

## *Supporting Information*

### **Theoretical Study in Rhodium- and Cobalt-Catalyzed Decarboxylative Transformation of Isoxazolone: Origin of Product Selectivity**

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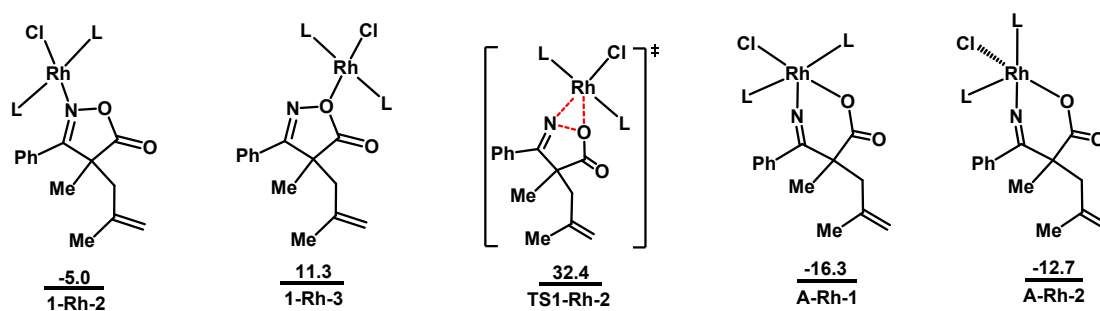
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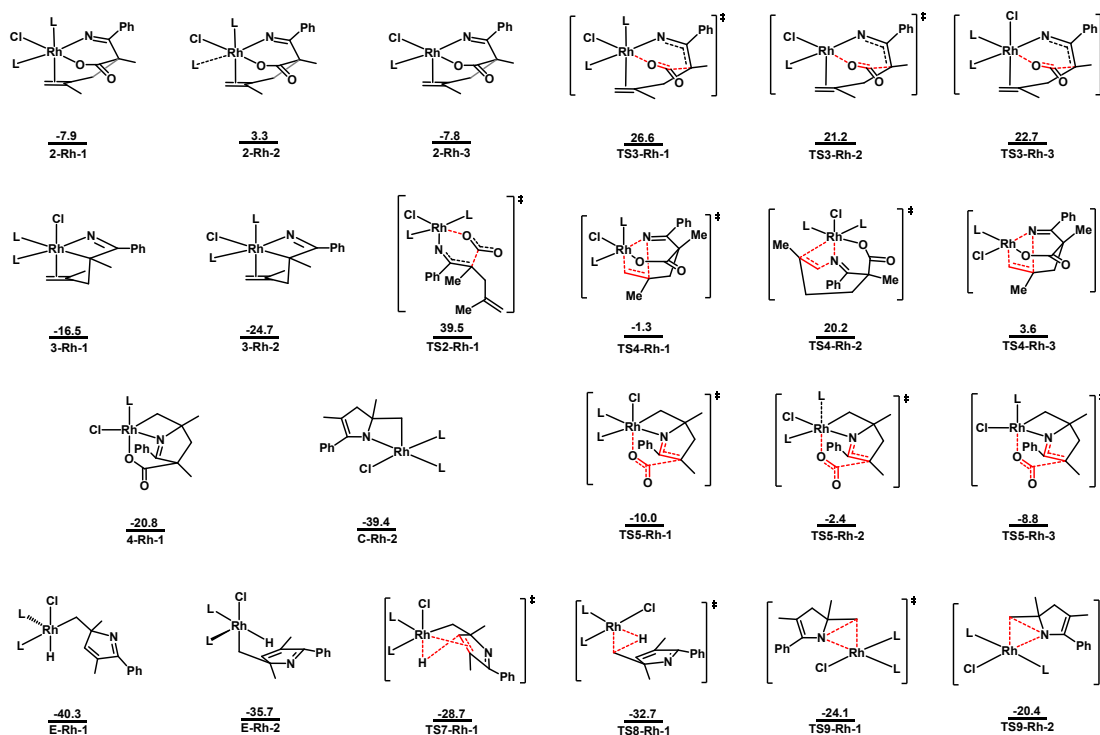
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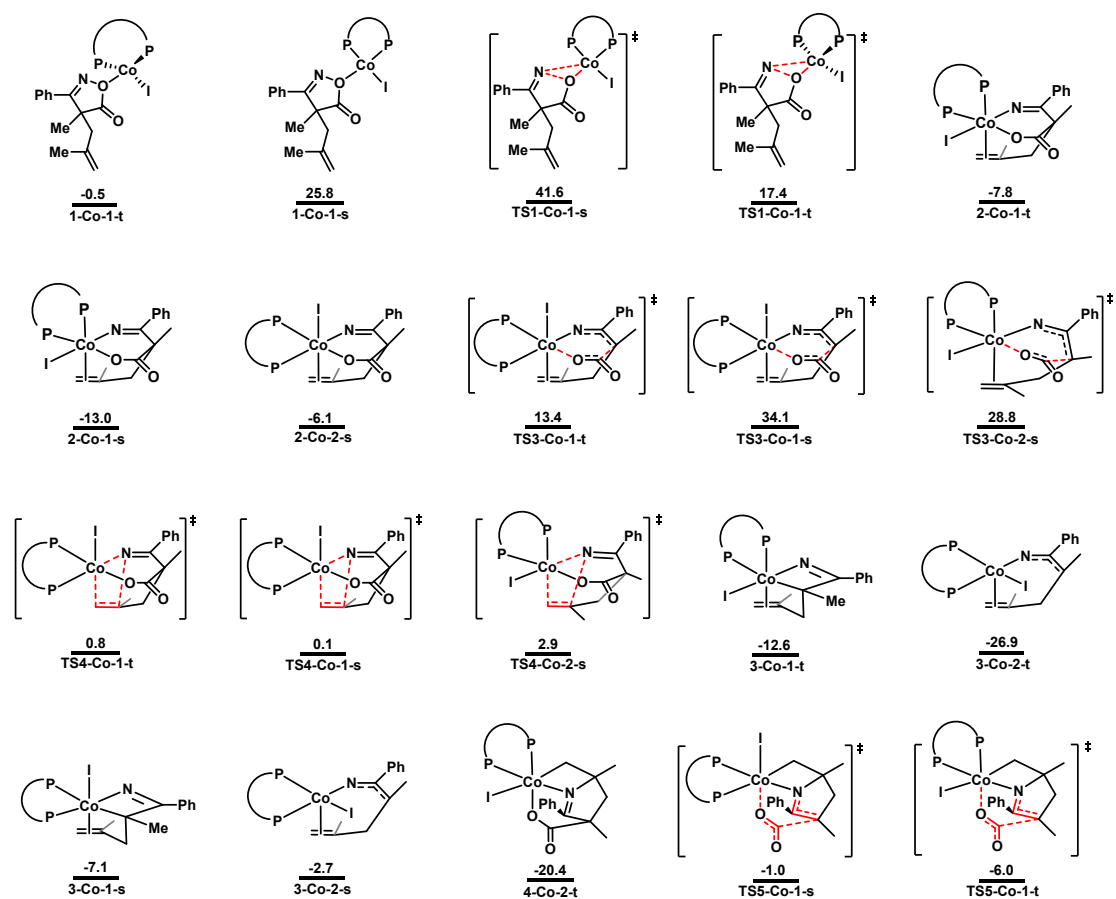
## Section 1. Other possible pathways



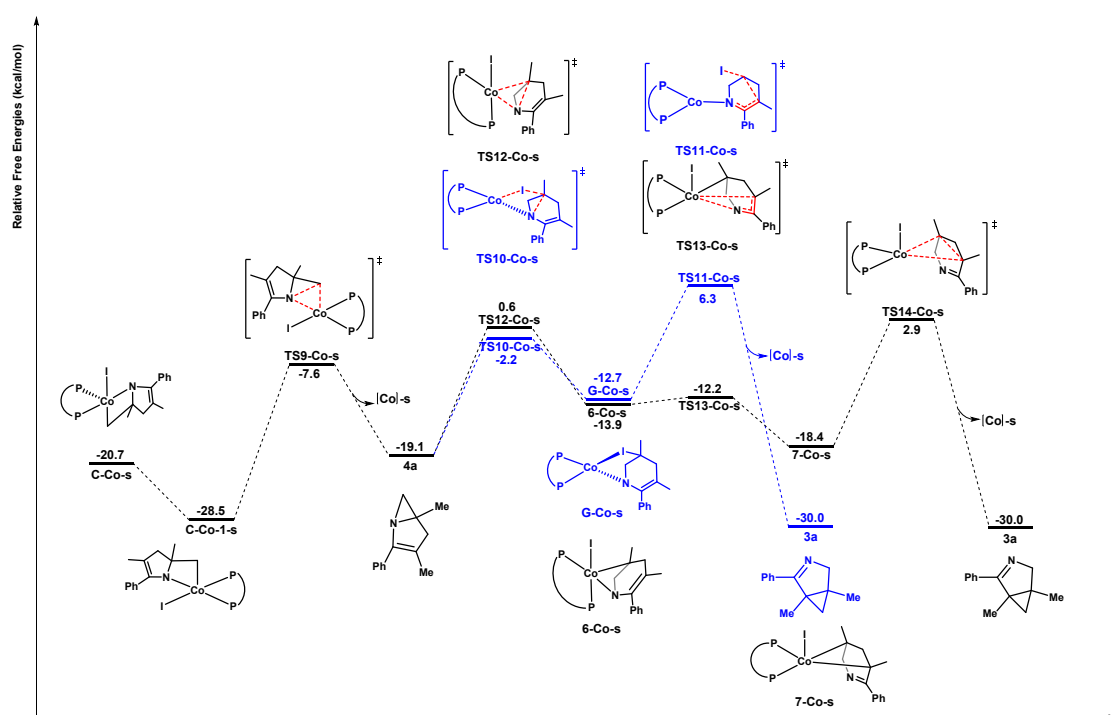
**Fig. S1** Other possible isomers of 1-Rh, TS1-Rh and A-Rh. Values shown are relative free energies in kcal/mol.



**Fig. S2** Other possible isomers of key species labeled in Figs. 2 and 3. Values shown are relative free energies in kcal/mol.

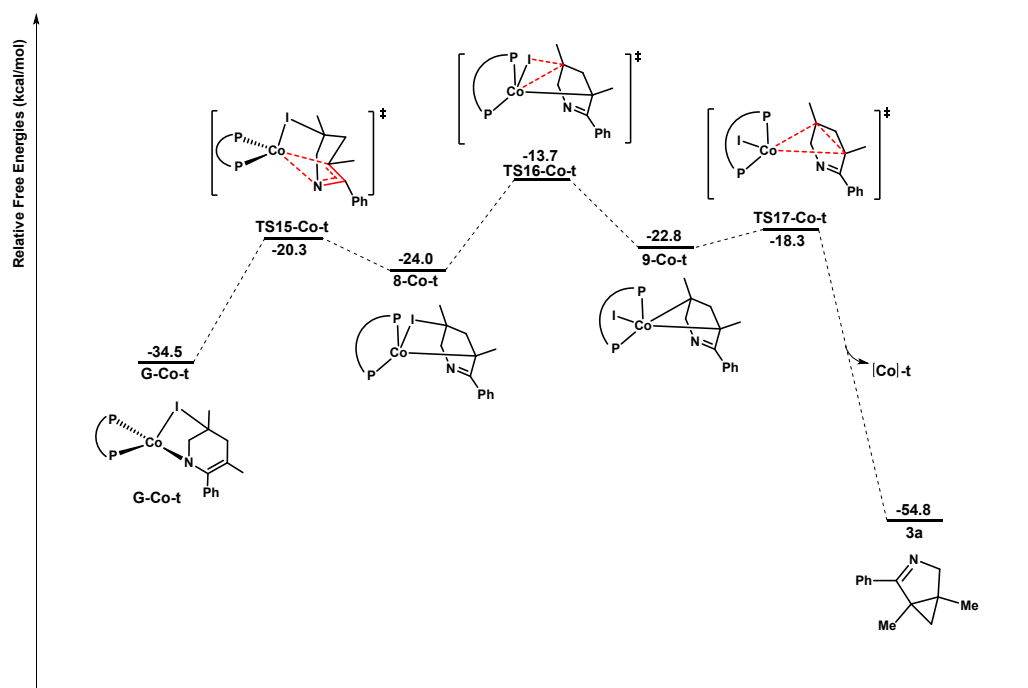


**Fig. S3** Other possible isomers of key species labeled in Fig. 4. Values shown are relative free energies in kcal/mol.



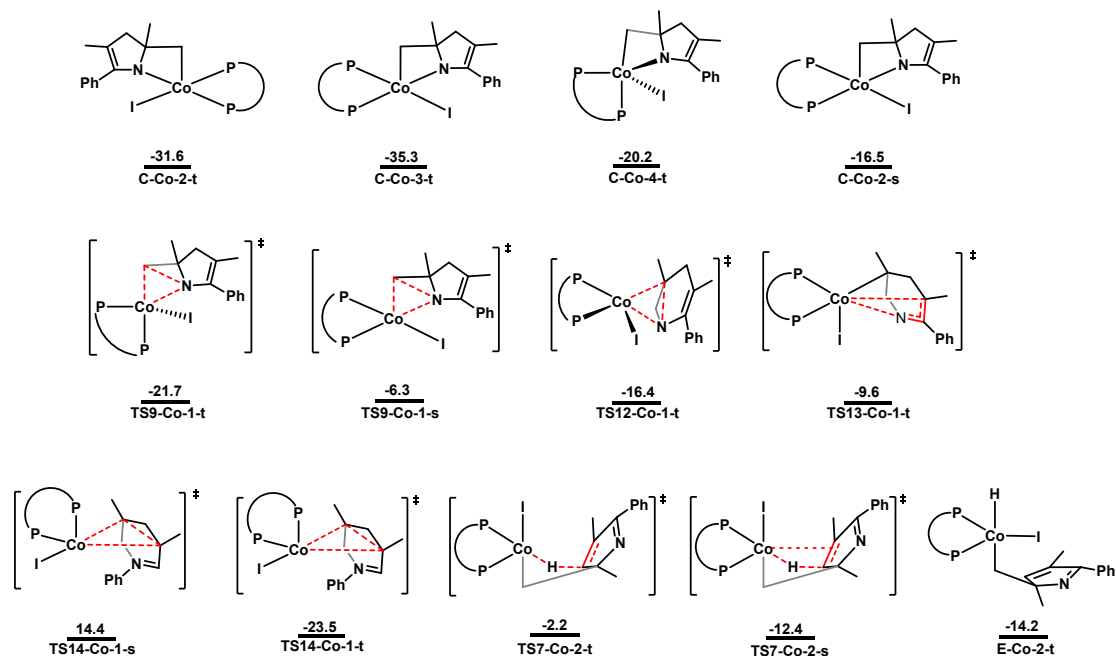
**Fig. S4** Calculated energy profiles for processes from C-Co-s to product 3a. Values

shown are relative free energies in kcal/mol.



**Fig. S5** Other possible mechanism of transformation from **G-Co-t** to **3a**. Values

shown are relative free energies in kcal/mol.



**Fig. S6** Other possible isomers of key species labeled in Figs. 5, 6 and S4. Values

shown are relative free energies in kcal/mol.

## Section 2. Table of energy values.

**Table S1.** Energies (in Hartree) of All TS and Intermediates.

Geometry	E <sub>0</sub>	E	H <sub>298.15</sub>	G <sub>298.15</sub>	E <sub>(sol,M06)</sub>
1a	-747.581783	-747.558003	-747.556821	-747.641450	-747.3503822
1-Rh	-4076.955293	-4076.850623	-4076.849441	-4077.118076	-4077.1286222
1-Rh-1	-4076.948696	-4076.843312	-4076.842130	-4077.116856	-4077.1059969
1-Rh-2	-4076.952383	-4076.848495	-4076.847313	-4077.113600	-4077.1222908
1-Rh-3	-4076.932040	-4076.826437	-4076.825256	-4077.101650	-4077.0872935
2a	-559.034734	-559.015043	-559.013861	-559.087955	-558.8667092
2-Rh	-4076.973458	-4076.869665	-4076.868483	-4077.131362	-4077.1519555
2-Rh-1	-4076.966440	-4076.863167	-4076.861985	-4077.126169	-4077.1299195
2-Rh-2	-4076.977805	-4076.873138	-4076.871956	-4077.146540	-4077.1018865
2-Rh-3	-2697.210785	-2697.144643	-2697.143461	-2697.327061	-2697.6897003
3-Rh	-3888.332107	-3888.232189	-3888.231007	-3888.486703	-3888.5680843
3-Rh-1	-3888.322838	-3888.222663	-3888.221481	-3888.481045	-3888.5502985
3-Rh-2	-3888.322249	-3888.221422	-3888.220240	-3888.479071	-3888.5662094
4-Rh	-4076.996550	-4076.895453	-4076.894271	-4077.150534	-4077.1741132
4-Rh-1	-2697.235549	-2697.170355	-2697.169173	-2697.347127	-2697.7168527
5-Rh	-3888.352481	-3888.253018	-3888.251837	-3888.507476	-3888.5916938
A-Rh	-4076.977451	-4076.872844	-4076.871662	-4077.138223	-4077.1450767
A-Rh-1	-4076.979196	-4076.874170	-4076.872988	-4077.143499	-4077.1371883
A-Rh-2	-4076.972960	-4076.868253	-4076.867072	-4077.136591	-4077.1329948
B-Rh	-3888.329256	-3888.229551	-3888.228369	-3888.487136	-3888.5541421
C-Rh	-3888.353822	-3888.253975	-3888.252793	-3888.509618	-3888.5896708
C-Rh-1	-3888.358810	-3888.259892	-3888.258710	-3888.513058	-3888.5921943
C-Rh-2	-3888.358810	-3888.259892	-3888.258710	-3888.513058	-3888.5921943
E-Rh	-3888.378236	-3888.278527	-3888.277345	-3888.537811	-3888.5858696
E-Rh-1	-3888.365180	-3888.264713	-3888.263532	-3888.524432	-3053.863246
E-Rh-2	-3888.362750	-3888.263072	-3888.261890	-3888.522269	-3888.5782679
RhL <sub>2</sub> Cl	-3329.369866	-3329.290786	-3329.289604	-3329.505434	-3329.7286976
TS1-Rh	-4076.942991	-4076.837944	-4076.836762	-4077.110868	-4077.1128318
TS1-Rh-1	-4076.914272	-4076.809100	-4076.807918	-4077.079760	-4077.0703724
TS1-Rh-2	-4076.903287	-4076.798673	-4076.797491	-4077.071601	-4077.0521053
TS2-Rh	-4076.910751	-4076.804493	-4076.803312	-4077.079405	-4077.0760702
TS2-Rh-1	-4076.886124	-4076.779529	-4076.778347	-4077.055180	-4077.0376813
TS3-Rh	-4076.913624	-4076.808336	-4076.807154	-4077.077347	-4077.0863772
TS3-Rh-1	-4076.893423	-4076.787998	-4076.786816	-4077.056788	-4077.0661548
TS3-Rh-2	-2697.161405	-2697.094215	-2697.093033	-2697.277891	-2697.6392233
TS3-Rh-3	-4076.904702	-4076.799421	-4076.798240	-4077.068865	-4077.0718795
TS4-Rh	-4076.942958	-4076.839902	-4076.838720	-4077.101092	-4077.1245016
TS4-Rh-1	-4076.948396	-4076.846681	-4076.845500	-4077.101530	-4077.1253861

TS4-Rh-2	-4076.909199	-4076.805750	-4076.804569	-4077.070443	-4077.0825511
TS4-Rh-3	-2697.197227	-2697.131723	-2697.130541	-2697.311981	-2697.6720483
TS5-Rh	-4076.962321	-4076.858553	-4076.857371	-4077.121209	-4077.1408319
TS5-Rh-1	-4076.952420	-4076.849191	-4076.848009	-4077.113389	-4077.1284911
TS5-Rh-2	-4076.976350	-4076.872443	-4076.871261	-4077.148846	-4077.104129
TS5-Rh-3	-2697.215411	-2697.149502	-2697.148320	-2697.330140	-2697.691107
TS6-Rh	-3888.352093	-3888.253996	-3888.252814	-3888.504322	-3888.5926207
TS7-Rh	-3888.338232	-3888.239667	-3888.238486	-3888.490467	-3888.5801207
TS7-Rh-1	-3888.328704	-3888.228965	-3888.227784	-3888.485818	-3888.5678931
TS8-Rh	-3888.356018	-3888.255088	-3888.253907	-3888.522692	-3888.5699704
TS8-Rh-1	-3888.352653	-3888.253232	-3888.252050	-3888.510731	-3888.5725764
TS9-Rh	-3888.318364	-3888.218660	-3888.217479	-3888.472378	-3888.5694647
TS9-Rh-1	-3888.321919	-3888.222267	-3888.221085	-3888.476846	-3888.5662879
TS9-Rh-2	-3888.316253	-3888.216064	-3888.214882	-3888.474222	-3888.5564987
3a	-559.011173	-558.992120	-558.990938	-559.063239	-558.8542337
4a	-558.995258	-558.976155	-558.974973	-559.047649	-558.8363596
1-Co-1-s	-2591.880626	-2591.810657	-2591.809475	-2592.004805	-4115.3329765
1-Co-1-t	-2591.931782	-2591.860847	-2591.859666	-2592.064174	-4115.3651935
1-Co-s	-2591.895764	-2591.826313	-2591.825131	-2592.016941	-4115.3629023
1-Co-t	-2591.938332	-2591.867799	-2591.866617	-2592.066669	-4115.3858981
2-Co-1-s	-2591.930072	-2591.861544	-2591.860362	-2592.044404	-4115.4066319
2-Co-1-t	-2591.912602	-2591.843377	-2591.842195	-2592.030925	-4115.3929908
2-Co-2-s	-2591.921746	-2591.852956	-2591.851774	-2592.038121	-4115.3928937
2-Co-s	-2591.932225	-2591.863480	-2591.862299	-2592.049104	-4115.4046156
2-Co-t	-2591.948759	-2591.877886	-2591.876705	-2592.075338	-4115.3900862
3-Co-1-s	-2403.271550	-2403.206052	-2403.204870	-2403.384328	-3926.8039603
3-Co-1-t	-2403.272408	-2403.206457	-2403.205275	-2403.389415	-3926.8079678
3-Co-2-s	-2403.264111	-2403.198217	-2403.197035	-2403.379905	-3926.7927398
3-Co-2-t	-2403.303420	-2403.236938	-2403.235757	-2403.421999	-3926.827502
3-Co-s	-2403.276816	-2403.211034	-2403.209852	-2403.390174	-3926.8120355
3-Co-t	-2403.293272	-2403.227074	-2403.225893	-2403.409771	-3926.8191314
4-Co-1-s	-2591.947695	-2591.880159	-2591.878977	-2592.061462	-4115.4260682
4-Co-1-t	-2403.326573	-2403.261328	-2403.260146	-2403.443388	-3926.8514166
4-Co-2-t	-2591.954732	-2591.885797	-2591.884615	-2592.076992	-4115.4094408
4-Co-s	-2591.943678	-2591.875713	-2591.874531	-2592.060053	-4115.4205307
4-Co-t	-2591.955636	-2591.887424	-2591.886242	-2592.076350	-4115.4122698
5-Co-1-s	-2403.284220	-2403.219956	-2403.218774	-2403.396255	-3926.8262672
5-Co-1-t	-2403.310900	-2403.245862	-2403.244680	-2403.426658	-3926.833656
5-Co-s	-2403.286708	-2403.222661	-2403.221479	-2403.397077	-3926.8285038
5-Co-t	-2403.304574	-2403.240402	-2403.239220	-2403.417480	-3926.8293215
6-Co-s	-2403.281564	-2403.217141	-2403.215960	-2403.394831	-3926.8160061
6-Co-t	-2403.313513	-2403.247610	-2403.246429	-2403.431982	-3926.834957
7-Co-s	-2403.278354	-2403.214415	-2403.213233	-2403.387411	-3926.8270128

7-Co-t	-2403.305492	-2403.240288	-2403.239106	-2403.421526	-3926.8311905
8-Co-t	-2403.294407	-2403.229430	-2403.228248	-2403.411386	-3926.8268479
9-Co-t	-2403.303777	-2403.239496	-2403.238314	-2403.418392	-3926.8271241
A-Co-s	-2591.939051	-2591.869661	-2591.868479	-2592.058747	-4115.4046416
A-Co-t	-2591.939008	-2591.869606	-2591.868424	-2592.062694	-4115.3943863
C-Co-1-s	-2403.305399	-2403.240907	-2403.239725	-2403.417782	-3926.8394763
C-Co-1-t	-2403.310368	-2403.244427	-2403.243245	-2403.429538	-3926.8284972
C-Co-2-s	-2403.289889	-2403.225413	-2403.224231	-2403.401880	-3926.8207248
C-Co-2-t	-2403.317502	-2403.251811	-2403.250629	-2403.436752	-3926.8350065
C-Co-3-t	-2403.319857	-2403.254413	-2403.253232	-2403.438543	-3926.8423964
C-Co-4-t	-2403.321737	-2403.255293	-2403.254112	-2403.444526	-3926.8117556
C-Co-s	-2403.295262	-2403.230725	-2403.229543	-2403.407889	-3926.826531
C-Co-t	-2403.320815	-2403.256462	-2403.255281	-2403.433994	-3926.8402681
Co-s	-1844.294782	-1844.251125	-1844.249943	-1844.386641	-3367.9549102
Co-t	-1844.341702	-1844.297553	-1844.296371	-1844.437202	-3367.9908106
E-Co-1-s	-2403.293639	-2403.228661	-2403.227479	-2403.408074	-3926.8197135
E-Co-1-t	-2403.289889	-2403.224043	-2403.222861	-2403.409417	-3926.8098773
E-Co-2-t	-2403.294295	-2403.228452	-2403.227271	-2403.414798	-3926.8030344
E-Co-s	-2403.287224	-2403.222541	-2403.221359	-2403.400060	-3926.8129289
G-Co-s	-2403.268668	-2403.204186	-2403.203005	-2403.382061	-3926.8132141
G-Co-t	-2403.312984	-2403.247726	-2403.246545	-2403.433641	-3926.8392463
TS1-Co-1-s	-2591.861483	-2591.791707	-2591.790526	-2591.984655	-4115.3065149
TS1-Co-1-t	-2591.913118	-2591.843455	-2591.842273	-2592.041799	-4115.337993
TS1-Co-s	-2591.889389	-2591.821222	-2591.820040	-2592.008516	-4115.3504697
TS1-Co-t	-2591.922942	-2591.853717	-2591.852535	-2592.047437	-4115.3858981
TS3-Co-1-s	-2591.852388	-2591.782169	-2591.780987	-2591.972436	-4115.3200818
TS3-Co-1-t	-2591.891978	-2591.822171	-2591.820989	-2592.013509	-4115.3507605
TS3-Co-2-s	-2591.857126	-2591.787698	-2591.786516	-2591.976698	-4115.3288722
TS3-Co-s	-2591.859990	-2591.789937	-2591.788755	-2591.980079	-4115.3297853
TS3-Co-t	-2591.897170	-2591.826997	-2591.825816	-2592.018559	-4115.3623557
TS4-Co-1-s	-2591.914002	-2591.846551	-2591.845369	-2592.027398	-4115.3862664
TS4-Co-1-t	-2591.919836	-2591.850402	-2591.849220	-2592.041501	-4115.3729977
TS4-Co-2-s	-2591.902173	-2591.834677	-2591.833496	-2592.015217	-4115.3816804
TS4-Co-s	-2591.914304	-2591.847756	-2591.846574	-2592.026260	-4115.3874582
TS4-Co-t	-2591.925597	-2591.855916	-2591.854734	-2592.048335	-4115.3810837
TS5-Co-1-s	-2591.907281	-2591.838502	-2591.837321	-2592.025462	-4115.3800933
TS5-Co-1-t	-2591.926883	-2591.857081	-2591.855899	-2592.050120	-4115.3818328
TS5-Co-s	-2591.917626	-2591.849359	-2591.848177	-2592.034039	-4115.3921896
TS5-Co-t	-2591.929786	-2591.859955	-2591.858773	-2592.052682	-3926.8514166
TS6-Co-s	-2403.291256	-2403.227816	-2403.226635	-2403.401292	-3926.8287582
TS6-Co-t	-2403.280770	-2403.219026	-2403.217844	-2403.389218	-3926.8114628
TS7-Co-1-s	-2403.277739	-2403.213766	-2403.212584	-2403.389584	-3926.8180643
TS7-Co-1-t	-2403.287407	-2403.221620	-2403.220438	-2403.407435	-3926.7983489

TS7-Co-2-s	-2403.273749	-2403.209797	-2403.208615	-2403.383067	-3926.8133494
TS7-Co-2-t	-2403.286724	-2403.223196	-2403.222015	-2403.402195	-3926.785347
TS8-Co-1-s	-2403.278557	-2403.213589	-2403.212408	-2403.395998	-3926.7964632
TS8-Co-s	-2403.282729	-2403.217585	-2403.216403	-2403.402106	-3926.7983191
TS8-Co-t	-2403.304053	-2403.238431	-2403.237249	-2403.427284	-3926.8058982
TS9-Co-1-s	-2403.258049	-2403.193375	-2403.192193	-2403.371830	-3926.8010737
TS9-Co-1-t	-2403.304073	-2403.239503	-2403.238322	-2403.421786	-3926.8198604
TS9-Co-s	-2403.265804	-2403.201087	-2403.199905	-2403.379492	-3926.8027068
TS9-Co-t	-2403.304939	-2403.239402	-2403.238220	-2403.424961	-3926.8261449
TS10-Co-s	-2403.255407	-2403.190774	-2403.189593	-2403.371081	-3926.7915098
TS10-Co-t	-2403.301445	-2403.235752	-2403.234571	-2403.424312	-3926.8194832
TS11-Co-s	-2403.257867	-2403.194656	-2403.193475	-2403.370403	-3926.7825048
TS11-Co-t	-2403.309867	-2403.245857	-2403.244675	-2403.429921	-3926.8114356
TS12-Co-1-t	-2403.291728	-2403.226398	-2403.225217	-2403.409885	-3926.8119609
TS12-Co-s	-2403.259707	-2403.196408	-2403.195227	-2403.370120	-3926.7937364
TS12-Co-t	-2403.297347	-2403.233005	-2403.231824	-2403.415689	-3926.8189533
TS13-Co-1-t	-2403.279870	-2403.214891	-2403.213710	-2403.395621	-3926.8039962
TS13-Co-s	-2403.278584	-2403.215305	-2403.214123	-2403.387243	-3926.8185501
TS13-Co-t	-2403.289584	-2403.224567	-2403.223386	-2403.404865	-3926.8241401
TS14-Co-1-s	-2403.227117	-2403.162843	-2403.161661	-2403.339492	-3926.7715469
TS14-Co-1-t	-2403.295235	-2403.230228	-2403.229047	-2403.412003	-3926.8257339
TS14-Co-s	-2403.239549	-2403.176655	-2403.175474	-2403.351580	-3926.7896481
TS14-Co-t	-2403.296358	-2403.231340	-2403.230158	-2403.414510	-3926.8271242
TS15-Co-t	-2403.286383	-2403.222249	-2403.221067	-2403.400852	-3926.8231734
TS16-Co-t	-2403.284689	-2403.219764	-2403.218583	-2403.402350	-3926.8075086
TS17-Co-t	-2403.292670	-2403.228891	-2403.227710	-2403.406219	-3926.8322529

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

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

$H_{298.15}$  = Sum of electronic and thermal enthalpies calculated by B3LYP in solvent

$G_{298.15}$  = Sum of electronic and thermal free energies calculated by B3LYP in solvent

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

### Section 3. Calculated imaginary frequencies of all transition states species.

Species	Frequency
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TS1-Rh	-74.39
TS1-Rh-1	-373.20
TS1-Rh-2	-375.76
TS2-Rh	-436.58
TS2-Rh-1	-243.12
TS3-Rh	-457.22
TS3-Rh-1	-455.52
TS3-Rh-2	-393.58
TS3-Rh-3	-460.09
TS4-Rh	-362.60
TS4-Rh-1	-341.28
TS4-Rh-2	-439.32
TS4-Rh-3	-283.01
TS5-Rh	-323.08
TS5-Rh-1	-301.25
TS5-Rh-2	-312.73
TS5-Rh-3	-356.00
TS6-Rh	-55.06
TS7-Rh	-652.33
TS7-Rh-1	-589.05
TS8-Rh	-875.02
TS8-Rh-1	-830.78
TS9-Rh	-327.15
TS9-Rh-1	-338.67
TS9-Rh-2	-387.87
TS1-Co-1-s	-233.49
TS1-Co-1-t	-885.85
TS1-Co-s	-323.63
TS1-Co-t	-505.75
TS3-Co-1-s	-388.06
TS3-Co-1-t	-394.40
TS3-Co-2-s	-376.79
TS3-Co-s	-439.70
TS3-Co-t	-401.47
TS4-Co-1-s	-269.32
TS4-Co-1-t	-456.16
TS4-Co-2-s	-393.08
TS4-Co-s	-330.41
TS4-Co-t	-468.96
TS5-Co-1-s	-263.63
TS5-Co-1-t	-419.38
TS5-Co-s	-272.48
TS5-Co-t	-391.82

TS6-Co-s	-27.69
TS6-Co-t	-222.38
TS7-Co-1-s	-734.61
TS7-Co-1-t	-1359.22
TS7-Co-2-s	-628.74
TS7-Co-2-t	-1318.43
TS8-Co-1-s	-936.47
TS8-Co-s	-792.45
TS8-Co-t	-100.11
TS9-Co-1-t	-449.56
TS9-Co-1-s	-361.19
TS9-Co-s	-420.29
TS9-Co-t	-320.73
TS10-Co-s	-144.40
TS10-Co-t	-375.78
TS11-Co-s	-136.33
TS11-Co-t	-99.22
TS12-Co-1-t	-361.06
TS12-Co-s	-175.35
TS12-Co-t	-743.76
TS13-Co-1-t	-207.46
TS13-Co-s	-58.56
TS13-Co-t	-149.98
TS14-Co-1-s	-217.89
TS14-Co-1-t	-204.13
TS14-Co-s	-173.98
TS14-Co-t	-207.52
TS15-Co-t	-40.57
TS16-Co-t	-249.63
TS17-Co-t	-187.82