Supporting Information

Mechanistic Molecular Motion of Transition-Metal Mediated β-Hydride Transfer: Quasiclassical Trajectories Reveal Dynamically Ballistic, Dynamically Unrelaxed, Two Step, and Concerted Mechanisms

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Table S1. M06/6-31G**[LANL2DZ for Co, Rh, and Ir] and M06/Def2-TZVPD absolute and relative energies. In the main manuscript, all reported structures and energies are for M06/6-31G**[LANL2DZ]. The geometry-optimized Def2-TZVPD electronic and free energies reported below are for basis set comparison, and were not included in the main manuscript. The Def2-TZVPD basis set is too large for direct dynamics trajectories.

Rhodium						
M06						
Absolute Energy (a.u.)						
Structure	Electronic	ZPE	Enthalpy	Free Energy	Def2-TZVPD Electronic	Def2-TZVPD Free Energy
1Rh	-656.806618	-656.466730	-656.446016	-656.512414	-658.080913	-657.786709
TS1Rh	-656.791761	-656.455685	-656.435046	-656.501536	-658.068218	-657.777993
2Rh	-656.793598	-656.456314	-656.435418	-656.502127	-658.069602	-657.778131
C-C Rotation	-656.799287	-656.460258	-656.439502	-656.506519	-658.070836	-657.778068
Relative Energies (kcal/mol)						
1Rh	0.0	0.0	0.0	0.0	0.0	0.0
TS1Rh	9.3	6.9	6.9	6.8	8.0	5.5
2Rh	8.2	6.5	6.7	6.5	7.1	5.4
C-C Rotation	4.6	4.1	4.1	3.7	6.3	5.4
MN15						
Absolute Energy (a.u.)						
1Rh	-656.322784	-655.979153	-655.958670	-656.024530	-657.613328	-657.315073
TS1Rh	-656.312908	-655.972334	-655.952093	-656.017477	-657.604851	-657.309419
2Rh	-656.316060	-655.974421	-655.953746	-656.020420	-657.607354	-657.311714
Relative Energies (kcal/mol)						
1Rh	0.0	0.0	0.0	0.0	0.0	0.0
TS1Rh	6.2	4.3	4.1	4.4	5.3	3.5
2Rh	4.2	3.0	3.1	2.6	3.7	2.1
ωB97X-D						
Absolute Energy (a.u.)						
1Rh	-657.105463	-656.759283	-656.738917	-656.804992	-658.387472	-658.087001
TS1Rh	-657.094007	-656.750737	-656.730659	-656.796059	-658.378756	-658.080808
2Rh	-657.096268	-656.751854	-656.731435	-656.797915	-658.380404	-658.082051
Relative Energies (kcal/mol)						
1Rh	0.0	0.0	0.0	0.0	0.0	0.0
TS1Rh	7.2	5.4	5.2	5.6	5.5	3.9
2Rh	5.8	4.7	4.7	4.4	4.4	3.1
Cobalt						
M06						
Absolute Energy (a.u.)						

Structure	Electronic	ZPE	Enthalpy	Free Energy	Def2-TZVPD Electronic	Def2-TZVPD Free Energy
1Co	-692.372691	-692.031560	-692.011432	-692.075882	-1930.215989	-1929.91918
2Co	-692.356409	-692.018815	-691.999699	-692.061400	-1930.199988	-1929.904979
Relative Energies (kcal/mol)						
1Co	0.0	0.0	0.0	0.0	0.0	0.0
2Co	10.2	8.0	7.4	9.1	10.0	8.9
ωB97X-D						
Absolute Energy (a.u.)						
1Co	-692.636687	-692.289074	-692.269207	-692.333361	-1930.575728	-1930.272402
2Co	-692.621114	-692.277123	-692.257488	-692.320845	-1930.561800	-1930.261532
Relative Energies (kcal/mol)						
1Co	0.0	0.0	0.0	0.0	0.0	0.0
2Co	9.8	7.5	7.4	7.9	8.7	6.8
Iridium						
M06						
Absolute Energy (a.u.)						
Structure	Electronic	ZPE	Enthalpy	Free Energy	Def2-TZVPD Electronic	Def2-TZVPD Free Energy
1Ir	-651.977051	-651.636556	-651.616128	-651.682439	-651.872166	-651.5775547
TS1Ir	-651.970097	-651.632421	-651.612398	-651.677884	-651.865801	-651.5735878
2Ir	-651.976711	-651.637766	-651.617313	-651.683714	-651.870828	-651.5778312
Relative Energies (kcal/mol)						
1Ir	0.0	0.0	0.0	0.0	0.0	0.0
TS1Ir	4.4	2.6	2.3	2.9	4.0	2.5
2Ir	0.2	-0.8	-0.7	-0.8	0.8	-0.2
MN15						
Absolute Energy (a.u.)						
1Ir	-651.5332167	-651.189949	-651.169699	-651.236067	-651.4755014	-651.1766898
TS1Ir	-651.524333	-651.182629	-651.162696	-651.228560	-651.472335	-651.176562
2Ir	-651.533217	-651.189949	-651.169699	-651.236067	-651.479212	-651.182063
Relative Energies (kcal/mol)						
1Ir	0.0	0.0	0.0	0.0	0.0	0.0
TS1Ir	2.4	0.9	0.8	0.5	2.0	0.1
2Ir	-3.2	-3.7	-3.6	-4.2	-2.3	-3.4
ωB97X-D						
Absolute Energy (a.u.)						
1Ir	-652.306923	-651.960367	-651.940364	-652.005808	-652.213929	-651.912814
TS1Ir	-652.303219	-651.958711	-651.939084	-652.004053	-652.210405	-651.911239
Relative Energies (kcal/mol)						
1Ir	0.0	0.0	0.0	0.0	0.0	0.0
TS1Ir	2.3	1.0	0.8	1.1	2.2	1.0