SUPPORTING INFORMATION

(“Bis(allyl)-Ruthenium(IV) Complexes as Highly Efficient Catalysts for the Redox Isomerization of Allylic Alcohols into Carbonyl Compounds in Organic Aqueous Media: Scope, Limitations and Theoretical Analysis on the Mechanism” by *Victorio Cadierno, Sergio García-Garrido, José Gimeno, Adrián Varela-Álvarez, and José A. Sordo*)

Complete reference 29

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Table S1. B3LYP/6-31G(d,p)+LANL2DZ Cartesian coordinates (angstroms).

I0:

Ru	0	-0.18993	0.03674	0.01974
Cl	0	-0.2049	2.52262	-0.29892
C	0	0.87043	-0.68667	-1.79135
C	0	1.06766	0.31033	1.82391
C	0	-0.24281	0.43916	2.29616
C	0	-0.371	-0.26089	-2.27339
C	0	1.70948	0.28935	-1.18939
C	0	1.41103	-0.94094	1.24245
C	0	2.71964	-1.19492	0.53132
C	0	2.98734	-0.05786	-0.45966
H	0	1.07579	-1.74937	-1.69925
H	0	1.69872	1.1869	1.71304
H	0	-0.6165	1.41175	2.59394
H	0	-0.75757	-0.44052	2.66823
H	0	-1.07318	-0.99768	-2.64534
H	0	-0.51758	0.76736	-2.58901
H	0	1.62924	1.30635	-1.55923
H	0	0.8716	-1.81452	1.59874
H	0	3.54082	-1.30182	1.2537
H	0	2.65018	-2.1541	0.00792
H	0	3.3391	0.83521	0.06723
H	0	3.78153	-0.32288	-1.17134
C	0	-2.59065	0.47475	0.68604
O	0	-0.90632	-1.90675	0.29238
C	0	-2.21157	-1.83988	-0.22312
C	0	-2.53858	-0.35743	-0.39568
H	0	-2.76854	1.53778	0.57249
H	0	-2.62577	0.06842	1.68875
H	0	-2.30944	-2.35483	-1.19568
H	0	-2.92966	-2.32009	0.46416
H	0	-2.7639	0.04486	-1.37799

TS1:

6	0	-0.16994	0.57186	2.27463
6	0	1.14601	0.35668	1.87892

6	0	1.47401	-0.89079	1.25463
6	0	2.80721	-1.11016	0.57415
6	0	3.06054	0.01226	-0.44563
6	0	1.78516	0.33862	-1.19252
6	0	0.97708	-0.68276	-1.79906
6	0	-0.2668	-0.31134	-2.29133
44	0	-0.02953	0.10794	0.0134
8	0	-0.90645	-1.66342	0.46671
6	0	-2.1361	-1.89703	-0.18433
6	0	-2.98015	-0.64483	-0.36537
6	0	-3.78558	-0.1497	0.57944
17	0	-0.22086	2.50696	-0.36433
1	0	1.2298	-1.73557	-1.69981
1	0	1.82769	1.20142	1.81519
1	0	-0.50306	1.57014	2.53427
1	0	-0.8132	-0.26571	2.52269
1	0	-0.96594	-1.0687	-2.62524
1	0	-0.46412	0.71532	-2.58556
1	0	1.73542	1.32866	-1.63686
1	0	0.94321	-1.77462	1.59723
1	0	3.62196	-1.1621	1.30969
1	0	2.7872	-2.08442	0.07466
1	0	3.40525	0.92004	0.06079
1	0	3.86083	-0.26664	-1.14572
1	0	-4.33432	0.77672	0.43777
1	0	-3.92173	-0.65877	1.53168
1	0	-1.99687	-2.39216	-1.16166
1	0	-2.68532	-2.61079	0.4499
1	0	-2.89	-0.10989	-1.30978

II:

6	0	0.52443	0.39303	2.39706
44	0	0.16415	0.28225	0.11348
17	0	1.17326	2.48977	-0.01718
6	0	1.48986	-0.38027	1.76006
6	0	1.04755	-1.51152	0.99427
6	0	1.9809	-2.2715	0.07782
6	0	2.69542	-1.29515	-0.87169
6	0	1.72956	-0.22963	-1.3438
6	0	0.45176	-0.56169	-1.90923
6	0	-0.4573	0.47511	-2.10905
8	0	-1.50676	-0.64415	0.68091
6	0	-2.6023	-1.04357	-0.11297
6	0	-3.63148	0.05094	-0.24091
6	0	-4.91293	-0.07581	0.10234
1	0	0.12572	-1.59683	-1.99003
1	0	2.50258	0.00145	1.6564
1	0	0.78607	1.3685	2.79083
1	0	-0.42857	-0.03669	2.68827

1	0	-1.48127	0.2579	-2.39135
1	0	-0.11142	1.49284	-2.26332
1	0	2.17207	0.71181	-1.65565
1	0	0.18245	-2.04949	1.37285
1	0	2.70785	-2.85692	0.65798
1	0	1.39363	-2.99969	-0.49194
1	0	3.52721	-0.80308	-0.35689
1	0	3.13971	-1.83051	-1.7226
1	0	-5.62211	0.73842	-0.01485
1	0	-5.30152	-1.00483	0.51406
1	0	-2.27022	-1.35338	-1.11775
1	0	-3.06808	-1.92942	0.3464
1	0	-3.26107	0.99828	-0.63406

TS2:

C	0	0.26246	0.95153	2.23142
C	0	1.37126	0.21996	1.8145
C	0	1.138	-1.07943	1.24876
C	0	2.22962	-1.85887	0.54929
C	0	2.90323	-0.97641	-0.51447
C	0	1.86192	-0.14691	-1.23522
C	0	0.68696	-0.73602	-1.81581
C	0	-0.31078	0.12884	-2.25997
Ru	0	0.12223	0.3933	-0.00138
O	0	-1.47154	-0.63209	0.61109
C	0	-2.37197	-1.45274	-0.09436
C	0	-3.7678	-0.89651	0.03306
C	0	-4.80391	-1.56476	0.53846
Cl	0	0.85112	2.66401	-0.47377
H	0	0.49297	-1.80326	-1.73089
H	0	2.33462	0.71239	1.70732
H	0	0.36383	2.00811	2.4513
H	0	-0.64903	0.44973	2.54034
H	0	-1.27808	-0.25708	-2.56162
H	0	-0.06867	1.1408	-2.57002
H	0	2.21445	0.77863	-1.68096
H	0	0.31973	-1.65434	1.67453
H	0	2.96668	-2.23452	1.27279
H	0	1.78265	-2.74498	0.08568
H	0	3.62098	-0.29575	-0.04492
H	0	3.48161	-1.58683	-1.22211
H	0	-5.79611	-1.12645	0.59476
H	0	-4.69799	-2.58082	0.91229
H	0	-2.11825	-1.52257	-1.16422
H	0	-2.34753	-2.47887	0.30877
H	0	-3.89058	0.12697	-0.32102

I2:

C	0	0.25593	0.07486	-2.21882
Ru	0	0.22844	0.0372	0.07356
Cl	0	2.66999	0.11039	-0.02432
C	0	-0.03514	1.33527	-1.69521
C	0	-1.19063	1.44252	-0.85881
C	0	-1.48326	2.68092	-0.04038
C	0	-0.23465	3.07518	0.76253
C	0	0.42852	1.83634	1.32591
C	0	-0.3028	0.83925	2.04882
C	0	0.35689	-0.36052	2.32354
O	0	-1.50583	-1.08541	0.09771
C	0	-0.82138	-2.2789	-0.00038
C	0	-1.27662	-3.16436	-1.13208
C	0	-1.50049	-4.47116	-0.99955
H	0	1.21964	-0.1163	-2.67664
H	0	-0.55117	-0.61955	-2.43024
H	0	0.71317	2.12252	-1.7307
H	0	-2.03382	0.79879	-1.09501
H	0	-1.81701	3.50731	-0.6832
H	0	-2.31938	2.46386	0.63229
H	0	-0.48498	3.78098	1.56664
H	0	0.4859	3.59204	0.1204
H	0	1.49353	1.91214	1.5286
H	0	-1.38007	0.90722	2.17304
H	0	1.43481	-0.39063	2.44717
H	0	-0.21361	-1.20756	2.69025
H	0	-0.78941	-2.85005	0.9439
H	0	0.29715	-2.05465	-0.21326
H	0	-1.4319	-2.67209	-2.09014
H	0	-1.36766	-4.97794	-0.04639
H	0	-1.82799	-5.08263	-1.83489

TS3:

C	0	2.10748	0.52689	-0.03349
C	0	1.48523	0.84963	-1.2625
C	0	0.82611	-0.2145	-1.9285
C	0	-0.13829	-0.05355	-3.08863
C	0	-1.17075	1.04073	-2.78766
C	0	-1.6691	0.9313	-1.36054
C	0	-2.08861	-0.2658	-0.73737
C	0	-2.21242	-0.2475	0.67554
Ru	0	-0.09074	0.13306	0.09465
O	0	0.25138	-2.06789	0.2285
C	0	0.37762	-1.97629	1.48741
C	0	1.66239	-2.21514	2.17004
C	0	1.71457	-2.48622	3.47887
Cl	0	-0.28456	2.41506	0.99963
H	0	2.47037	1.32425	0.60425
H	0	2.58561	-0.44204	0.0768

H	0	1.31392	1.88743	-1.53183
H	0	1.25034	-1.20803	-1.80074
H	0	0.40002	0.15588	-4.02412
H	0	-0.64291	-1.01383	-3.24231
H	0	-2.00452	1.00721	-3.50364
H	0	-0.71389	2.02905	-2.90657
H	0	-1.95621	1.86297	-0.88314
H	0	-2.09159	-1.21218	-1.2728
H	0	-2.51978	0.65931	1.18601
H	0	-2.42413	-1.18195	1.18724
H	0	-0.51245	-2.03774	2.13262
H	0	0.28013	-0.11552	1.69206
H	0	2.55286	-2.21855	1.54819
H	0	0.81617	-2.49022	4.09178
H	0	2.64976	-2.71084	3.98092

I3:

C	0	0.85314	0.13926	-2.15553
Ru	0	0.4633	-0.0019	0.01674
Cl	0	2.82337	0.64619	0.32031
C	0	0.43604	1.41521	-1.66979
C	0	-0.85339	1.48703	-1.10412
C	0	-1.40162	2.59635	-0.22086
C	0	-0.42869	2.94693	0.91348
C	0	0.19329	1.70849	1.53342
C	0	-0.46886	0.53376	1.94
C	0	0.34023	-0.62975	2.13195
O	0	-1.33507	-1.21373	-0.34878
C	0	-1.37138	-2.44674	-0.42867
C	0	-2.61641	-3.17051	-0.64867
C	0	-2.62055	-4.50909	-0.7388
H	0	1.88697	0.00753	-2.45164
H	0	0.12973	-0.50008	-2.65741
H	0	1.17249	2.19538	-1.50253
H	0	-1.6063	0.82449	-1.52624
H	0	-1.65395	3.49194	-0.80758
H	0	-2.34887	2.24105	0.20102
H	0	-0.91993	3.57366	1.67254
H	0	0.39427	3.55046	0.51543
H	0	1.21431	1.83226	1.87886
H	0	-1.55169	0.44366	1.87577
H	0	1.34474	-0.52789	2.52952
H	0	-0.15301	-1.57365	2.34828
H	0	-0.44333	-3.03026	-0.33484
H	0	1.22164	-1.41326	-0.15704
H	0	-3.5239	-2.57894	-0.73667
H	0	-1.7015	-5.08318	-0.64917
H	0	-3.53411	-5.07053	-0.90433

TS4:

C,0,2.0469141561,0.9067781747,0.0688826332
 Ru,0,-0.1041626571,0.4320225518,0.2094308729
 Cl,0,-0.4413527802,2.8120239362,0.674085479
 C,0,1.4526117664,1.0505284531,-1.2205114326
 C,0,0.8722486606,-0.1049533752,-1.7832319915
 C,0,-0.1146145776,-0.1597315823,-2.9386661885
 C,0,-1.2703371772,0.8326082603,-2.7415815468
 C,0,-1.7713414553,0.8526634711,-1.3077687831
 C,0,-2.0712826316,-0.2592815666,-0.494649463
 C,0,-2.1544405787,-0.0208258065,0.910579764
 O,0,0.3756994398,-1.7286435215,0.6531239495
 C,0,0.530671869,-2.7542426274,1.3048775446
 C,0,1.8007610337,-3.1572586433,1.905820879
 C,0,1.8942220035,-4.3008804891,2.5992386917
 H,0,2.3694792446,1.7959083526,0.5974377154
 H,0,2.5823805398,-0.0098561012,0.3058885898
 H,0,1.2236289206,2.0411801836,-1.6022307078
 H,0,1.3506621454,-1.0517561338,-1.538905174
 H,0,0.3841089968,0.0115510274,-3.9040084603
 H,0,-0.5093455851,-1.1813365186,-2.9855614032
 H,0,-2.0870352047,0.6281823565,-3.4499232678
 H,0,-0.9241863942,1.8460389731,-2.9722858758
 H,0,-2.1320129801,1.8163464086,-0.962262285
 H,0,-1.9974252985,-1.2755253738,-0.8767719393
 H,0,-2.5540367927,0.919774884,1.2756219095
 H,0,-2.26887542,-0.8698580937,1.5776803383
 H,0,-0.322640139,-3.4421267544,1.4673759762
 H,0,0.1718808172,0.5361507162,1.7902246756
 H,0,2.6454681342,-2.4868294679,1.7724761457
 H,0,1.0344172862,-4.9553424676,2.7241635422
 H,0,2.8216119723,-4.6191786236,3.0637364307

I4:

C	0	0.72585	-0.08772	-2.02801
C	0	0.21616	1.21069	-1.71724
C	0	-1.09426	1.27469	-1.2044
C	0	-1.72664	2.44784	-0.47435
C	0	-0.79627	2.99688	0.61557
C	0	-0.12333	1.8878	1.40341
C	0	-0.73269	0.73649	1.94261
C	0	0.13832	-0.33221	2.31487
Ru	0	0.29323	0.02043	0.13476
O	0	-1.45059	-1.33346	-0.04225
C	0	-1.56305	-2.51636	-0.3782
C	0	-0.50906	-3.37912	-0.89263
C	0	-0.79196	-4.64959	-1.22051
Cl	0	2.59958	0.84639	0.39762

H	0	1.77187	-0.184	-2.29508
H	0	0.05479	-0.8211	-2.47282
H	0	0.89904	2.05024	-1.63067
H	0	-1.79507	0.52269	-1.56139
H	0	-2.02215	3.24567	-1.17165
H	0	-2.65833	2.09056	-0.02072
H	0	-1.33465	3.689	1.27996
H	0	0.00086	3.58868	0.15239
H	0	0.87249	2.12363	1.76498
H	0	-1.80318	0.56485	1.85126
H	0	1.12064	-0.11219	2.72008
H	0	-0.29941	-1.27534	2.62796
H	0	-2.5634	-2.97509	-0.28613
H	0	1.15222	-1.3351	0.22122
H	0	0.4845	-2.95059	-0.9804
H	0	-1.79551	-5.0553	-1.11089
H	0	-0.03337	-5.32297	-1.60587

TS5:

C	0	2.32489	0.00134	0.3125
C	0	1.81999	-1.24016	-0.18415
C	0	1.00851	-1.99232	0.68741
C	0	0.06958	-3.12389	0.31011
C	0	-0.80615	-2.76477	-0.89815
C	0	-1.33237	-1.342	-0.8
C	0	-1.92538	-0.74012	0.3294
C	0	-2.00953	0.68461	0.32566
Ru	0	0.11386	0.0834	0.24908
O	0	0.39918	0.73742	-1.86133
C	0	0.51671	1.84613	-2.37471
C	0	0.20369	3.15439	-1.74738
C	0	-1.01517	3.69288	-1.72607
Cl	0	0.04291	0.13916	2.70878
H	0	2.86886	0.64875	-0.36957
H	0	2.59306	0.09589	1.35966
H	0	1.8613	-1.46032	-1.24906
H	0	1.22325	-1.90689	1.74784
H	0	-0.56781	-3.31457	1.18038
H	0	0.6196	-4.05963	0.13118
H	0	-1.62448	-3.49039	-1.01589
H	0	-0.21363	-2.83344	-1.81779
H	0	-1.4863	-0.84125	-1.75453
H	0	-2.05825	-1.28668	1.25801
H	0	-2.31634	1.19193	1.2327
H	0	-2.2407	1.19826	-0.60462
H	0	0.91539	1.87992	-3.40578
H	0	1.0665	3.69817	-1.36257
H	0	-1.88167	3.17836	-2.13092
H	0	-1.18531	4.67226	-1.29137

H	0	0.36509	1.63845	0.5664
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I5:

Ru	0	0.1136	0.08028	0.2862
Cl	0	0.00008	-0.10735	2.73588
C	0	2.32563	-0.07696	0.34241
C	0	1.77983	-1.24491	-0.26805
C	0	0.94442	-2.04601	0.53758
C	0	-0.0254	-3.1157	0.07026
C	0	-0.87822	-2.64125	-1.11316
C	0	-1.36505	-1.21751	-0.9056
C	0	-1.94939	-0.69105	0.26291
C	0	-1.99976	0.73192	0.37948
H	0	2.87766	0.62446	-0.27547
H	0	2.59164	-0.08918	1.39432
H	0	1.81055	-1.36315	-1.34894
H	0	1.16713	-2.06359	1.59966
H	0	-0.67613	-3.35015	0.91982
H	0	0.49911	-4.05183	-0.17197
H	0	-1.71526	-3.33209	-1.2922
H	0	-0.27954	-2.65523	-2.03119
H	0	-1.48182	-0.63173	-1.8152
H	0	-2.11095	-1.30799	1.14175
H	0	-2.31939	1.16273	1.3215
H	0	-2.21108	1.32285	-0.50958
O	0	0.40729	0.90358	-1.77122
C	0	0.41159	1.91722	-2.47356
C	0	0.01904	3.28654	-2.13371
C	0	-0.37518	3.71019	-0.92129
H	0	0.76049	1.79132	-3.51443
H	0	0.08565	3.98546	-2.96504
H	0	-0.43034	3.03394	-0.07372
H	0	-0.63363	4.75304	-0.76135
H	0	0.48288	1.5602	0.78561

TS6:

C	0	0.57509	0.03568	-2.17438
Ru	0	0.20274	-0.05934	0.00572
Cl	0	2.52548	0.69377	0.28058
C	0	0.0897	1.29535	-1.72287
C	0	-1.20836	1.30283	-1.16621
C	0	-1.81693	2.41188	-0.32955
C	0	-0.84308	2.87334	0.76078
C	0	-0.15644	1.69557	1.42259
C	0	-0.78029	0.51672	1.89115
C	0	0.07751	-0.57974	2.16916
O	0	-1.60646	-1.3695	-0.24152
C	0	-1.6409	-2.62764	-0.26052

C	0	-0.50505	-3.48195	-0.24637
C	0	0.7149	-3.06336	-0.73592
H	0	1.61266	-0.04515	-2.47959
H	0	-0.12481	-0.65346	-2.6452
H	0	0.77285	2.12983	-1.59581
H	0	-1.91442	0.57616	-1.56117
H	0	-2.13379	3.25743	-0.95717
H	0	-2.73212	2.01924	0.12768
H	0	-1.35024	3.50544	1.50424
H	0	-0.06078	3.49987	0.31893
H	0	0.84729	1.89133	1.78627
H	0	-1.854	0.36818	1.80651
H	0	1.07648	-0.40328	2.55454
H	0	-0.3593	-1.54772	2.39555
H	0	-2.64148	-3.08329	-0.19674
H	0	1.0303	-1.52494	0.03965
H	0	-0.59757	-4.41823	0.29832
H	0	0.77691	-2.43085	-1.60718
H	0	1.61292	-3.63962	-0.52542

I6:

Ru	0	-0.12606	0.00429	0.21033
Cl	0	-0.01778	0.05207	2.63102
C	0	2.1787	0.26529	0.10649
C	0	1.76402	-0.95073	-0.42859
C	0	1.03084	-1.84154	0.42827
C	0	0.33628	-3.07471	-0.11046
C	0	-0.55057	-2.70217	-1.31074
C	0	-1.25164	-1.38796	-1.04436
C	0	-2.00917	-1.16565	0.15367
C	0	-2.42702	0.1314	0.43512
H	0	2.55787	1.04613	-0.54202
H	0	2.35096	0.37325	1.17329
H	0	1.80821	-1.11685	-1.5025
H	0	1.34096	-1.88654	1.46852
H	0	-0.26992	-3.50753	0.69199
H	0	1.06715	-3.84736	-0.38797
H	0	-1.27682	-3.49928	-1.52268
H	0	0.05517	-2.59718	-2.21715
H	0	-1.51074	-0.78362	-1.90993
H	0	-2.04778	-1.92072	0.93519
H	0	-2.79727	0.37768	1.42377
H	0	-2.59652	0.84701	-0.36284
O	0	-0.43538	1.18616	-1.41115
C	0	0.48366	1.92403	-2.0387
C	0	0.96357	3.11493	-1.61709
C	0	0.59756	3.81323	-0.34233
H	0	0.79918	1.54178	-3.01693
H	0	1.63739	3.63334	-2.29713

H	0	0.22251	4.82496	-0.54261
H	0	1.466	3.92844	0.31979
H	0	-0.17202	3.26653	0.20876

TS7:

C	0	2.43716	0.04147	-0.06528
C	0	1.85714	-1.14418	-0.47027
C	0	1.01986	-1.85093	0.46357
C	0	0.2596	-3.0947	0.05071
C	0	-0.59341	-2.8001	-1.19332
C	0	-1.22634	-1.4342	-1.05318
C	0	-1.9097	-1.04077	0.13868
C	0	-2.23261	0.31648	0.26995
Ru	0	-0.01388	0.03302	0.04454
O	0	-0.18198	1.00545	-1.77968
C	0	0.66418	2.00123	-1.57265
C	0	0.50064	3.04826	-0.7099
C	0	-0.7221	3.46555	0.05013
Cl	0	0.14109	0.3537	2.45308
H	0	2.96247	0.66988	-0.77358
H	0	2.54746	0.28018	0.98775
H	0	1.88977	-1.4342	-1.5178
H	0	1.31455	-1.8026	1.5084
H	0	-0.37646	-3.40788	0.88489
H	0	0.95086	-3.9292	-0.13263
H	0	-1.35593	-3.57761	-1.34086
H	0	0.0269	-2.80852	-2.09592
H	0	-1.48048	-0.91075	-1.97158
H	0	-1.96561	-1.6993	1.0012
H	0	-2.56144	0.70467	1.22716
H	0	-2.45172	0.90275	-0.61649
H	0	1.59931	1.96564	-2.14681
H	0	1.35454	3.72183	-0.64133
H	0	-0.93643	4.52276	-0.15011
H	0	-0.57968	3.36548	1.13317
H	0	-1.59659	2.87851	-0.23049

I7:

Ru	0	-0.10771	0.07231	0.05304
C	0	-0.61557	-0.17106	2.32979
C	0	0.7649	-0.18654	2.10431
C	0	1.29165	-1.22288	1.28555
C	0	2.7338	-1.23911	0.82451
C	0	3.08886	0.11522	0.19916
C	0	1.94876	0.57272	-0.68379
C	0	1.29377	-0.2874	-1.60689
C	0	0.11262	0.20353	-2.18498
H	0	-1.05285	0.64725	2.88964

H	0	-1.19746	-1.08476	2.26739
H	0	1.37634	0.66174	2.403
H	0	0.78008	-2.1799	1.30873
H	0	3.4077	-1.48493	1.65691
H	0	2.85716	-2.04223	0.09078
H	0	3.2522	0.86661	0.97912
H	0	4.02753	0.06104	-0.36994
H	0	1.86652	1.64247	-0.86063
H	0	1.54884	-1.33994	-1.68291
H	0	0.0242	1.26642	-2.37847
H	0	-0.52255	-0.46548	-2.75245
Cl	0	-1.20627	-2.10048	-0.32415
C	0	-2.32749	1.04532	-0.30352
C	0	-1.47673	1.87847	0.45095
C	0	-2.69202	1.19386	-1.75571
O	0	-0.32177	2.27624	0.03071
H	0	-1.74691	2.09238	1.49287
H	0	-3.08969	0.54849	0.29493
H	0	-3.68896	1.65238	-1.81155
H	0	-2.00041	1.83845	-2.29759
H	0	-2.7572	0.2236	-2.25496

TS8:

C	0	-1.13247	0.86385	-2.03952
C	0	-2.27408	0.29429	-1.48027
C	0	-2.24669	-1.11413	-1.20023
C	0	-3.32367	-1.79693	-0.38329
C	0	-3.53228	-1.05306	0.94545
C	0	-2.19864	-0.61157	1.50711
C	0	-1.10336	-1.51988	1.68829
C	0	0.14353	-0.97884	1.98562
Ru	0	-0.68712	-0.14594	-0.00384
Cl	0	0.7657	-1.77817	-1.14396
O	0	-0.75225	1.61883	0.97909
C	0	-1.06822	2.82234	0.49025
C	0	-0.21234	3.68956	-0.09168
H	0	-0.61892	4.6701	-0.33601
O	0	2.72697	0.28742	0.36836
C	0	4.01032	-0.07539	0.86645
C	0	5.0462	-0.15065	-0.22186
C	0	5.81581	-1.21289	-0.45928
H	0	-1.02916	1.94194	-2.07853
H	0	-0.45322	0.27044	-2.64448
H	0	-1.72661	-1.74318	-1.91703
H	0	-3.05505	0.93248	-1.07306
H	0	-4.26396	-1.86269	-0.94866
H	0	-3.01081	-2.82962	-0.19753
H	0	-4.15551	-0.16538	0.79282
H	0	-4.0724	-1.68213	1.66673

H	0	-2.20129	0.2779	2.13161
H	0	-1.17789	-2.55554	1.36601
H	0	0.23457	-0.02157	2.48794
H	0	1.03461	-1.58968	1.90895
H	0	2.41668	-0.41297	-0.23245
H	0	3.97903	-1.02841	1.41827
H	0	4.27721	0.70873	1.58605
H	0	5.13524	0.7418	-0.84102
H	0	-2.104	3.13796	0.66647
C	0	1.24496	3.45996	-0.35753
H	0	5.73526	-2.11804	0.13904
H	0	6.55479	-1.22118	-1.25518
H	0	1.47405	3.57468	-1.426
H	0	1.85606	4.20669	0.16711
H	0	1.57556	2.46809	-0.04165

I8:

C	0	0.01248	-1.24522	2.01733
C	0	-1.35919	-1.28884	1.72336
C	0	-2.00175	-0.04075	1.4941
C	0	-3.40063	0.09737	0.92951
C	0	-3.52023	-0.7228	-0.35982
C	0	-2.26533	-0.57253	-1.19143
C	0	-1.65902	0.67559	-1.51803
C	0	-0.3812	0.62281	-2.08158
Ru	0	-0.3824	-0.33976	-0.01075
Cl	0	-0.01356	-2.66236	-0.93611
O	0	0.22417	1.47511	0.8019
C	0	-0.36625	2.65369	0.5991
C	0	0.20377	3.73211	0.02245
H	0	-0.3754	4.65351	0.02519
O	0	1.87028	-0.4713	-0.44906
C	0	2.8665	-0.12377	0.53779
C	0	4.22942	-0.0794	-0.08496
C	0	5.26554	-0.80153	0.34217
H	0	-2.0462	1.61694	-1.1396
H	0	-1.82885	-2.23002	1.45126
H	0	0.58319	-2.16747	2.02078
H	0	0.42781	-0.38875	2.54063
H	0	0.21124	1.52782	-2.15146
H	0	-0.07324	-0.22612	-2.68394
H	0	-2.03903	-1.40599	-1.84892
H	0	-1.62406	0.80222	2.0649
H	0	-4.15668	-0.20593	1.66695
H	0	-3.58612	1.15708	0.724
H	0	-3.64089	-1.78521	-0.12324
H	0	-4.41034	-0.43706	-0.9376
H	0	-1.38811	2.75856	0.99246
C	0	1.59239	3.78132	-0.5451

H	0	6.24504	-0.72742	-0.1204
H	0	5.17359	-1.48897	1.1803
H	0	4.34122	0.60002	-0.92883
H	0	2.83944	-0.83394	1.37334
H	0	2.54914	0.85589	0.90423
H	0	1.90965	-1.42219	-0.67034
H	0	1.60553	4.24938	-1.53789
H	0	2.27157	4.37236	0.08554
H	0	2.01288	2.7762	-0.63262

TS9:

C	0	-0.62488	-1.10373	2.05289
C	0	-1.89538	-0.87393	1.51407
C	0	-2.23181	0.47644	1.21145
C	0	-3.45425	0.88141	0.41591
C	0	-3.49427	0.10397	-0.90425
C	0	-2.10474	0.00993	-1.49368
C	0	-1.22205	1.11749	-1.64534
C	0	0.10838	0.82304	-1.9765
Ru	0	-0.45134	-0.12354	0.00763
Cl	0	-0.40539	-2.43276	-0.96472
O	0	0.26224	1.54389	1.02735
C	0	0.17214	2.8082	0.61979
C	0	1.21685	3.59574	0.28594
H	0	1.00239	4.64122	0.07228
O	0	1.86662	-0.5353	0.21138
C	0	2.50462	-1.79606	0.54459
C	0	3.99317	-1.66786	0.42327
C	0	4.72895	-2.41318	-0.40338
H	0	-1.49058	2.11426	-1.30969
H	0	-2.47794	-1.70483	1.12592
H	0	-0.25496	-2.12054	2.1217
H	0	-0.13123	-0.33926	2.6454
H	0	0.84703	1.61717	-1.92173
H	0	0.33842	-0.05158	-2.57893
H	0	-1.92904	-0.84411	-2.13921
H	0	-1.80187	1.23424	1.85918
H	0	-4.37263	0.72576	0.99898
H	0	-3.3978	1.95803	0.22249
H	0	-3.85605	-0.91555	-0.73422
H	0	-4.19381	0.5597	-1.61906
H	0	-0.83471	3.25445	0.62217
C	0	2.65165	3.15337	0.27926
H	0	5.80771	-2.3042	-0.46514
H	0	4.27603	-3.16986	-1.03994
H	0	4.46493	-0.91439	1.0531
H	0	2.10634	-2.59426	-0.08765
H	0	2.20534	-1.98823	1.5788
H	0	2.22157	-0.24745	-0.64055

H	0	3.13872	3.35813	-0.68426
H	0	3.24122	3.68301	1.04047
H	0	2.72058	2.08338	0.49034

I9:

C	0	0.22582	0.08269	-2.19229
C	0	1.5871	-0.08118	-1.89527
C	0	2.17834	0.90034	-1.05801
C	0	3.54649	0.77808	-0.42583
C	0	3.66484	-0.5708	0.28815
C	0	2.37964	-0.88553	1.0214
C	0	1.70641	0.00518	1.90634
C	0	0.42978	-0.38761	2.31972
Ru	0	0.50775	-0.12813	0.04084
Cl	0	0.24787	-2.57122	-0.33398
O	0	0.11565	1.96697	0.21859
C	0	-0.8702	2.37424	1.00168
C	0	-2.03019	2.94375	0.57879
C	0	-2.36229	3.26719	-0.85116
O	0	-1.75378	-0.18861	0.23704
C	0	-2.6848	-0.84774	-0.65243
C	0	-4.03349	-0.99217	-0.00983
C	0	-4.61151	-2.1672	0.23871
H	0	2.05	1.02397	2.06495
H	0	2.07308	-1.03332	-2.08799
H	0	-0.31541	-0.72609	-2.66961
H	0	-0.19818	1.08003	-2.25184
H	0	-0.20502	0.29982	2.86552
H	0	0.16316	-1.43871	2.366
H	0	2.17652	-1.9426	1.16182
H	0	1.77054	1.90441	-1.12127
H	0	4.34064	0.90779	-1.17428
H	0	3.66528	1.59986	0.28838
H	0	3.84047	-1.37138	-0.43825
H	0	4.52207	-0.59061	0.97575
H	0	-0.7342	2.25796	2.08637
H	0	-2.70857	3.30426	1.34988
H	0	-1.61846	2.84139	-1.52856
H	0	-2.37615	4.35272	-1.0186
H	0	-3.35427	2.89725	-1.14132
H	0	-5.59929	-2.23541	0.68507
H	0	-4.11558	-3.1047	-0.00062
H	0	-4.55334	-0.06679	0.24161
H	0	-2.75398	-0.272	-1.58631
H	0	-2.23985	-1.81946	-0.86792
H	0	-2.0347	0.73773	0.4169

TS10:

C	0	2.23263	0.40853	0.46837
C	0	1.76726	1.73663	0.40884
C	0	1.04677	2.09485	-0.7607
C	0	0.25217	3.37391	-0.93008
C	0	-0.67103	3.57697	0.27488
C	0	-1.30493	2.2612	0.67524
C	0	-1.96558	1.37443	-0.21694
C	0	-2.26368	0.09138	0.25837
Ru	0	-0.00585	0.43093	0.3095
O	0	0.01256	-1.70367	0.30365
C	0	0.74322	-2.57753	1.15085
C	0	1.92278	-3.19444	0.44794
C	0	2.08316	-4.50472	0.25799
Cl	0	-0.00763	0.43762	2.74511
O	0	0.22344	-0.55768	-1.71011
C	0	-0.65837	-0.5256	-2.75804
C	0	-1.5142	-1.48688	-3.12669
C	0	-1.73871	-2.81838	-2.46798
H	0	2.62364	0.0217	1.40217
H	0	2.53794	-0.09479	-0.44451
H	0	1.74421	2.35212	1.30306
H	0	1.35012	1.59848	-1.68
H	0	0.91845	4.23545	-1.07687
H	0	-0.33873	3.29115	-1.84924
H	0	-1.43461	4.34063	0.07058
H	0	-0.09668	3.9469	1.13082
H	0	-1.55476	2.16303	1.72657
H	0	-2.02213	1.58249	-1.28325
H	0	-2.44872	-0.08416	1.31266
H	0	-2.58435	-0.67799	-0.4344
H	0	0.17949	-1.39943	-1.02025
H	0	-0.57095	0.39543	-3.33066
H	0	-2.08392	-1.27936	-4.0302
H	0	-1.38521	-3.63707	-3.10829
H	0	-1.23474	-2.8966	-1.50216
H	0	1.06795	-2.02628	2.04303
H	0	0.06926	-3.37504	1.49866
H	0	2.68146	-2.50239	0.08209
H	0	1.34399	-5.22217	0.60818
H	0	2.95731	-4.9121	-0.24215
H	0	-2.80891	-2.99187	-2.30142

I10:

44	0	-0.47019	-0.22674	-0.07219
17	0	-0.87218	-2.2805	-1.31479
6	0	-0.18914	-1.55157	1.71689
6	0	-1.5396	-1.16347	1.61372
6	0	-1.79616	0.23075	1.67896
6	0	-3.12145	0.88588	1.3461

6	0	-3.63143	0.37464	-0.00435
6	0	-2.48932	0.28222	-0.99465
6	0	-1.56113	1.32296	-1.26411
6	0	-0.41978	0.98903	-2.00429
1	0	0.09075	-2.5741	1.49209
1	0	0.48803	-0.97934	2.34464
1	0	-2.28712	-1.86412	1.25415
1	0	-1.12421	0.81117	2.30767
1	0	-3.85701	0.71641	2.14487
1	0	-2.96678	1.97004	1.30554
1	0	-4.44365	1.00623	-0.39093
1	0	-4.05794	-0.62756	0.10989
1	0	-2.59385	-0.48076	-1.75897
1	0	-1.59951	2.26817	-0.72678
1	0	-0.44258	0.18479	-2.73172
1	0	0.4034	1.69091	-2.07034
8	0	1.61052	-0.38651	-0.45948
8	0	0.84279	1.31233	0.96832
1	0	1.54913	0.71857	0.44405
6	0	2.40895	-1.55799	-0.47621
6	0	3.3134	-1.63681	0.72488
6	0	4.6453	-1.66987	0.66413
6	0	0.87816	2.66792	0.75548
6	0	1.77288	3.3494	0.03059
6	0	2.93401	2.79907	-0.74806
1	0	0.08375	3.17699	1.29579
1	0	1.65077	4.43052	0.0407
1	0	3.88722	3.09225	-0.28929
1	0	2.90914	1.70946	-0.82214
1	0	1.76058	-2.44248	-0.5299
1	0	3.01972	-1.55868	-1.39219
1	0	2.81923	-1.66797	1.69634
1	0	5.16929	-1.63703	-0.28885
1	0	5.2619	-1.74093	1.55579
1	0	2.94058	3.2029	-1.76781

TS11:

C	0	-2.37161	-1.17003	-0.287
C	0	-2.11953	-1.42407	1.07626
C	0	-0.79783	-1.86115	1.38835
C	0	-0.26322	-1.97187	2.79883
C	0	-0.56563	-0.67748	3.56758
C	0	-0.32113	0.51737	2.66935
C	0	0.89778	0.69132	1.94461
C	0	0.96371	1.68608	0.97617
Ru	0	-0.71625	0.1225	0.46313
O	0	0.01626	0.19949	-1.41421
C	0	-0.53504	-0.03798	-2.69816
C	0	0.14589	-1.20175	-3.37099

C	0	0.77383	-1.13052	-4.5447
Cl	0	-2.41518	1.77245	0.83652
O	0	2.46364	-0.79854	-0.68069
C	0	3.68795	-0.24956	-0.91053
C	0	4.01273	0.81235	-1.66103
C	0	3.08727	1.67666	-2.47261
H	0	-3.27756	-0.65111	-0.57965
H	0	-1.90198	-1.79539	-1.04011
H	0	-2.80356	-1.08438	1.84734
H	0	-0.29281	-2.472	0.63656
H	0	-0.68867	-2.84936	3.30509
H	0	0.81659	-2.14479	2.7478
H	0	0.03221	-0.62129	4.48785
H	0	-1.6133	-0.66295	3.88659
H	0	-0.88667	1.41459	2.89958
H	0	1.67296	-0.07181	1.95787
H	0	0.32484	2.56208	1.0312
H	0	1.80461	1.72259	0.29421
H	0	1.73606	-0.32877	-1.14655
H	0	4.45741	-0.80384	-0.378
H	0	5.07162	1.05746	-1.69393
H	0	3.27242	1.5593	-3.54877
H	0	2.03336	1.44724	-2.29286
H	0	-1.61651	-0.22372	-2.62788
H	0	-0.40113	0.86682	-3.30941
H	0	0.10384	-2.14998	-2.83441
H	0	0.84339	-0.19545	-5.09568
H	0	1.23841	-2.00021	-4.99992
H	0	3.23734	2.73937	-2.24314

II1:

C	0	2.02426	0.90376	0.48118
Ru	0	-0.16907	0.38594	0.17286
Cl	0	-0.61223	2.66919	0.89233
C	0	1.65798	0.97774	-0.8661
C	0	1.12545	-0.21171	-1.47045
C	0	0.46271	-0.19121	-2.83147
C	0	-0.58963	0.92835	-2.88692
C	0	-1.35607	0.99175	-1.5827
C	0	-1.96989	-0.17467	-1.00505
C	0	-2.45488	-0.07628	0.2915
O	0	-0.0239	-1.44103	0.92172
C	0	0.96458	-2.43614	0.88319
C	0	0.70253	-3.41622	1.99883
C	0	1.6008	-3.77103	2.9166
H	0	2.2079	1.81434	1.03966
H	0	2.39728	-0.02135	0.90876
H	0	1.55456	1.94717	-1.34529
H	0	1.58488	-1.1539	-1.18509

H	0	1.209	-0.06949	-3.62887
H	0	-0.00756	-1.1657	-3.00327
H	0	-1.27016	0.78123	-3.73731
H	0	-0.10651	1.89717	-3.05157
H	0	-1.80217	1.95181	-1.33848
H	0	-1.85171	-1.15308	-1.4643
H	0	-2.76739	0.87928	0.70111
H	0	-2.70327	-0.9729	0.84811
H	0	0.92054	-2.97893	-0.08038
H	0	1.9927	-2.04654	0.98218
H	0	-0.30196	-3.83661	2.01649
H	0	2.60484	-3.3525	2.92463
H	0	1.37012	-4.49514	3.69248

TS12:

C	0	-0.13568	-0.39464	-2.21797
Ru	0	0.30133	-0.4182	0.00988
Cl	0	2.07075	-1.97475	-0.5396
C	0	0.64022	0.70601	-1.83965
C	0	0.08788	1.57151	-0.83886
C	0	0.90311	2.64422	-0.1486
C	0	2.21842	2.04933	0.38068
C	0	1.96746	0.67636	0.97191
C	0	0.94619	0.45259	1.95595
C	0	0.60916	-0.86011	2.26941
O	0	-1.64528	-0.57202	0.31507
C	0	-3.01522	-0.68056	0.53113
C	0	-3.84091	0.19999	-0.37653
C	0	-4.69306	1.13275	0.05004
H	0	0.31099	-1.19804	-2.79222
H	0	-1.2184	-0.34835	-2.17461
H	0	1.68977	0.76078	-2.1143
H	0	-0.98982	1.72309	-0.86077
H	0	1.09491	3.48489	-0.83007
H	0	0.30882	3.0537	0.67526
H	0	2.68284	2.72217	1.11515
H	0	2.94246	1.94579	-0.43419
H	0	2.81535	-0.00191	0.98085
H	0	0.29257	1.26321	2.27139
H	0	1.329	-1.66538	2.15879
H	0	-0.29152	-1.06938	2.83578
H	0	-3.28368	-1.73667	0.35142
H	0	-3.28383	-0.46407	1.58159
H	0	-3.7021	0.03709	-1.446
H	0	-4.84885	1.31334	1.11176
H	0	-5.27308	1.74281	-0.63667

2-propen-1-ol:

C	0.49233	0.1025	-1.50822
C	-0.60672	0.01917	-0.76025
C	-0.61787	0.01968	0.74681
O	0.66581	-0.04525	1.34293
H	0.44682	0.08982	-2.59229
H	1.47309	0.20229	-1.05284
H	-1.58613	-0.06154	-1.23217
H	-1.27041	-0.79665	1.10301
H	-1.07151	0.94991	1.11323
H	1.07531	-0.86993	1.04751

1-propen-1-ol:

C	0.13762	-0.84965	0.21281
C	1.56499	-0.38422	0.13147
C	-0.9573	-0.11018	0.00469
O	-1.0289	1.2135	-0.32344
H	-0.02732	-1.89287	0.46625
H	2.12749	-0.94515	-0.62507
H	1.65964	0.67735	-0.1278
H	2.08751	-0.52367	1.08588
H	-1.95486	-0.53087	0.08505
H	-0.13303	1.57145	-0.39071

Propanal:

C	0.84879	-0.19255	-0.04315
O	1.72937	0.46484	0.46498
C	-0.49957	0.34403	-0.4681
C	-1.65934	-0.48967	0.09854
H	0.99177	-1.28294	-0.2346
H	-0.56325	1.39375	-0.16753
H	-0.53009	0.30689	-1.56722
H	-2.61782	-0.12929	-0.28436
H	-1.69039	-0.43334	1.19091
H	-1.5645	-1.54464	-0.18078

Table S2. B3LYP/6-31G(d,p)+LANL2DZ at 348.15 K.

Structure	U(au)	H(au)	S (cal/K·mol)	G(au)
I0	-1058.691703	-1058.411598	129.7	-1058.483529
TS1	-1058.681804	-1058.403759	132.9	-1058.477475
I1	-1058.687229	-1058.407977	137.5	-1058.484247
TS2	-1058.687016	-1058.408981	132.6	-1058.482541
I2	-1058.684736	-1058.407034	136.9	-1058.483003
TS3	-1058.670678	-1058.397389	133.3	-1058.471369
I3	-1058.681826	-1058.406183	139.6	-1058.483614
TS4	-1058.671081	-1058.397115	138.7	-1058.474072
I4	-1058.680501	-1058.404829	137.7	-1058.481202
TS5	-1058.662518	-1058.388595	135.7	-1058.463870
I5	-1058.673190	-1058.397503	138.1	-1058.474122
TS6	-1058.658891	-1058.386006	131.4	-1058.458935
I6	-1058.706923	-1058.427910	139.8	-1058.505471
TS7	-1058.705631	-1058.427375	132.0	-1058.500608
I7	-1058.708800	-1058.429167	132.9	-1058.502901
TS8	-1251.837745	-1251.464540	175.1	-1251.561690
I8	-1251.850181	-1251.475252	169.3	-1251.569188
TS9	-1251.840547	-1251.466916	168.2	-1251.560227
I9	-1251.847365	-1251.472817	172.7	-1251.568627
TS10	-1251.836258	-1251.465779	165.9	-1251.557849
I10	-1251.836277	-1251.463830	170.0	-1251.558148
TS11	-1251.821453	-1251.448314	171.9	-1251.543667
II1	-1058.686403	-1058.407384	137.9	-1058.483913
TS12	-1058.669338	-1058.392929	131.8	-1058.466029
2-propen-1-ol	-193.124026	-193.031394	71.7	-193.071150
1-propen-1-ol	-193.135592	-193.042916	73.9	-193.083932
Propanal	-193.151756	-193.059671	73.8	-193.100638

Table S3. B3LYP/6-31G(d,p)+LANL2DZ (kcal/mol) at 348.15 K.

STRUCTURE	ΔU	ΔH	ΔS	ΔG
I0 + 2-propen-1-ol	0.0	0.0	0.0	0.0
TS1 + 2-propen-1-ol	6.2	4.9	3.2	3.8
I1 + 2-propen-1-ol	2.8	2.3	7.8	-0.5
TS2 + 2-propen-1-ol	2.9	1.6	2.9	0.6
I2 + 2-propen-1-ol	4.4	2.9	7.3	0.3
TS3 + 2-propen-1-ol	13.2	8.9	3.7	7.6
I3 + 2-propen-1-ol	6.2	3.4	9.9	-0.1
TS4 + 2-propen-1-ol	12.9	9.1	9.1	5.9
I4 + 2-propen-1-ol	7.0	4.2	8.0	1.5
TS5 + 2-propen-1-ol	18.3	14.4	6.0	12.3
I5 + 2-propen-1-ol	11.6	8.8	8.4	5.9
TS6 + 2-propen-1-ol	20.6	16.1	1.8	15.4
I6 + 2-propen-1-ol	-9.6	-10.2	10.1	-13.8
TS7 + 2-propen-1-ol	-8.7	-9.9	2.3	-10.7
I7 + 2-propen-1-ol	-10.7	-11.0	3.2	-12.2
TS8	-13.8	-13.5	-26.2	-4.4
I8	-21.6	-20.2	-32.0	-9.1
TS9	-15.6	-15.0	-33.2	-3.5
I9	-19.9	-18.7	-28.7	-8.8
TSI10	-12.9	-14.3	-35.4	-2.0
I10	-12.9	-13.1	-31.4	-2.2
TS11	-3.6	-3.3	-29.5	6.9
I11 + 1-propen-1-ol	-3.9	-4.6	10.5	-8.3
I11 + propanal	-14.1	-15.1	10.4	-18.7
TSI2 + propanal	-3.4	-6.0	4.2	-7.5
I1 + propanal	-14.6	-15.5	9.9	-19.0

Table S4. B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p)+LANL2DZ (au) at 348.15 K. Solvation energies in kcal/mol.

Structure	U	H	G	$\Delta G^{\text{solv}}(\text{H}_2\text{O})$	$\Delta G^{\text{solv}}(\text{THF})$
I0	-1058.850031	-1058.569927	-1058.641858	3.0	3.0
TS1	-1058.841514	-1058.563469	-1058.637185	7.4	6.7
I1	-1058.847982	-1058.568730	-1058.645000	6.8	6.5
TS2	-1058.847878	-1058.569843	-1058.643403	7.1	6.8
I2	-1058.845033	-1058.567332	-1058.643301	5.0	4.6
TS3	-1058.831435	-1058.558146	-1058.632126	4.3	4.1
I3	-1058.842971	-1058.567328	-1058.644759	2.7	3.1
TS4	-1058.833006	-1058.559040	-1058.635997	3.9	4.0
I4	-1058.841607	-1058.565935	-1058.642308	2.3	2.6
TS5	-1058.824390	-1058.550467	-1058.625742	2.8	3.3
I5	-1058.834218	-1058.558531	-1058.635150	3.7	3.7
TS6	-1058.820139	-1058.547254	-1058.620183	4.9	4.6
I6	-1058.865887	-1058.586874	-1058.664435	9.1	8.1
TS7	-1058.863264	-1058.585008	-1058.658241	7.1	6.4
I7	-1058.866389	-1058.586756	-1058.660490	4.8	4.4
TS8	-1252.054658	-1251.681453	-1251.778603	15.3	14.0
I8	-1252.065936	-1251.691007	-1251.784943	12.0	10.8
TS9	-1252.056608	-1251.682977	-1251.776288	10.2	10.0
I9	-1252.063100	-1251.688552	-1251.784362	11.8	10.7
TS10	-1252.050619	-1251.680140	-1251.772210	12.1	10.9
I10	-1252.050908	-1251.678462	-1251.772780	12.1	10.9
TS11	-1252.038773	-1251.665634	-1251.760987	14.7	13.2
II1	-1058.847358	-1058.568339	-1058.644868	6.2	6.2
TS12	-1058.832206	-1058.555797	-1058.628897	9.5	8.7
2-propen-1-ol	-193.182050	-193.089418	-193.129174	0.9	0.8
1-propen-1-ol	-193.192293	-193.099618	-193.140634	1.3	1.0
Propanal	-193.205892	-193.113807	-193.154774	1.1	1.0

Table S5. B3LYP/6-311+G(d,p)//B3LYP/6-31G(d,p)+LANL2DZ (kcal/mol) at 348.15 K.

STRUCTURE	ΔU	ΔH	ΔG	$\Delta G^{\text{total}}(\text{H}_2\text{O})$	$\Delta G^{\text{total}}(\text{THF})$
I0 + 2-propen-1-ol	0.0	0.0	0.0	0.0	0.0
TS1 + 2-propen-1-ol	5.3	4.1	2.9	7.3	6.7
I1 + 2-propen-1-ol	1.3	0.8	-2.0	1.9	1.6
TS2 + 2-propen-1-ol	1.4	0.1	-1.0	3.1	2.8
I2 + 2-propen-1-ol	3.1	1.6	-0.9	1.0	0.7
TS3 + 2-propen-1-ol	11.7	7.4	6.1	7.4	7.2
I3 + 2-propen-1-ol	4.4	1.6	-1.8	-2.1	-1.7
TS4 + 2-propen-1-ol	10.7	6.8	3.7	4.6	4.7
I4 + 2-propen-1-ol	5.3	2.5	-0.3	-1.0	-0.7
TS5 + 2-propen-1-ol	16.1	12.2	10.1	9.9	10.4
I5 + 2-propen-1-ol	9.9	7.2	4.2	4.9	4.9
TS6 + 2-propen-1-ol	18.8	14.2	13.6	15.5	15.2
I6 + 2-propen-1-ol	-9.9	-10.6	-14.2	-8.1	-9.1
TS7 + 2-propen-1-ol	-8.3	-9.5	-10.3	-6.2	-6.9
I7 + 2-propen-1-ol	-10.3	-10.6	-11.7	-9.9	-10.3
TS8	-14.2	-13.9	-4.8	6.6	5.4
I8	-21.2	-19.9	-8.7	-0.6	-1.8
TS9	-15.4	-14.8	-3.3	3.1	2.9
I9	-19.5	-18.3	-8.4	-0.5	-1.4
TSI10	-11.6	-13.0	-0.7	7.4	6.4
I10	-11.8	-12.0	-1.1	7.1	6.1
TS11	-4.2	-3.9	6.3	17.1	15.7
I11 + 1-propen-1-ol	-4.8	-5.4	-8.3	-4.7	-4.9
I11 + propanal	-13.3	-14.3	-18.0	-14.6	-14.5
TSI2 + propanal	-3.8	-6.4	-7.9	-1.2	-2.1
I1 + propanal	-13.7	-14.6	-18.0	-14.0	-14.3

Figure S1. B3LYP/6-31G(d,p)+LANL2DZ structures (distances in Å).

Figure S1 (cont.).

Figure S1 (cont.).

Figure S1 (cont.).

Figure S1 (cont.).

Figure S1 (cont.).