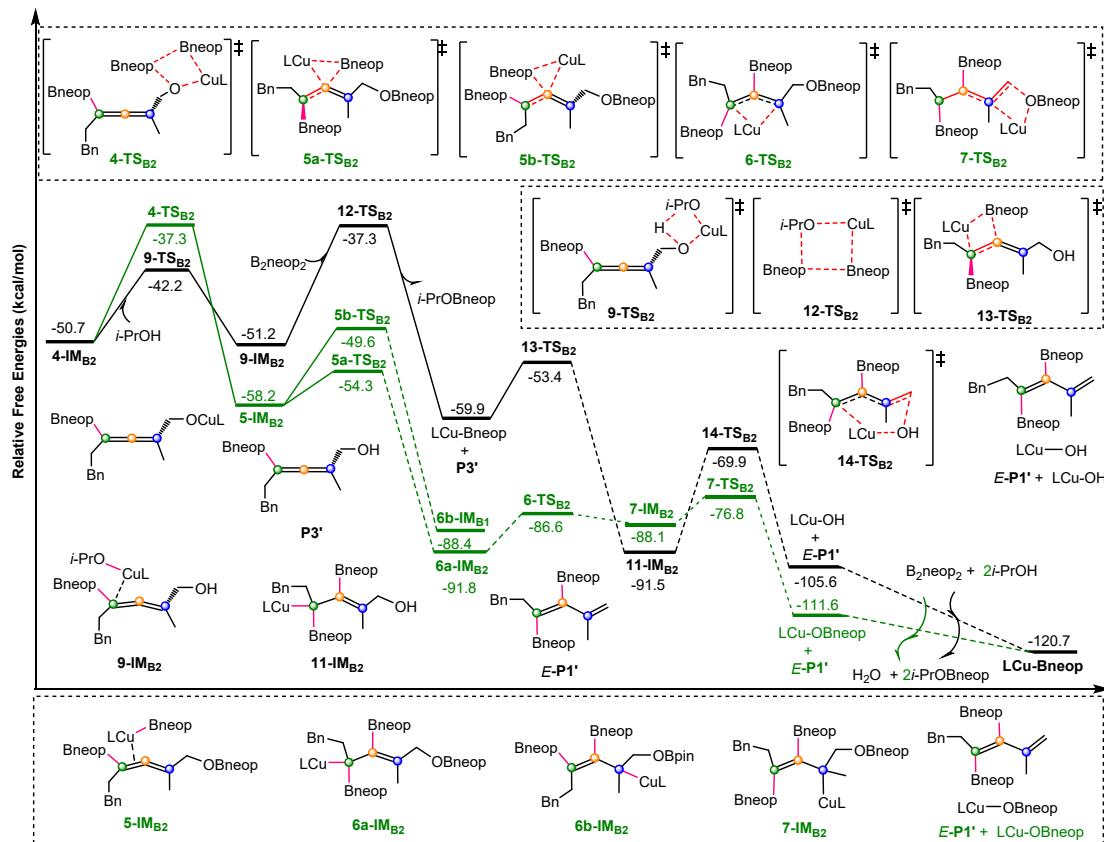
Fig. S9 Calculated free-energy profiles for other possible pathways for **4-IM$_{B2}$** → *E*-**P1'** with B$_2$neop$_2$ substrate. Values shown are relative free energies in kcal/mol.
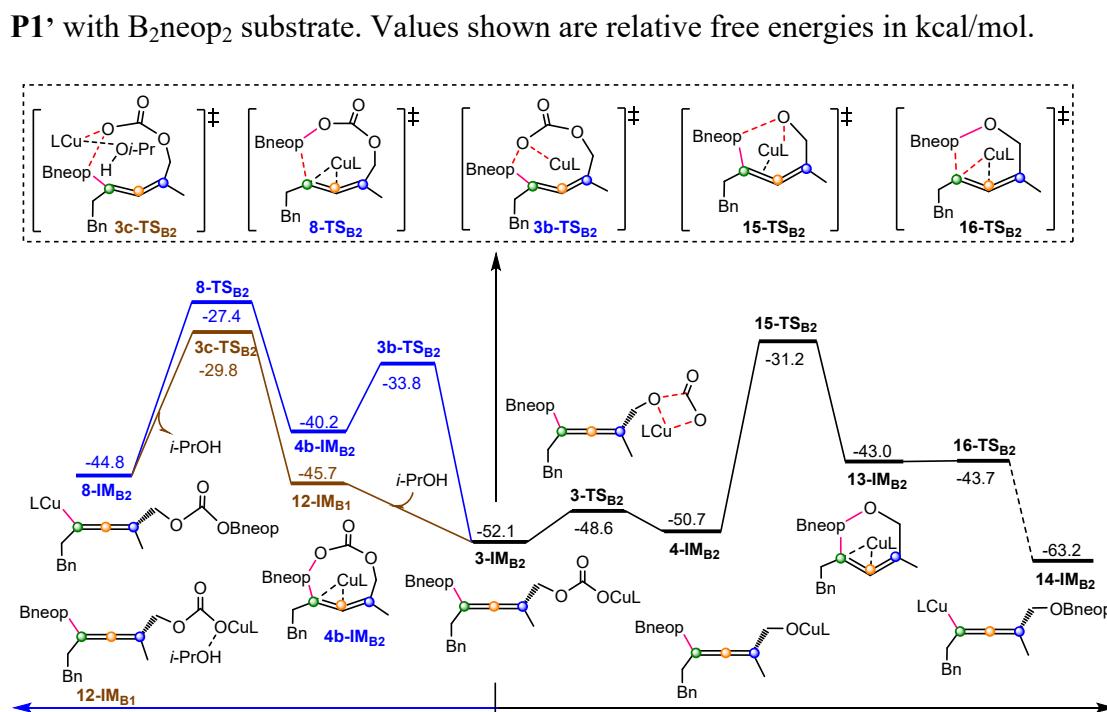
Fig. S10 Calculated free-energy profiles for other possible pathways from **3-IM$_{B2}$** with B$_2$neop$_2$ substrate. Values shown are relative free energies in kcal/mol.
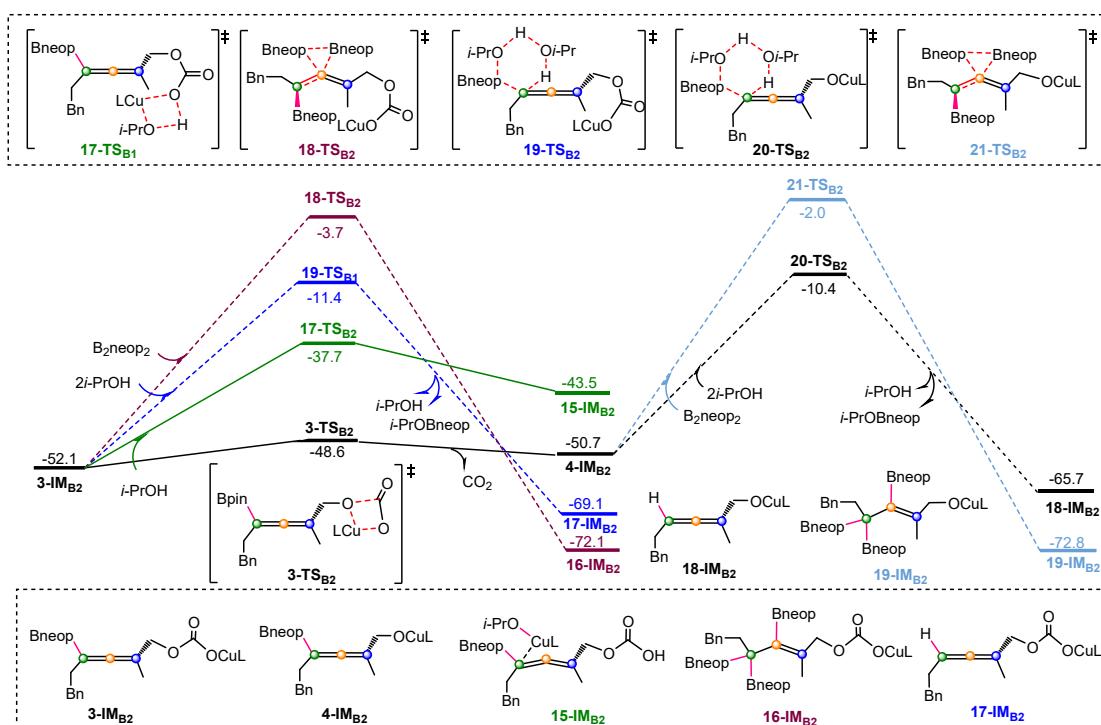
Fig. S11 Calculated free-energy profiles for other possible pathways from **3-IM$_{B2}$** with B$_2$neop$_2$ substrate. Values shown are relative free energies in kcal/mol.

Section 4. First three steps of most favorable pathways to afford *E*-P1' and P2 with B₂neop₂ substrate
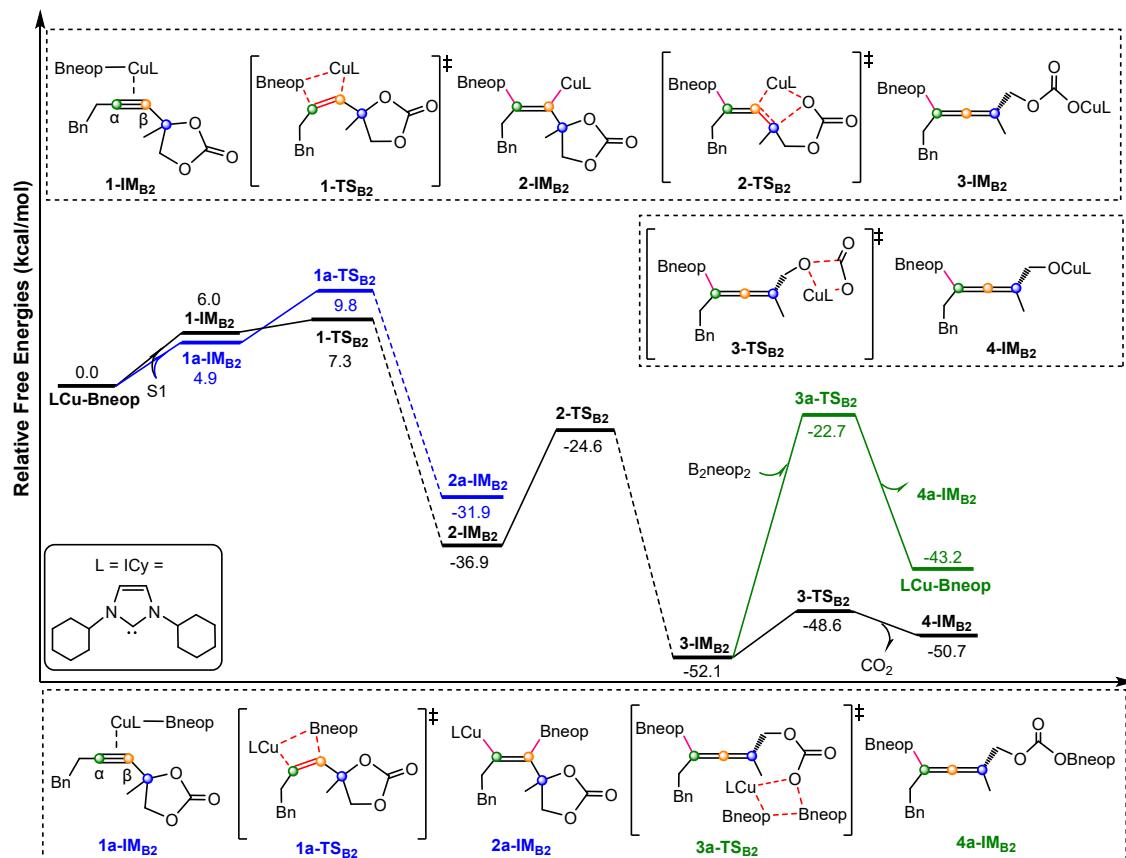
Fig. S12 Calculated free-energy profiles for first three steps of most favorable pathways to afford *E*-**P1'** and **P2** with B₂neop₂ substrate. The first step, i.e., C$_\beta$-borylation, is shown in blue. For comparison, an experiment-based mechanism is shown in green. Values shown are relative free energies (kcal/mol).

Section 5. Catalyst regeneration process
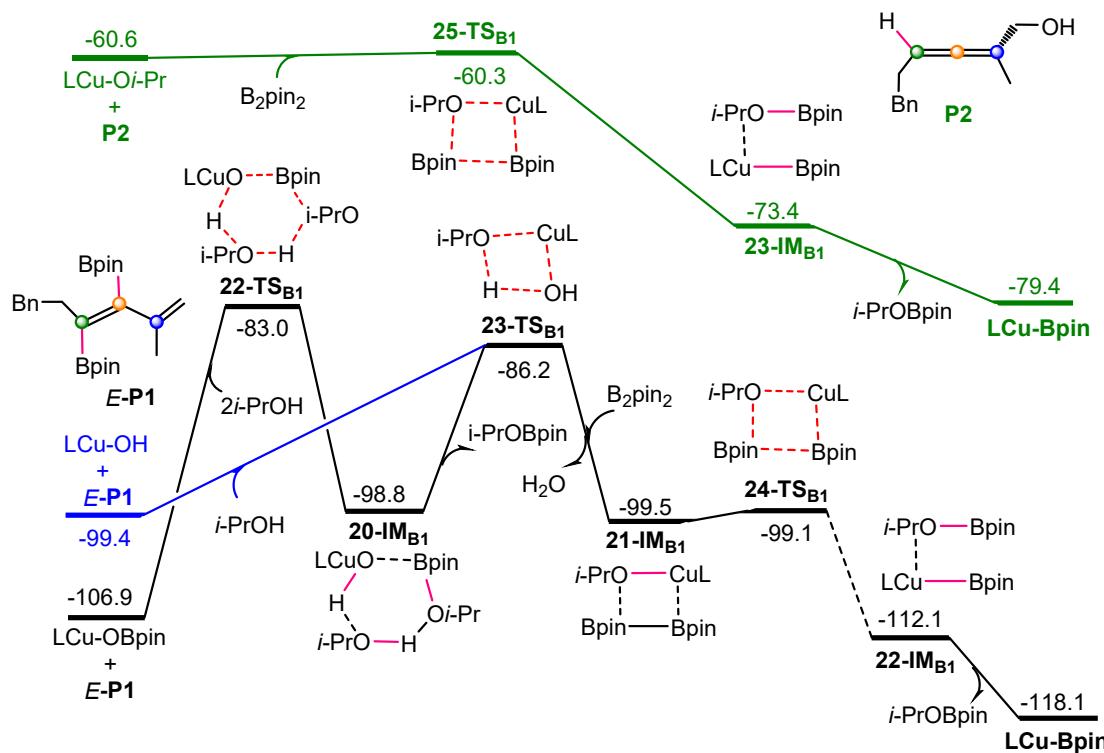
Fig. S13 Calculated free-energy profiles for catalyst regeneration for B$_2$pin$_2$ system.

Values shown are relative free energies in kcal/mol.
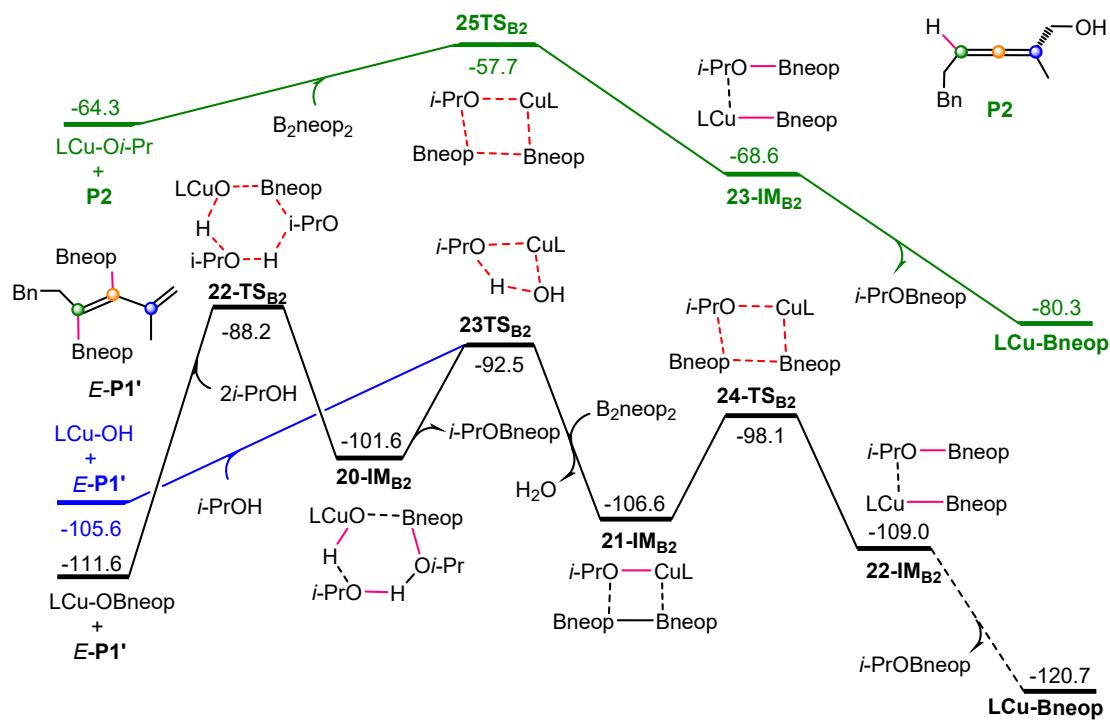
Fig. S14 Calculated free-energy profiles for catalyst regeneration for B_2neop_2 system. Values shown are relative free energies in kcal/mol.

Section 6. The metathesis and protonation steps with the B₂cat₂ substrate
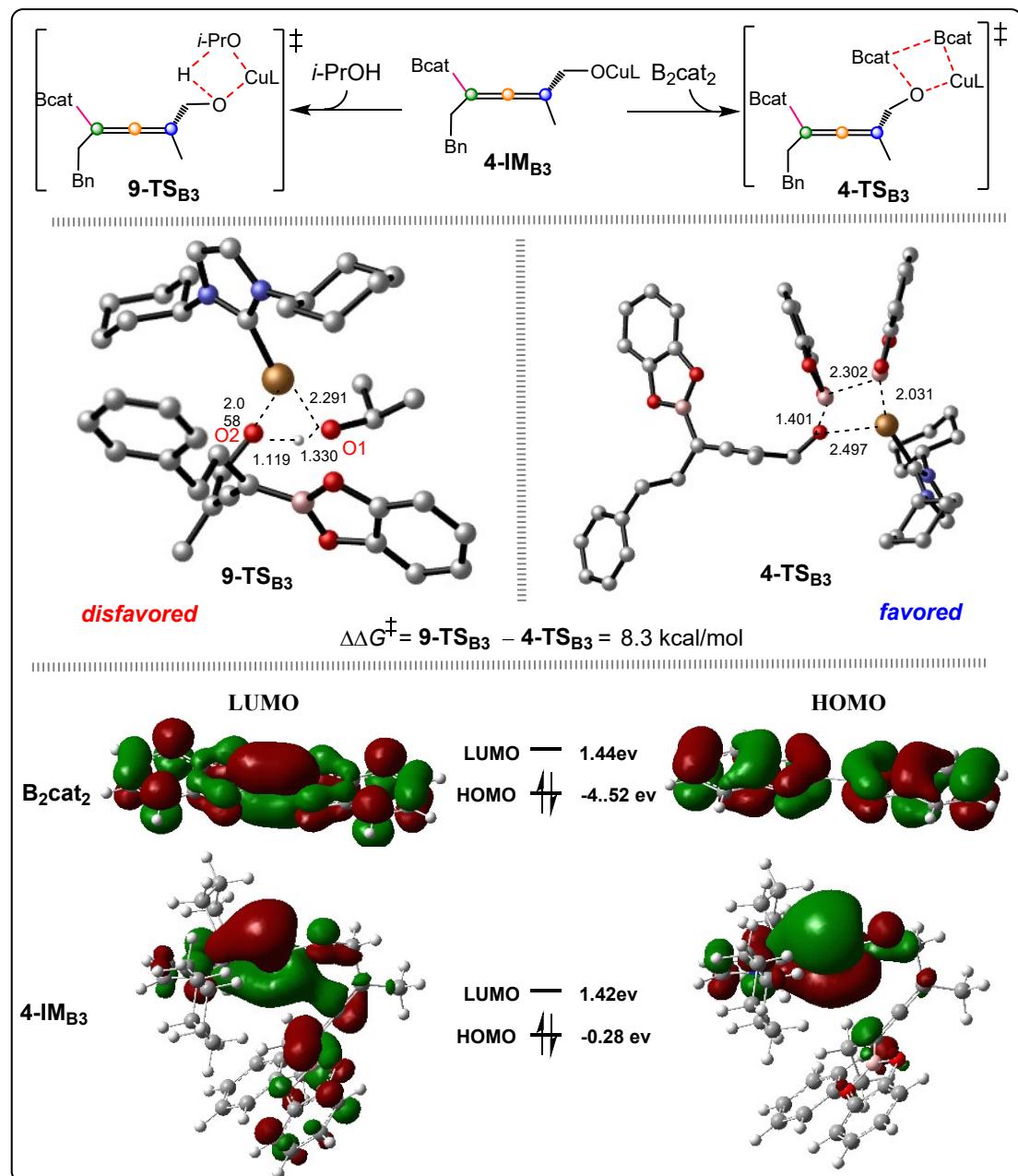
Fig. S15 Optimized structures for product-selectivity-determining transition states **4-TS_B3** and **9-TS_B3** along with interatomic distances (angstroms). Frontier molecular orbitals calculated for B₂cat₂ and **4-IM_B3**. Orbital energies are given in eV.

Section 7. Energies (in Hartree) of All TSs and Intermediates.

| Geometry	E_0	E	$H_{323.15}$	$G_{323.15}$	$E_{(sol,M06)}$
S1	-767.300942	-767.283142	-767.282119	-767.352085	-767.2568272
i-PrOH	-194.253721	-194.247587	-194.246564	-194.283871	-194.2882389
B_2pin_2	-822.181612	-822.158744	-822.157721	-822.233848	-822.2501967
i-PrOBpin	-604.840886	-604.823884	-604.822861	-604.886146	-604.8718168
H_2O	-76.392569	-76.389496	-76.388473	-76.412044	-76.4249529
CO_2	-188.568634	-188.565367	-188.564344	-188.588155	-188.5602234
LCu-Bpin	-1302.466603	-1302.433548	-1302.432525	-1302.538738	-1303.7657053
1-IM$_{B1}$	-2069.760543	-2069.708239	-2069.707216	-2069.857750	-2071.0413925
1-TS$_{B1}$	-2069.754239	-2069.702982	-2069.701959	-2069.848443	-2071.037284
2-IM$_{B1}$	-2069.837892	-2069.786459	-2069.785436	-2069.932156	-2071.1126026
2-TS$_{B1}$	-2069.813976	-2069.762185	-2069.761162	-2069.909257	-2071.0856894
3-IM$_{B1}$	-2069.862171	-2069.809358	-2069.808335	-2069.960841	-2071.1214245
3-TS$_{B1}$	-2069.845156	-2069.793485	-2069.792462	-2069.944627	-2071.1074421
4-IM$_{B1}$	-1881.270235	-1881.220467	-1881.219444	-1881.363491	-1882.5432862
1a-IM$_{B1}$	-2069.763036	-2069.710336	-2069.709313	-2069.861723	-2071.0396906
1a-TS$_{B1}$	-2069.742231	-2069.691360	-2069.690337	-2069.834340	-2071.0274163
2a-IM$_{B1}$	-2069.830128	-2069.778840	-2069.777817	-2069.924658	-2071.1045037
3a-TS$_{B1}$	-2892.015601	-2891.938600	-2891.937578	-2892.141232	-2893.3670994
4a-IM$_{B1}$	-1589.562255	-1589.519536	-1589.518514	-1589.644745	-1589.5936927
4-TS$_{B1}$	-2703.446495	-2703.372950	-2703.371927	-2703.568502	-2704.8067253
5-IM$_{B1}$	-2703.460925	-2703.386531	-2703.385508	-2703.581883	-2704.8367367
5a-TS$_{B1}$	-2703.455431	-2703.381872	-2703.380849	-2703.576165	-2704.8323836
6a-IM$_{B1}$	-2703.517577	-2703.444194	-2703.443171	-2703.637477	-2704.8967468
5b-TS$_{B1}$	-2703.442934	-2703.369247	-2703.368224	-2703.563373	-2704.8214172
6b-IM$_{B1}$	-2703.496013	-2703.424111	-2703.423088	-2703.613732	-2704.8753964
5c-TS$_{B1}$	-2703.445188	-2703.371407	-2703.370384	-2703.566225	-2704.8228389
6c-IM$_{B1}$	-2703.491811	-2703.419509	-2703.418486	-2703.609079	-2704.8709604
5d-TS$_{B1}$	-2703.442054	-2703.368999	-2703.367976	-2703.559523	-2704.8211061
6d-IM$_{B1}$	-2703.513169	-2703.440004	-2703.438981	-2703.631649	-2704.8986373
6-TS$_{B1}$	-2703.504701	-2703.432878	-2703.431855	-2703.620508	-2704.8873953
6a-TS$_{B1}$	-2703.487915	-2703.415358	-2703.414335	-2703.605584	-2704.8695573
7-IM$_{B1}$	-2703.510797	-2703.437510	-2703.436487	-2703.629422	-2704.8888626
7-TS$_{B1}$	-2703.495648	-2703.422625	-2703.421602	-2703.614306	-2704.8703516
LCu-OBpin	-1377.790717	-1377.756975	-1377.755952	-1377.861197	-1379.0898920
E-P1	-1325.754391	-1325.716190	-1325.715167	-1325.827995	-1325.8027605
3b-TS$_{B1}$	-2069.828191	-2069.776592	-2069.775569	-2069.922890	-2071.0947855
4b-IM$_{B1}$	-2069.830531	-2069.779493	-2069.778470	-2069.922880	-2071.1074240
8-TS$_{B1}$	-2069.815314	-2069.763683	-2069.762661	-2069.908146	-2071.0898190
8-IM$_{B1}$	-2069.847621	-2069.794773	-2069.793751	-2069.945871	-2071.1118037
9-TS$_{B1}$	-2075.519814	-2075.462780	-2075.461757	-2075.622745	-2076.8324817

9-IM$_{B1}$	-2075.524302	-2075.467327	-2075.466304	-2075.623528	-2076.8628252
10-TS$_{B1}$	-2075.507225	-2075.451056	-2075.450033	-2075.606109	-2076.8471330
10-IM$_{B1}$	-1470.727256	-1470.688444	-1470.687421	-1470.809746	-1471.9727981
11-TS$_{B1}$	-1859.219003	-1859.165286	-1859.164263	-1859.318611	-1860.5561335
LCu-O*i*-Pr	-1085.068520	-1085.041214	-1085.040191	-1085.132678	-1086.3569275
P2	-579.925030	-579.908076	-579.907053	-579.974205	-579.9094569
12-TS$_{B1}$	-1907.246838	-1907.195347	-1907.194324	-1907.338268	-1908.6316958
P3	-990.444135	-990.415458	-990.414435	-990.508029	-990.4603392
13-TS$_{B1}$	-2292.892312	-2292.829954	-2292.828931	-2292.999478	-2294.2457988
11-IM$_{B1}$	-2292.953458	-2292.893476	-2292.892453	-2293.053293	-2294.3129281
14-TS$_{B1}$	-2292.924617	-2292.862869	-2292.861846	-2293.027724	-2294.2734702
LCu-OH	-967.214348	-967.191724	-967.190701	-967.269878	-968.4942868
3c-TS$_{B1}$	-2264.077025	-2264.017114	-2264.016091	-2264.182487	-2265.3971073
12-IM$_{B1}$	-2264.116139	-2264.055388	-2264.054365	-2264.226536	-2265.4228527
15-TS$_{B1}$	-1881.244219	-1881.195310	-1881.194287	-1881.335118	-1882.5197576
13-IM$_{B1}$	-1881.254318	-1881.205158	-1881.204135	-1881.350009	-1882.5291535
16-TS$_{B1}$	-1881.248027	-1881.200284	-1881.199261	-1881.336054	-1882.5298632
14-IM$_{B1}$	-1881.290479	-1881.240894	-1881.239871	-1881.382970	-1882.5658304
17-TS$_{B1}$	-2264.109846	-2264.049847	-2264.048824	-2264.219271	-2265.4127146
15-IM$_{B1}$	-2264.096657	-2264.037467	-2264.036444	-2264.200106	-2265.4235899
18-TS$_{B1}$	-2891.974614	-2891.897630	-2891.896607	-2892.101107	-2893.3321402
16-IM$_{B1}$	-2892.078156	-2892.002708	-2892.001685	-2892.199555	-2893.4447170
19-TS$_{B1}$	-2458.322495	-2458.255337	-2458.254314	-2458.439025	-2459.6746087
17-IM$_{B1}$	-1659.344544	-1659.303363	-1659.302340	-1659.430889	-1660.5671533
20-TS$_{B1}$	-2269.729884	-2269.665998	-2269.664975	-2269.840736	-2271.0933918
18-IM$_{B1}$	-1470.749322	-1470.711323	-1470.710300	-1470.829142	-1471.9829007
21-TS$_{B1}$	-2703.379488	-2703.305797	-2703.304774	-2703.499133	-2704.7477201
19-IM$_{B1}$	-2703.482764	-2703.410473	-2703.409450	-2703.598152	-2704.8591509
22-TS$_{B1}$	-1766.282971	-1766.235268	-1766.234245	-1766.372603	-1767.6667750
20-IM$_{B1}$	-1766.305337	-1766.257037	-1766.256014	-1766.395152	-1767.6984418
23-TS$_{B1}$	-1161.467254	-1161.437530	-1161.436507	-1161.534096	-1162.7771243
21-IM$_{B1}$	-1907.257275	-1907.205627	-1907.204604	-1907.348865	-1908.6333018
24-TS$_{B1}$	-1907.246838	-1907.195347	-1907.194324	-1907.338268	-1908.6316958
22-IM$_{B1}$	-1907.277374	-1907.224599	-1907.223576	-1907.374842	-1908.6479110
25-TS$_{B1}$	-1907.246838	-1907.195347	-1907.194324	-1907.338268	-1908.6316958
23-IM$_{B1}$	-1907.277374	-2212.797345	-1907.224599	-1907.374842	-1908.6479110
4-TS$_{B1}$-D3	-2703.624308	-2703.552714	-2703.551691	-2703.740997	-2704.8127938
9-TS$_{B1}$-D3	-2075.653771	-2075.597880	-2075.596857	-2075.751347	-2076.8421352
4-TS$_{B1}$-BW91	-2703.148801	-2703.073309	-2703.072286	-2703.270154	-2704.7971231
4-TS$_{B1}$-M06	-2701.750184	-2701.677964	-2701.676941	-2701.864786	-2704.8240284
9-TS$_{B1}$-BW91	-2075.324750	-2075.266405	-2075.265382	-2075.429706	-2076.8225735
9-TS$_{B1}$-M06	-2074.205950	-2074.150942	-2074.149919	-2074.297110	-2076.8574140
LCu-Bneop	-1263.165511	-1263.134225	-1263.133202	-1263.234278	-1264.456198

B$_2$neop$_2$	-743.588922	-743.569254	-743.568232	-743.639275	-743.6390471
LCu-OBenop	-1338.492600	-1338.460535	-1338.459513	-1338.562221	-1339.782325
i-PrOBenop	-565.541524	-565.526122	-565.525099	-565.585609	-565.5671958
1-IM$_{B2}$	-2030.460772	-2030.410993	-2030.409970	-2030.554481	-2031.730735
1-TS$_{B2}$	-2030.455997	-2030.406427	-2030.405404	-2030.548783	-2031.729686
2-IM$_{B2}$	-2030.538371	-2030.488726	-2030.487703	-2030.631444	-2031.802617
2-TS$_{B2}$	-2030.517495	-2030.467427	-2030.466404	-2030.610740	-2031.779668
3-IM$_{B2}$	-2030.568055	-2030.516891	-2030.515868	-2030.666590	-2031.819122
3-TS$_{B2}$	-2030.549743	-2030.498137	-2030.497115	-2030.646470	-2031.812248
4-IM$_{B2}$	-1841.974425	-1841.926440	-1841.925417	-1842.066080	-1843.238596
1a-IM$_{B2}$	-2030.462794	-2030.411874	-2030.410851	-2030.559670	-2031.729263
1a-TS$_{B2}$	-2030.451165	-2030.401513	-2030.400490	-2030.545192	-2031.724018
2a-IM$_{B2}$	-2030.532689	-2030.483979	-2030.482956	-2030.623235	-2031.796939
3a-TS$_{B2}$	-2774.120634	-2774.048595	-2774.047572	-2774.243973	-2775.436579
4a-IM$_{B2}$	-1510.974765	-1510.935282	-1510.934259	-1511.055204	-1510.988116
4-TS$_{B2}$	-2585.551307	-2585.482392	-2585.481370	-2585.669782	-2586.879739
5-IM$_{B2}$	-2585.570971	-2585.501585	-2585.500562	-2585.690319	-2586.914521
5a-TS$_{B2}$	-2585.562383	-2585.493817	-2585.492794	-2585.680581	-2586.908749
6a-IM$_{B2}$	-2585.627667	-2585.559349	-2585.558326	-2585.743509	-2586.973122
5b-TS$_{B2}$	-2585.555189	-2585.486606	-2585.485583	-2585.671794	-2586.902085
6b-IM$_{B2}$	-2585.619374	-2585.552435	-2585.551412	-2585.732790	-2586.001051
6-TS$_{B2}$	-2585.616142	-2585.548297	-2585.547274	-2585.731256	-2586.9644345
7-IM$_{B2}$	-2585.606514	-2585.538402	-2585.537379	-2585.722661	-2586.968481
7-TS$_{B2}$	-2585.606514	-2585.538402	-2585.537379	-2585.722661	-2586.9466922
3b-TS$_{B2}$	-2030.533408	-2030.484240	-2030.483217	-2030.627124	-2031.792853
4b-IM$_{B2}$	-2030.539801	-2030.489730	-2030.488707	-2030.631146	-2031.806378
8-TS$_{B2}$	-2030.513915	-2030.463695	-2030.462672	-2030.607255	-2031.782578
8-IM$_{B2}$	-2030.556847	-2030.505816	-2030.504793	-2030.652965	-2031.809961
3c-TS$_{B2}$	-2224.787051	-2224.728937	-2224.727914	-2224.890682	-2226.096468
12-IM$_{B2}$	-2224.827963	-2224.768760	-2224.767737	-2224.938181	-2226.11775
9-TS$_{B2}$	-2036.224599	-2036.169132	-2036.168109	-2036.326854	-2037.529574
9-IM$_{B2}$	-2036.226665	-2036.172005	-2036.170982	-2036.324062	-2037.552312
10-TS$_{B2}$	-2036.208653	-2036.153106	-2036.152083	-2036.309604	-2037.53444
10-IM$_{B2}$	-1470.727256	-1470.688444	-1470.687421	-1470.809746	-1471.972798
10a-TS$_{B2}$	-2230.433672	-2230.373511	-2230.372488	-2230.541624	-2231.775509
10b-TS$_{B2}$	-1145.343287	-1145.309313	-1145.308290	-1145.415041	-1145.390814
10c-TS$_{B2}$	-1339.607074	-1339.566182	-1339.565159	-1339.686054	-1339.712398
11-TS$_{B2}$	-1859.219003	-1859.165286	-1859.164263	-1859.318611	-1860.556134
12-TS$_{B2}$	-1828.648872	-1828.600768	-1828.599745	-1828.737780	-1830.009613
13-TS$_{B2}$	-2214.294673	-2214.235507	-2214.234484	-2214.400940	-2215.626495
11-IM$_{B2}$	-2214.359521	-2214.300668	-2214.299645	-2214.463153	-2215.692308
14-TS$_{B2}$	-2214.330913	-2214.272394	-2214.271371	-2214.432197	-2215.657543
15-TS$_{B2}$	-1841.941923	-1841.894998	-1841.893975	-1842.032185	-1843.207632

13-IM$_{B2}$	-1841.960213	-1841.913128	-1841.912105	-1842.049837	-1843.2273
16-TS$_{B2}$	-1841.954260	-1841.907513	-1841.906490	-1842.043582	-1843.227522
14-IM$_{B2}$	-1841.995739	-1841.947801	-1841.946778	-1842.088028	-1843.258808
17-TS$_{B2}$	-2224.818831	-2224.762146	-2224.761123	-2224.923978	-2226.104606
15-IM$_{B2}$	-2224.804148	-2224.746315	-2224.745292	-2224.905070	-2226.123085
18-TS$_{B2}$	-2774.083913	-2774.012132	-2774.011109	-2774.205382	-2775.407954
16-IM$_{B2}$	-2774.190999	-2774.120521	-2774.119498	-2774.310261	-2775.523336
19-TS$_{B2}$	-2419.029147	-2418.963790	-2418.962767	-2419.145084	-2420.37075
17-IM$_{B2}$	-1659.344544	-1659.303363	-1659.302340	-1659.430889	-1660.567153
20-TS$_{B2}$	-2230.433461	-2230.371524	-2230.370501	-2230.542623	-2231.791133
18-IM$_{B2}$	-1470.749322	-1470.711323	-1470.710300	-1470.829142	-1471.982901
21-TS$_{B2}$	-2585.487731	-2585.419016	-2585.417993	-2585.604570	-2586.824273
19-IM$_{B2}$	-2585.596720	-2585.528768	-2585.527745	-2585.710227	-2586.946075
22-TS$_{B2}$	-1726.987763	-1726.941704	-1726.940681	-1727.076386	-1728.36031
20-IM$_{B2}$	-1727.006882	-1726.960989	-1726.959966	-1727.094476	-1728.388481
23-TS$_{B2}$	-1161.467254	-1161.437530	-1161.436507	-1161.534096	-1162.777124
21-IM$_{B2}$	-1828.666426	-1828.617882	-1828.616859	-1828.756948	-1830.021932
24-TS$_{B2}$	-1828.648872	1828.600768	-1828.599745	-1828.737780	-1830.009613
22-IM$_{B2}$	-1828.680916	-1828.635206	-1828.634183	-1828.767238	-1830.031037
25-TS$_{B2}$	-1828.648872	1828.600768	-1828.599745	-1828.737780	-1830.009613
23-IM$_{B2}$	-1828.680916	-1828.635206	-1828.634183	-1828.767238	-1830.031037
E-P1'	-1247.164387	-1247.129331	-1247.128308	-1247.237013	-1247.193221
P3'	-951.148512	-951.121518	-951.120495	-951.210777	-951.1554424
B$_2$cat$_2$	-812.694320	-812.679496	-812.678473	-812.739902	-812.5782136
4-IM$_{B3}$	-1876.526955	-1876.481024	-1876.480001	-1876.619456	-1877.7101709
4-TS$_{B3}$	-2689.232003	-2689.169938	-2689.168915	-2689.345884	-2690.3076090
9-TS$_{B3}$	-2070.776840	-2070.723851	-2070.722828	-2070.877376	-2071.9993373
4-TS$_{B2}$-D3	-2585.715080	-2585.648634	-2585.647611	-2585.825056	-2586.8876495
9-TS$_{B2}$-D3	-2036.355070	-2036.300790	-2036.299768	-2036.451216	-2037.5369103
4-TS$_{B2}$-BW91	-2585.278982	-2585.209314	-2585.208291	-2585.397005	-2586.8703189
4-TS$_{B2}$-M06	-2583.936368	-2583.869936	-2583.868913	-2584.042998	-2586.8976101
9-TS$_{B2}$-BW91	-2036.036715	-2035.980099	-2035.979076	-2036.139842	-2037.5189986
9-TS$_{B2}$-M06	-2034.944645	-2034.890580	-2034.889558	-2035.038029	-2037.5497666

E_0 = Sum of electronic and zero-point energies calculated by B3LYP in solvent

E = Sum of electronic and thermal energies calculated by B3LYP in solvent

$H_{323.15}$ = Sum of electronic and thermal enthalpies calculated by B3LYP in solvent

$G_{323.15}$ = Sum of electronic and thermal free energies calculated by B3LYP in solvent

$E_{(M06)}$ = Single point energies calculated calculated by M06 in solvent

Section 8. Calculated imaginary frequencies of all transition states species.

Species	Frequency
1-TS$_{B1}$	-133.21
2-TS$_{B1}$	-195.51
3-TS$_{B1}$	-95.15
1a-TS$_{B1}$	-186.91
3a-TS$_{B1}$	-104.97
4-TS$_{B1}$	-57.72
5a-TS$_{B1}$	-105.20
5b-TS$_{B1}$	-97.84
5c-TS$_{B1}$	-138.78
5d-TS$_{B1}$	-143.78
6-TS$_{B1}$	-40.56
6a-TS$_{B1}$	-251.51
7-TS$_{B1}$	-86.37
3b-TS$_{B1}$	-118.93
8-TS$_{B1}$	-227.78
9-TS$_{B1}$	-442.69
10-TS$_{B1}$	-211.55
11-TS$_{B1}$	-1180.18
12-TS$_{B1}$	-89.66
13-TS$_{B1}$	-115.71
14-TS$_{B1}$	-330.96
3c-TS$_{B1}$	-131.58
15-TS$_{B1}$	-180.08
16-TS$_{B1}$	-47.01
17-TS$_{B1}$	-67.45
18-TS$_{B1}$	-420.08
19-TS$_{B1}$	-1107.65
20-TS$_{B1}$	-1118.25
21-TS$_{B1}$	-408.79
22-TS$_{B1}$	-852.26
23-TS$_{B1}$	-667.20
24-TS$_{B1}$	-89.66
25-TS$_{B1}$	-89.66
4-TS$_{B1}$-D3	-35.36
9-TS$_{B1}$-D3	-396.79
4-TS$_{B1}$-BW91	-78.44
9-TS$_{B1}$-BW91	-251.75
4-TS$_{B1}$-M06	-16.77

9-TS$_{B1}$-M06	-131.33
1-TS$_{B2}$	-125.19
2-TS$_{B2}$	-206.75
3-TS$_{B2}$	-97.44
1a-TS$_{B2}$	-135.97
3a-TS$_{B2}$	-107.74
4-TS$_{B2}$	-109.92
5a-TS$_{B2}$	-124.20
5b-TS$_{B2}$	-106.02
6-TS$_{B2}$	-26.78
7-TS$_{B2}$	-76.08
3b-TS$_{B2}$	-106.41
8-TS$_{B2}$	-277.63
9-TS$_{B2}$	-477.36
10-TS$_{B2}$	-222.52
10a-TS$_{B2}$	-1282.27
10b-TS$_{B2}$	-1328.00
10c-TS$_{B2}$	-1153.11
11-TS$_{B2}$	-1180.18
12-TS$_{B2}$	-113.56
13-TS$_{B2}$	-130.02
14-TS$_{B2}$	-331.45
15-TS$_{B2}$	-212.96
16-TS$_{B2}$	-57.98
17-TS$_{B2}$	-327.51
18-TS$_{B2}$	-413.31
19-TS$_{B2}$	-1055.71
20-TS$_{B2}$	-1125.16
21-TS$_{B2}$	-414.76
22-TS$_{B2}$	-593.39
23-TS$_{B2}$	-667.20
24-TS$_{B2}$	-113.56
25-TS$_{B2}$	-113.56
4-TS$_{B3}$	-104.48
9-TS$_{B3}$	-288.00
4-TS$_{B2}$-D3	-45.62
9-TS$_{B2}$-D3	-788.40
4-TS$_{B2}$-BW91	-78.57
9-TS$_{B2}$-BW91	-309.32
4-TS$_{B2}$-M06	-90.61
9-TS$_{B2}$-M06	-606.75