

Supporting Information

Mechanistic Insight into the Rhodium-Catalyzed O-H Insertion Reaction:

A DFT Study

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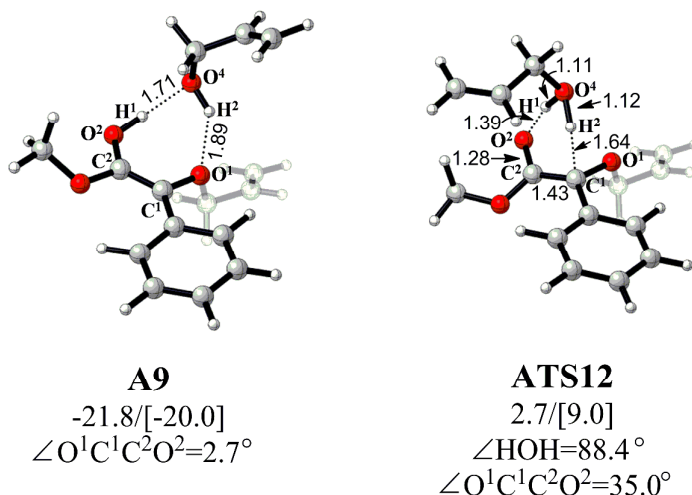


Figure S1 The relative free energies for A9 and A10 in kcal/mol along with the selected bond angles in degree.

Computed Energies of All stationary points

Table S1. Total free energy in solution (G_{sol} , in a.u., solvent = pentane), electronic (E, in a.u.), Sum of electronic and zero-point Energies (E+ZPE, in a.u.), Sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal free energies (G, in a.u.)

	G_{sol}	E	E+ZPE	H	G
Rh2L4	-975.349885	-975.812023	-975.710432	-975.695556	-975.750922
CB	-1473.07011	-1473.98274	-1473.73155	-1473.70505	-1473.78817
PA	-192.91614	-193.105502	-193.02104	-193.01571	-193.047467
A1	-1665.98251	-1667.09983	-1666.76225	-1666.72898	-1666.82913
ATS2	-1665.97948	-1667.09898	-1666.76062	-1666.72888	-1666.82311
A3	-1665.99205	-1667.10924	-1666.76879	-1666.73739	-1666.8301
ATS4	-1665.99007	-1667.10566	-1666.76875	-1666.73758	-1666.83042
A5	-1666.00169	-1667.12438	-1666.7842	-1666.75251	-1666.84633
A6	-690.64687	-691.305616	-691.067823	-691.051847	-691.111785
ATS7	-1665.96949	-1667.08874	-1666.75147	-1666.71974	-1666.81349
A8	-690.69959	-691.352156	-691.114209	-691.098388	-691.157258
A9	-883.587193	-884.434578	-884.109364	-884.087103	-884.164062
A10	-883.560542	-884.402064	-884.078976	-884.05725	-884.130938
ATS11	-883.542581	-884.381416	-884.061042	-884.039624	-884.113785
ATS12	-883.548218	-884.385737	-884.066429	-884.045285	-884.117765
A13	-883.613837	-884.459141	-884.133702	-884.110979	-884.190628
A14	-1665.99639	-1667.12701	-1666.78602	-1666.75442	-1666.84995
A15	-1858.91003	-1860.25096	-1859.823	-1859.78507	-1859.89663
ATS16	-1858.87059	-1860.20656	-1859.78433	-1859.74705	-1859.85738
A17	-1076.50871	-1077.56272	-1077.14973	-1077.12136	-1077.2125
ATS18	-1076.48717	-1077.53046	-1077.1249	-1077.0977	-1077.18501
A19	-1076.53695	-1077.58966	-1077.17635	-1077.14768	-1077.23979
A20	-1269.42731	-1270.69255	-1270.19229	-1270.15763	-1270.26545
ATS21	-1269.40885	-1270.66493	-1270.17129	-1270.13791	-1270.241
A22	-1269.45237	-1270.71813	-1270.2173	-1270.18227	-1270.29146
B1	-1665.98324	-1667.10087	-1666.76237	-1666.72959	-1666.8268
BTS2	-1665.97905	-1667.09743	-1666.75876	-1666.72712	-1666.82083
B3	-1665.99159	-1667.10653	-1666.76618	-1666.73485	-1666.82704
B4	-690.601314	-691.252756	-691.016207	-691.000039	-691.060403
B5	-1665.95788	-1667.0889	-1666.74884	-1666.71716	-1666.81243
B6	-883.55129	-884.389235	-884.065148	-884.043154	-884.117459
BTS7	-883.543715	-884.377504	-884.058245	-884.036774	-884.109964
B8	-883.610359	-884.458182	-884.13275	-884.109966	-884.189283
BTS9	-1665.97002	-1667.08615	-1666.74899	-1666.71731	-1666.81044
B10	-690.696419	-691.350444	-691.112589	-691.096669	-691.155621