Supporting Information

Dehydrogenation of Formic Acid Using Iridium-NSi Species as Catalyst Precursors

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General Procedure

Catalytic reactions were carried out on a microreactor (Man on the Moon series X102 Kit) with a total volume of 19 mL. Under an argon atmosphere, the reactor was filled with the desired amount of base (sodium formate or NEt_3) and of formic acid. The reactor was then closed and heated to the desire temperature in an oil bath. When the system is stabilized, the desired amount of complex, dissolved in a small amount of formic acid, is then injected with a microsyringe.

SF concentration effect: 500 µL of FA, 0.025 mol % of **1** (2.6 mg, 3.25 10^{-3} mmol), and 2.5 mol % of SF (22.5 mg, 0.33 mmol), or 5 mol % of SF (45.0 mg, 0.66 mmol), or 10 mol % of SF (90.0 mg, 1.32 mmol) at 80 ºC.

Complex 1 concentration effect: 500 µL of FA, 5 mol % of sodium formate (45.0 mg, 0.66 mmol), 0.025 mol % of **1** (2.6 mg, 3.25 10^{-3} mmol), or 0.05 mol % of **1** (5.2 mg, 6.50 10^{-3} mmol), or 0.1 mol % (10.4 mg, 0.013 mmol) at 80 ºC.

Effect of the silicon substituents in the FA dehydrogenation with SF as base: 500 µL of FA, 5 mol % of sodium formate (45.0 mg, 0.66 mmol), 0.025 mol % of **1** (2.6 mg, 3.25 10^{-3} mmol) or 0.025 mol % of **2** (2.25 mg, 3.25 10^{-3} mmol) at 80 ºC.

Effect of the silicon substituents in the FA dehydrogenation with NEt_3 as base: 500 µL of FA, 10 mol % of NEt_3 (186 µL, 1.32 mmol), 0.1 mol % of **1** (10.4 mg, 0.013 mmol) or 0.1 mol % of **2** (9 mg, 0.013 mmol mmol) at 80 ºC.

NEt_3 concentration effect: 500 µL of FA, 0.1 mol % of **2** (9 mg, 0.013 mmol) and 1.0 mol % (18.6 µL, 0.13 mmol), 2.5 mol % (46.5 µL, 0.32 mmol), 5.0 mol % (93 µL, 0.65 mmol) 10 mol % (186 µL, 1.32 mmol), 20 mol % (372 µL, 2.64 mmol) or 40 mol % (744 µL, 5.28 mmol) of NEt_3 at 80 ºC.

Temperature effect: 500 µL of FA, 0.1 mol % of **2** (9 mg, 0.013 mmol) and 10 mol % (186 µL, 1.32 mmol) of NEt_3 at different temperatures (from 40 to 100 ºC).

KIE Experiments: 250 µL of FA (HCOOH, HCOOD, DCOOH or DCOOD), 0.1 mol % of **2** (4.5 mg, 6.5 10^{-3} mmol) and 40 mol % (372 µL, 2.64 mmol) of NEt_3 at 80 ºC.

Studies of the black precipitated: Black precipitate was separated from the reaction medium and washed with distilled water and dried in vacuo for its measurements in TEM spectroscopy.

FT-IR and GC of gaseous product: FT-IR: Gaseous products from the catalysis were collected in a rubber balloon that was attached to a Schlenk containing the reaction mixture: 500 µL of FA, 0.1 mol % of **2** (9 mg, 0.013 mmol mmol) and 10 mol % of NEt_3 (186 µL, 1.32 mmol) at 80ºC. The gas sample was transferred to the cell and the FT-IR spectrum was acquired. GC: The gaseous mixture was taken directly from the microreactor and injected into the cell.

Mercury drop test: A drop of mercury was added to the microreactor together with 450 µL of FA, and 10 mol % (186 µL, 1.32 mmol) of NEt_3, the system was heated at 80ºC. When the system is stabilized, a solution of 0.1 mol % of **2** (9 mg, 0.013 mmol) in 50 µL of FA was injected to the reaction mixture.

NMR Studies

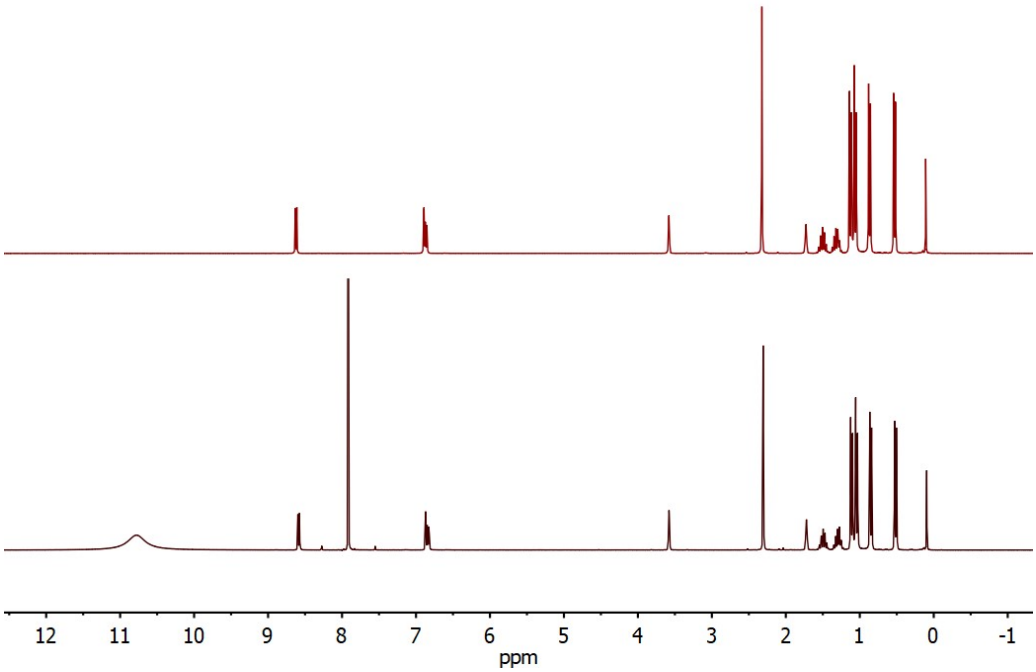


Figure S1. (up) ^{1}H NMR spectrum of **1** in thf-d_8; (down) ^{1}H NMR spectrum of **1** and HCOOH (20 eq.) in thf-d_8 after heating at 323 K for 3 h.

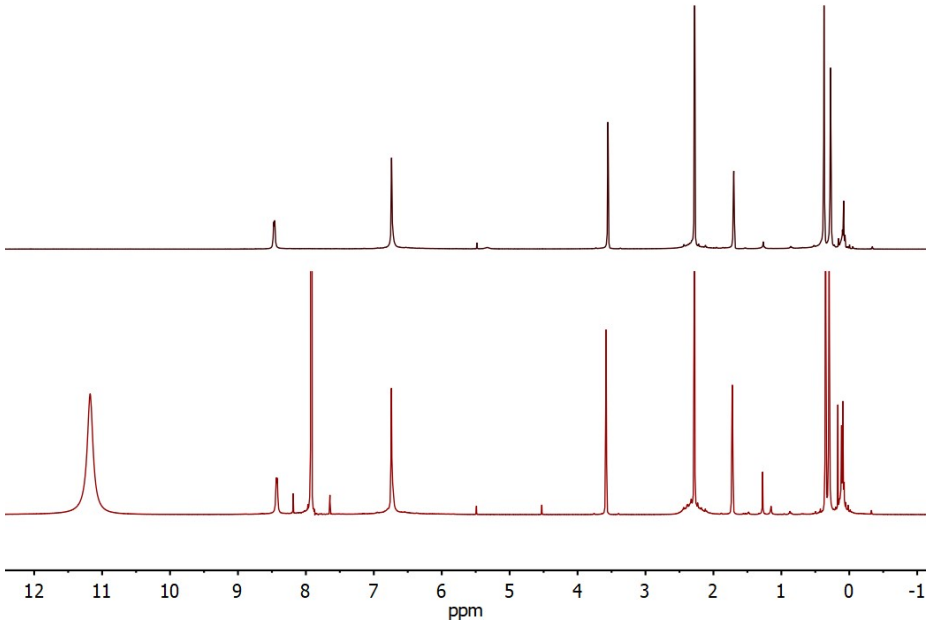


Figure S2. (up) ^{1}H NMR spectrum of **2** in thf-d_8; (down) ^{1}H NMR spectrum of **2** and HCOOH (20 eq.) in thf-d_8 after heating at 323 K for 3 h.

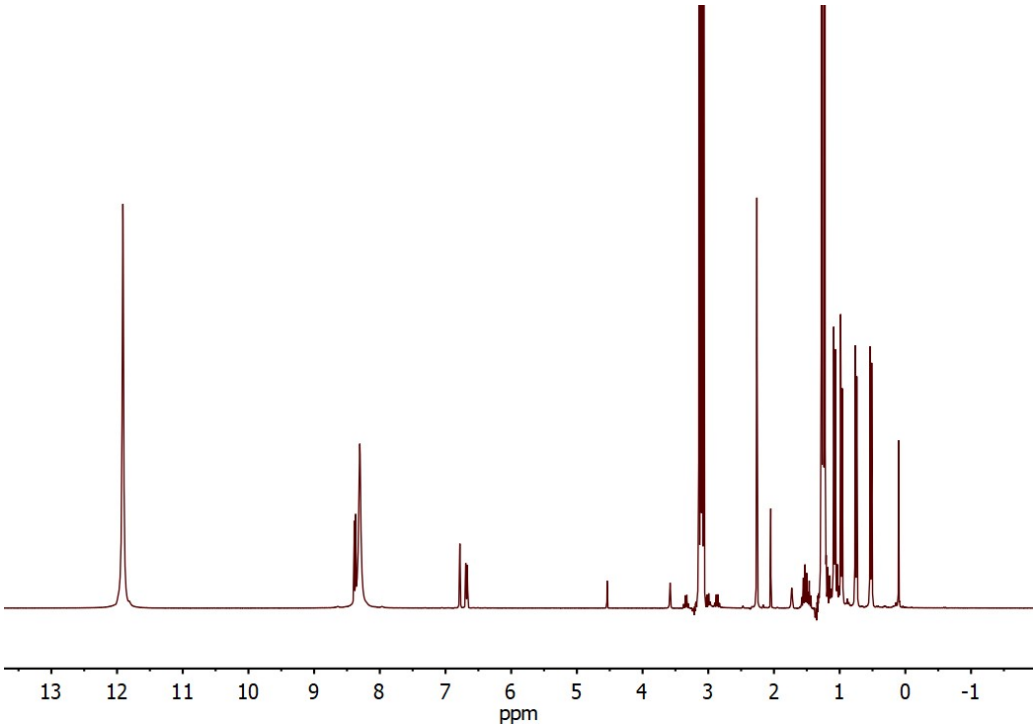


Figure S3. ^{1}H NMR spectrum of **1**, HCOOH (20 eq.), Et_3N (40 mol% to FA) in thf-d_8, after heating at 323 K for 30 min.

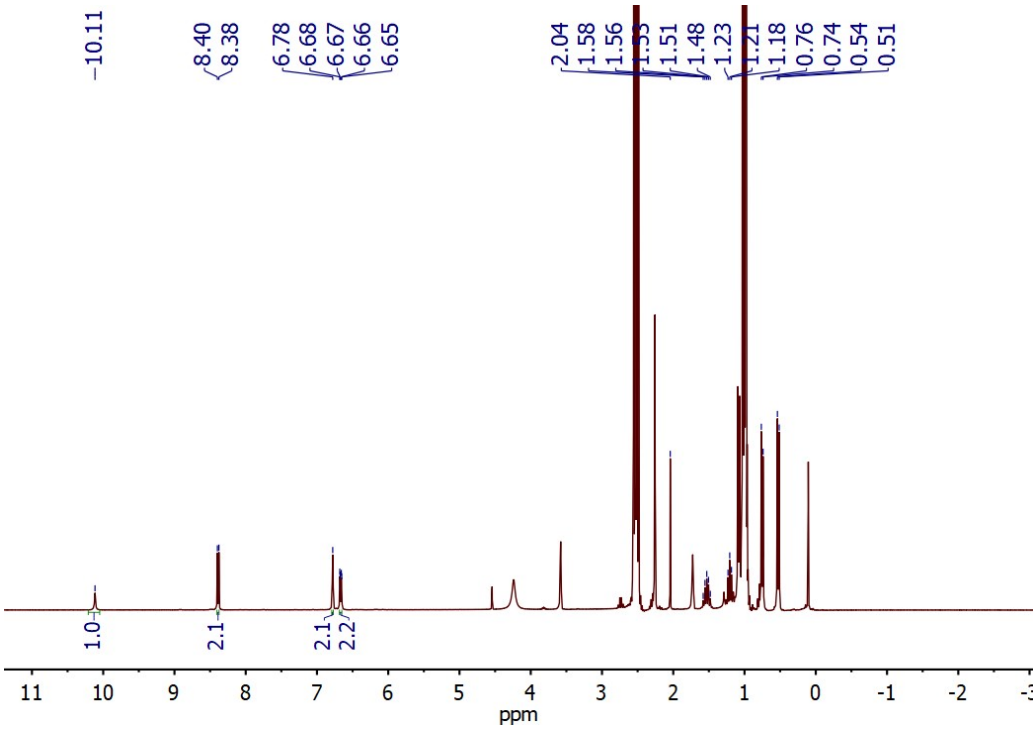


Figure S4. ^{1}H NMR spectrum of **1**-catalyzed FADH reaction in thf-d_8 once all the FA has been consumed. The only Ir-compound observed is species **3**.

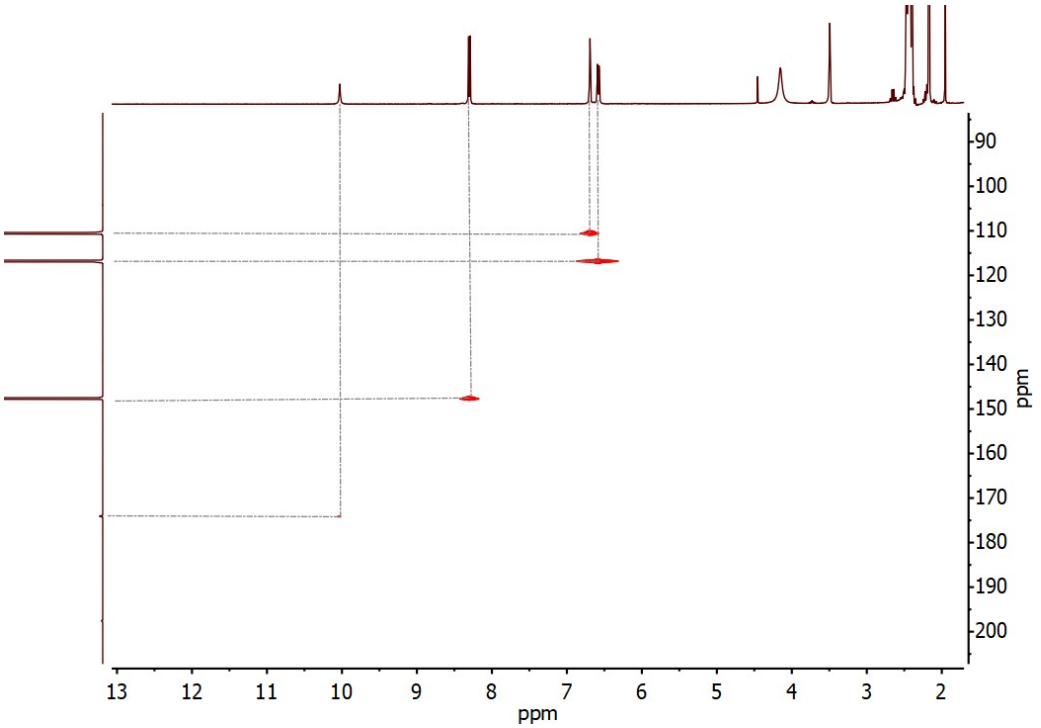


Figure S5. ^{1}H-^{13}C HSQC NMR spectrum of **3** solutions in thf-d_8.

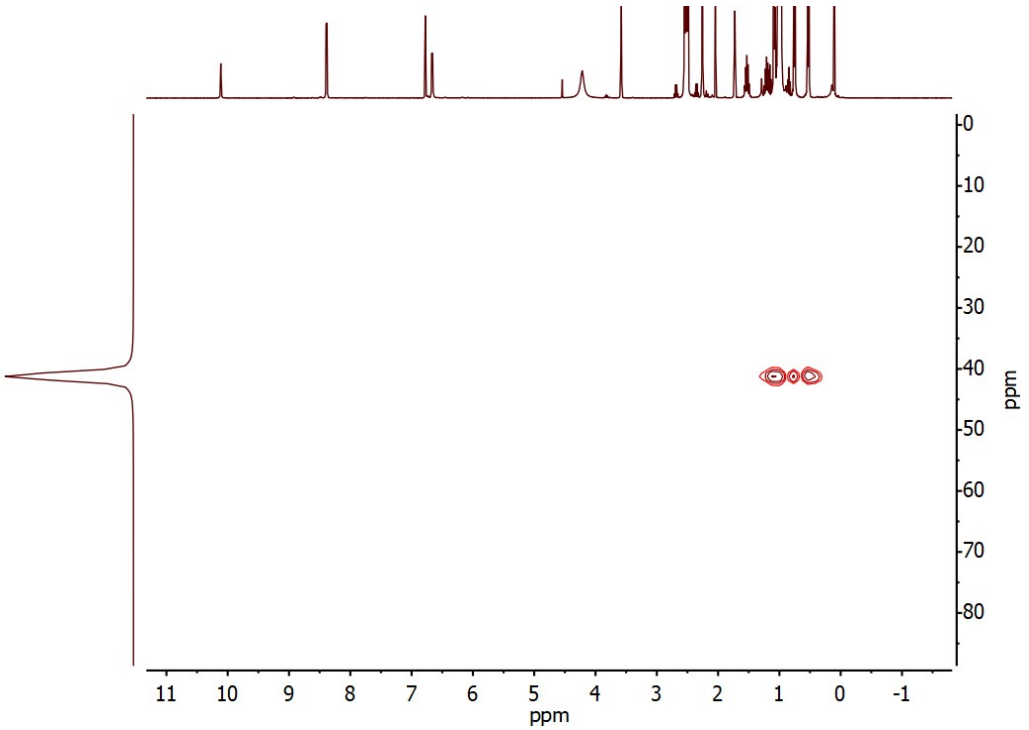


Figure S6. ^{1}H-^{29}Si HSQC NMR spectrum of **3** solutions in thf-d_8.

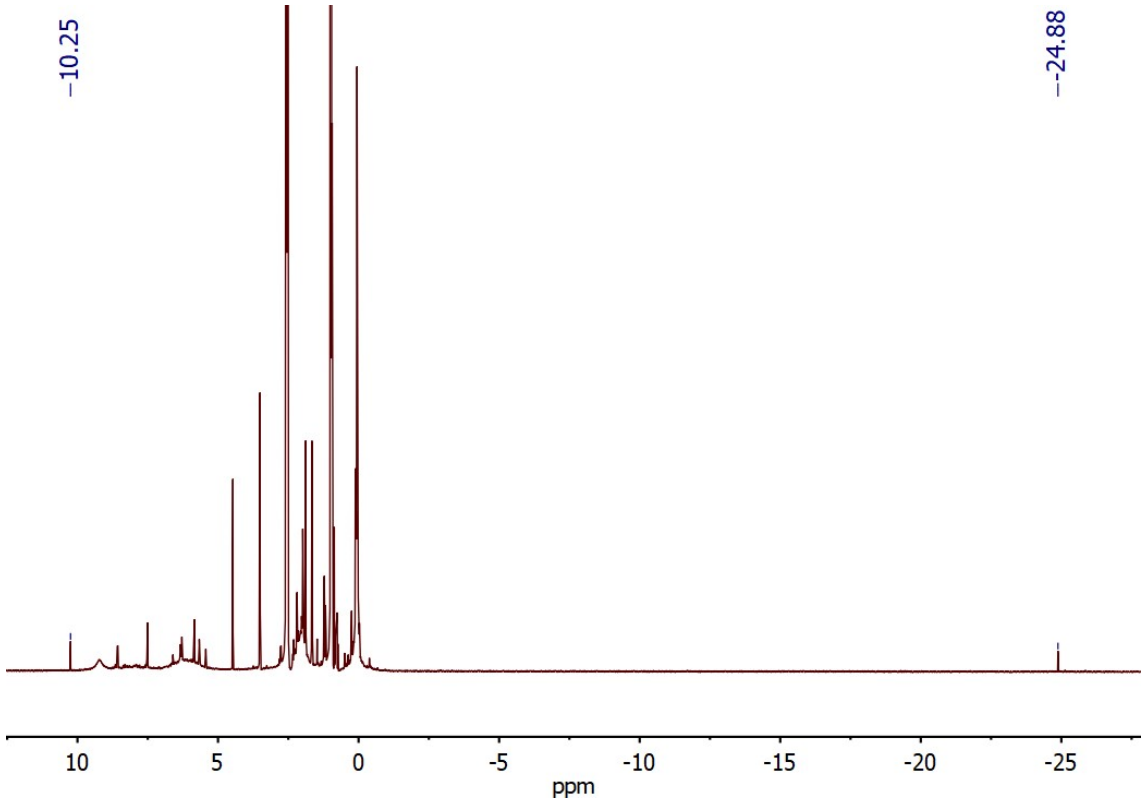


Figure S7. ^{1}H NMR spectrum of **2**-catalyzed FADH reaction in thf-d_8 once all the FA has been consumed.

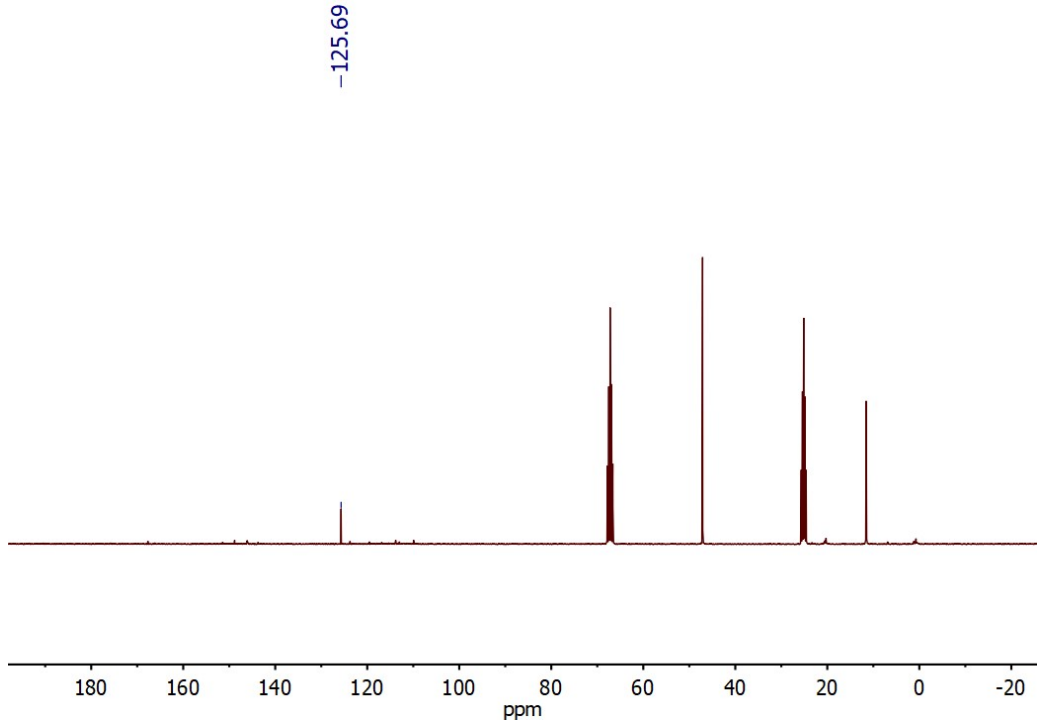


Figure S8. ^{1}H NMR spectrum of **2**-catalyzed FADH reaction in thf-d_8 once all the FA has been consumed.

TON and TOF determination

H_2 pressure: $P_{H2} = \frac{P_{measured}}{2}$

Amount of H_2 formed calculated with the Ideal Gas Law: $n_{H2} = \frac{P_{H2}V}{RT}$;

Total Volume = 0.019 L; R constant= 0.08314 bar L mol^{-1} K^{-1}

$$TON = \frac{n_{H2}}{n_{cat}}$$

$$TOF = \frac{TON}{t}$$

Effect of the silicon substituents with NEt_3 as base

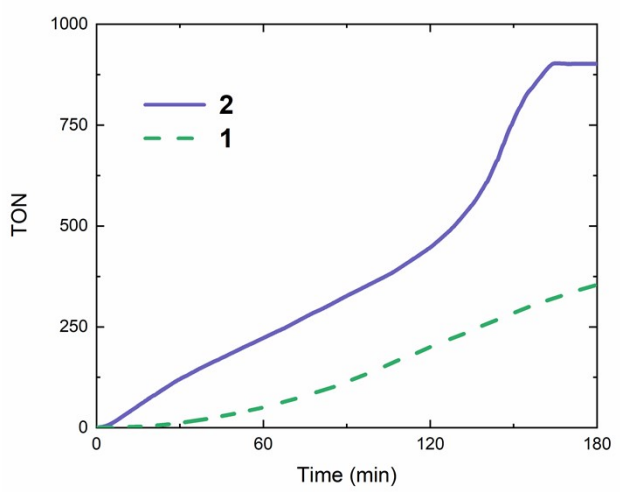


Figure S9. TON vs time comparison of the **1**- or **2**-catalyzed (0.1 mol %) solventless dehydrogenation of formic acid using triethylamine (10 mol %) at 80ºC.

NEt_3 concentration effect

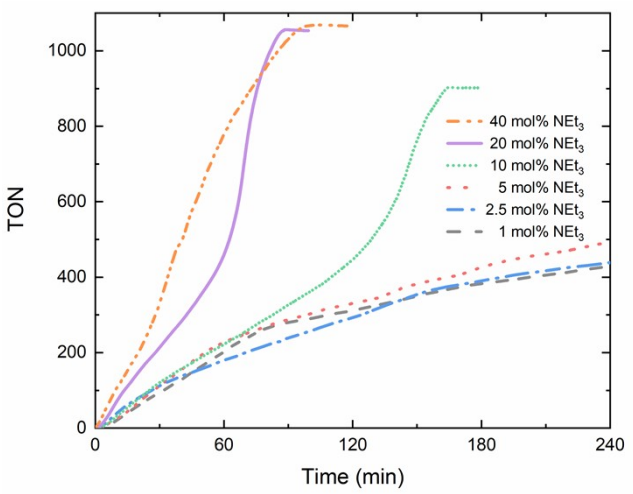


Figure S10. TON vs time representation of the 2-catalyzed (0.1 mol %) solvent-free FA dehydrogenation with different concentrations of NEt3 at 80ºC

Temperature effect

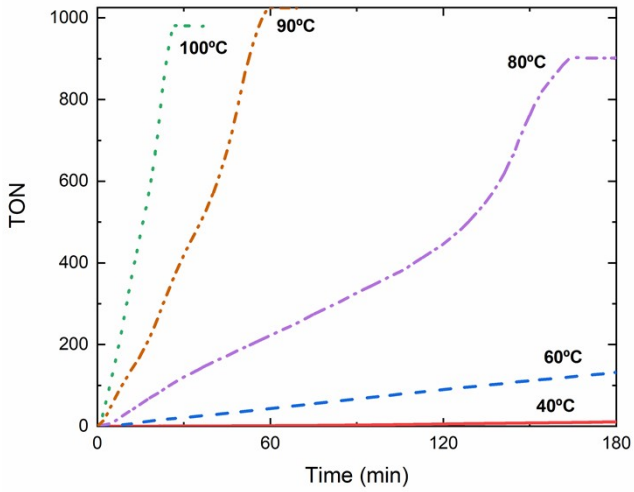


Figure S11. TON vs time representation of the **2**-catalyzed (0.1 mol %) solvent-free FA dehydrogenation with 10 mol % of NEt_3 at different temperatures.

2-Catalysed FA dehydrogenation with optimized conditions

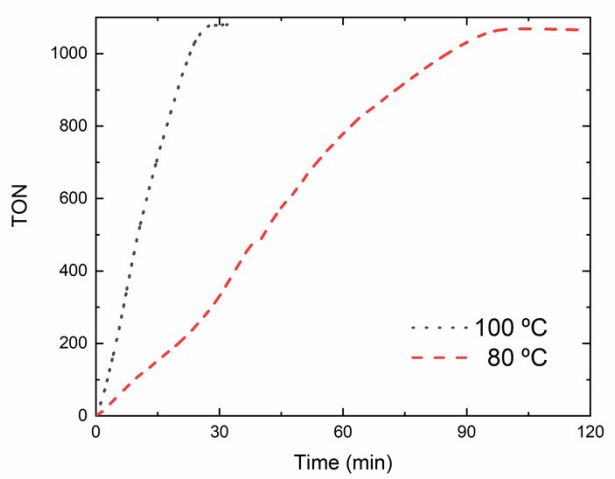


Figure S12. TON vs time representation of the 2-catalysed FA solvent-less dehydrogenation with NEt_3 (40 mol %) at 80 and 100 ºC.

FT-IR and GC of gaseous product

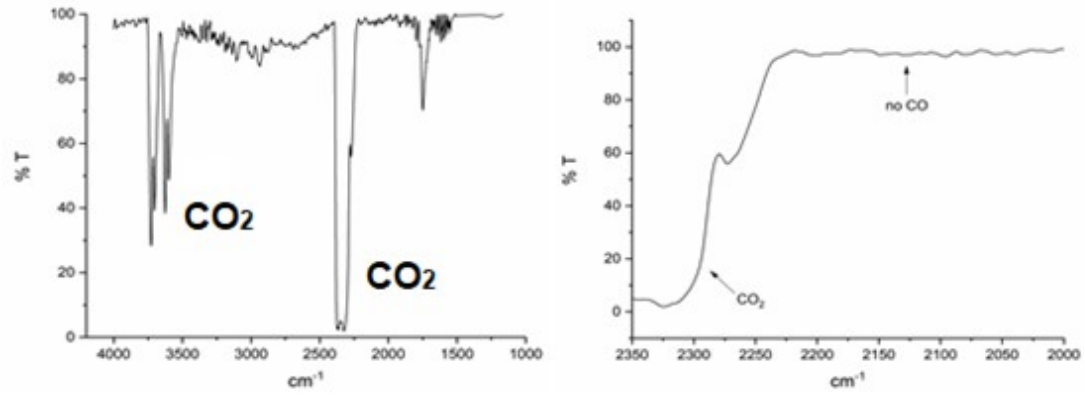


Figure S13. (Left) FT-IR spectrum of the gaseous product. (Right) Detail from the FT-IR spectrum showing the absence of CO signal.

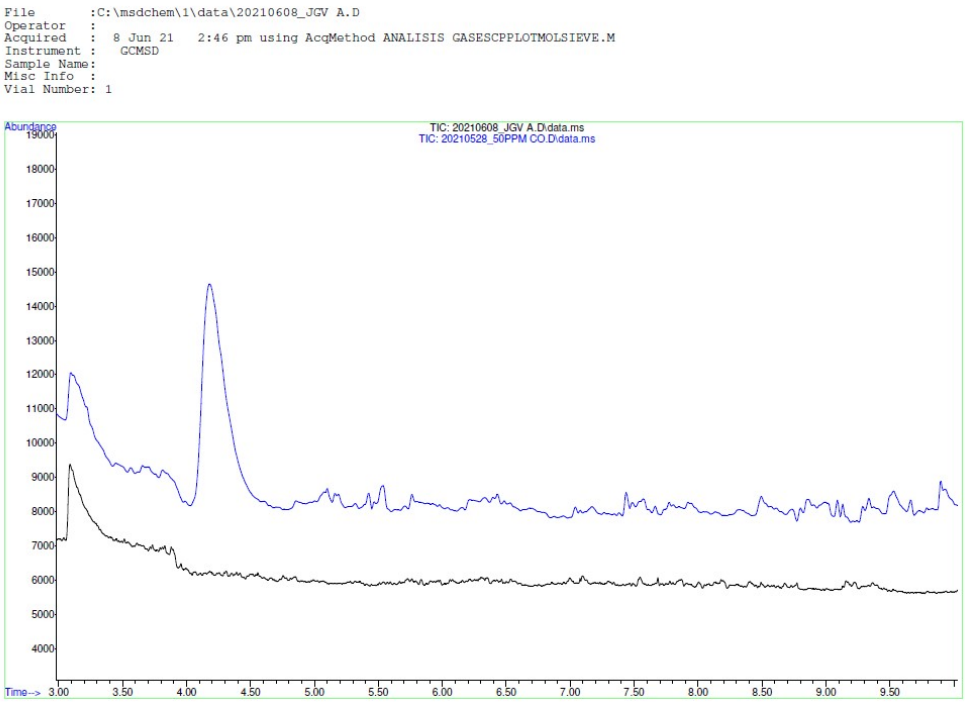


Figure S14. Gas chromatography of the gaseous mixture formed in the **2**-catalyzed (0.1 mol %) solvent-free FA dehydrogenation with 40 mol % of NEt_3 at 80ºC

Arrhenius Plot

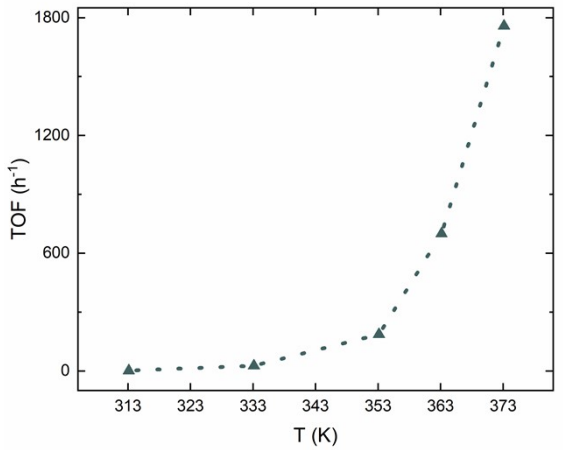


Figure S15. TOF_{5min} (h^{-1}) versus T (K) from the **2**-catalyzed solvent-free FA dehydrogenation.

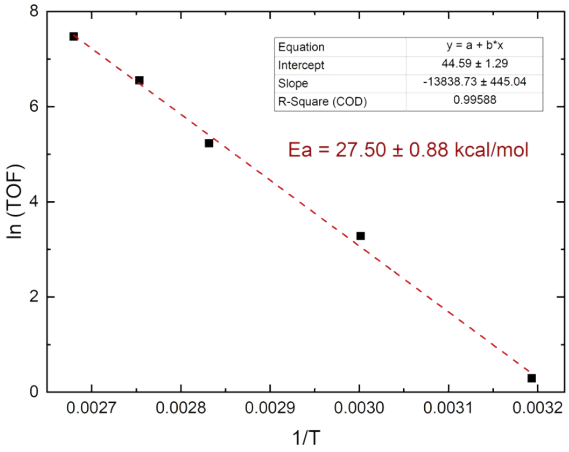
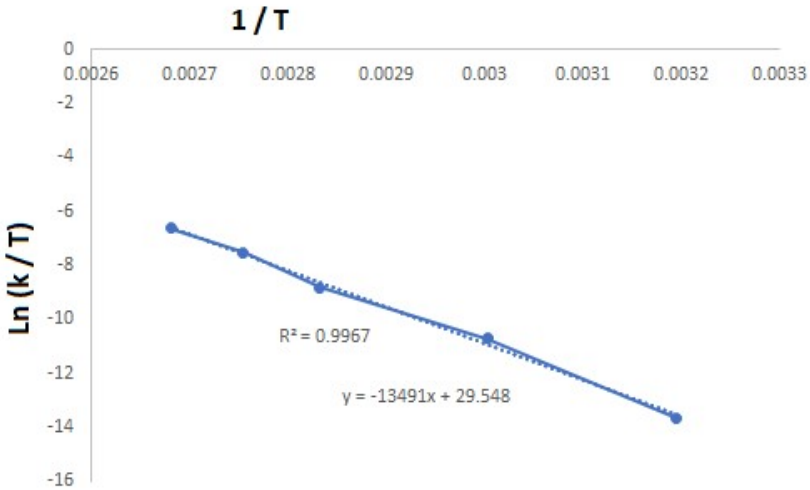


Figure S16. Arrhenius plot of the **2**-catalysed solvent-free FA dehydrogenation (apparent activation energy of 27.5 kcal mol^{-1})

Eyring plot



Data:

Point	T (°C)	T (K)	1/T (K^{-1})	k (h^{-1})	k (s^{-1})	k/T	Ln (k/T)
1	40	313.13	0.003194	1.3334	3.704 10^{-4}	1.183 10^{-6}	-13.65
2	60	333.13	0.003002	26.5894	7.386 10^{-3}	2.217 10^{-5}	-10.717
3	80	353.13	0.002832	186.3074	5.175 10^{-2}	1.465 10^{-4}	-8.828
4	90	363.13	0.002754	699.4523	1.943 10^{-1}	5.351 10^{-4}	-7.533
5	100	373.13	0.002680	1757.6207	4.882 10^{-1}	1.308 10^{-3}	-6.639

Figure S17. Representation of LnK versus 1/T; y = -13491x + 29.548; R2 = 0.9967; Activation Enthalpy = 112.2 ±1.7 kJ mol-1 (26.8 ±0.4 kcal mol^{-1}) Activation Entropy = 47.7 ±6 J K^{-1} mol^{-1} (11.4 ±1.5 cal K^{-1} mol^{-1}). The errors in the activation parameters were calculated following error propagation formulas (P. M. Morse, M. D. Spencer, S. R. Wilson, G. S. Girolami, Organometallics, 1994, 13, 1646-1655).

KIE Experiments

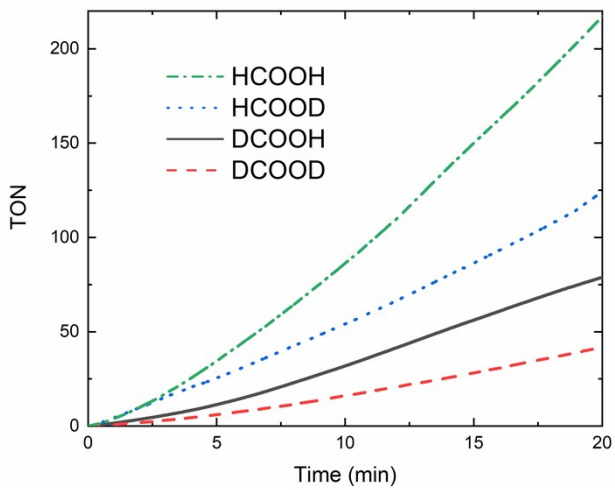


Figure S18. TON vs time representation of the **2**-catalyzed (0.1 mol %) solvent-free FA dehydrogenation with 40 mol % of NEt_3 at 80ºC

Studies of the black precipitate

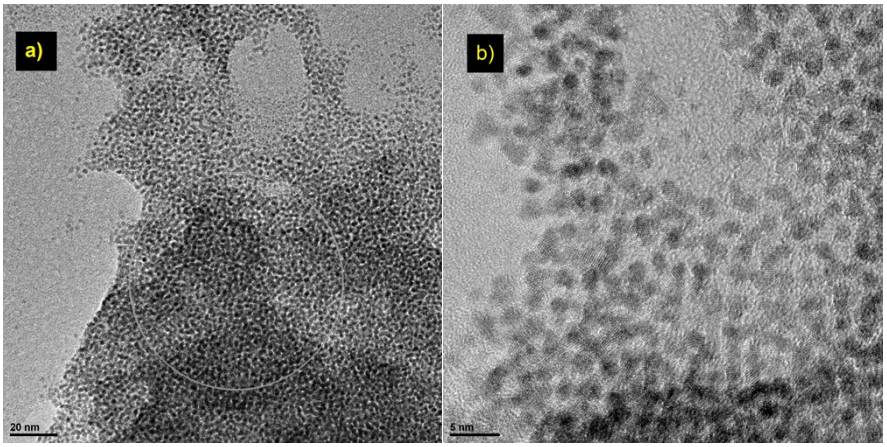


Figure S19. Transmission Electronic Microscopy images of the dark iridium nanoparticles. a) TEM image (20 nm). b) Closer image showing lattice fringes (5 nm).

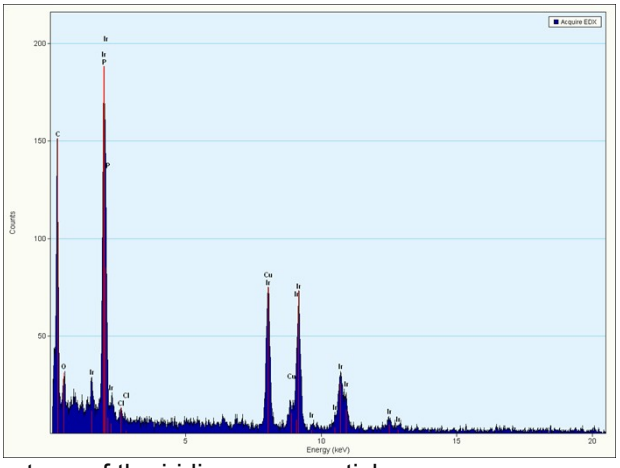


Figure S20. EDX spectrum of the iridium nanoparticles.

Mercury drop test

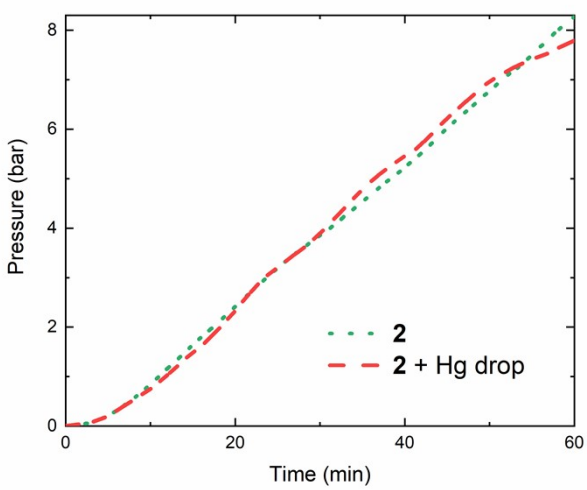


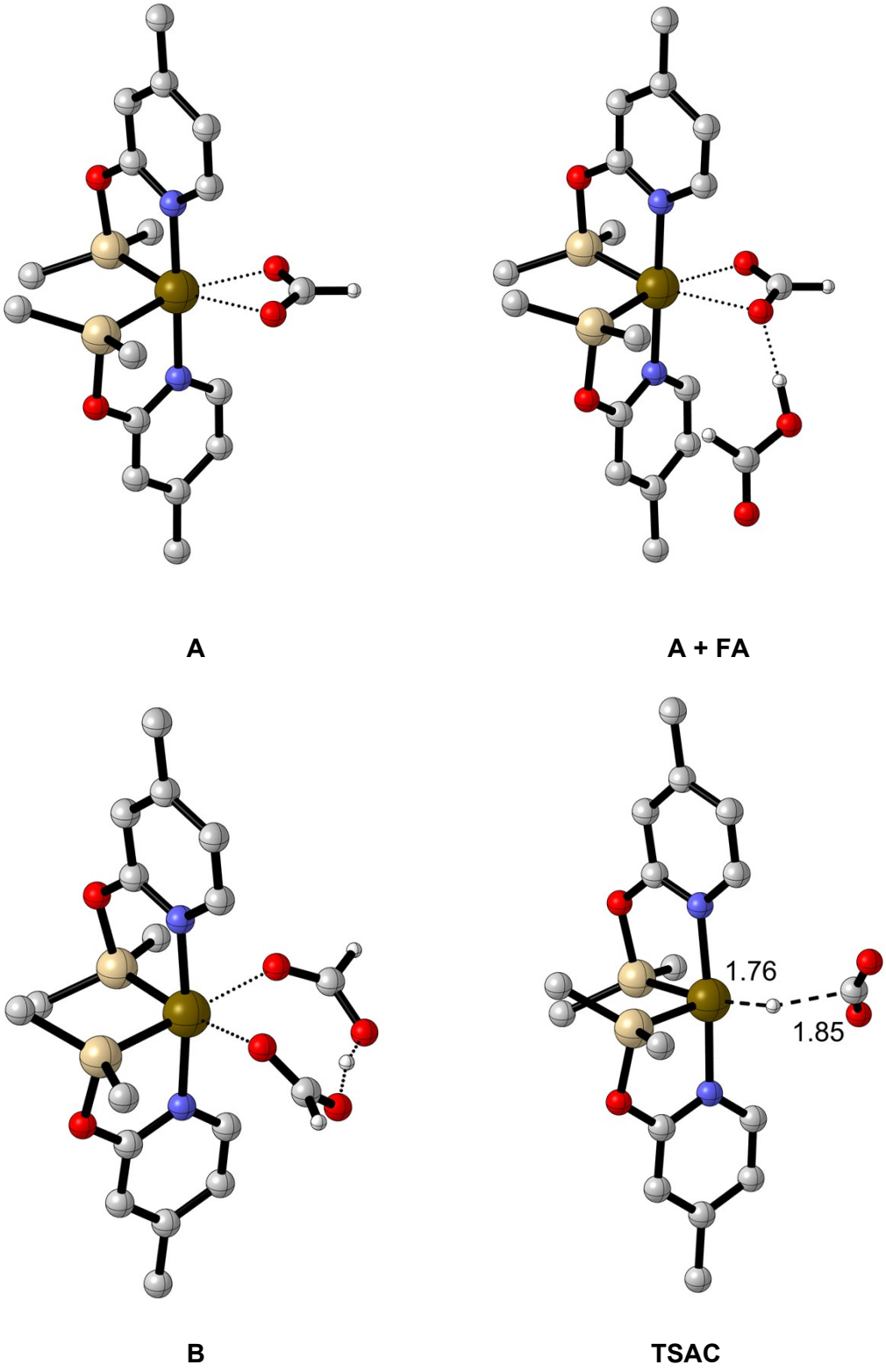
Figure S21. Pressure vs time representation of the **2**-catalysed (0.1 mol %) solvent-free dehydrogenation of FA with NEt_3 (10 mol %) at 80ºC both in presence and absence of a mercury drop.

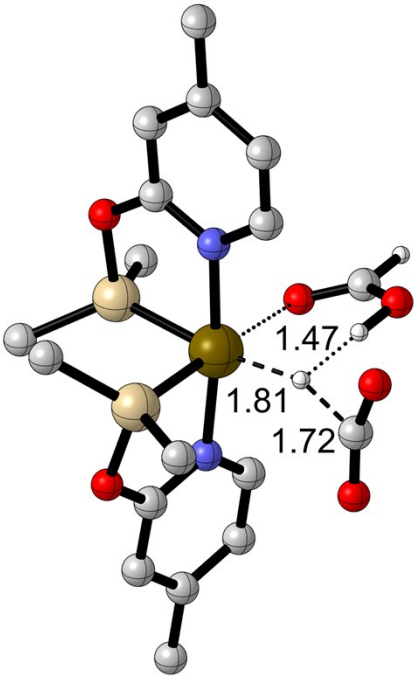
DFT Calculations

Table S1. Energetic values for all DFT calculated species. Geometrical optimizations performed at a B3LYP-D3(PCM)/def2-SVP level, E(DZ). Single point energies B3LYP-D3(BJ)/def2-TZVP, E(TZ). Frequencies were calculated at the same level than the optimization, G_{corr}, in the case of HCOOH the translational entropy contribution to the free energy was removed. Relative Gibbs free energies, ΔG, were calculated adding E(TZ) and G_{corr} and relative to **A** and isolated molecules. All absolute energies are given in a.u. and relative Gibbs free energies are given in kcal mol^{-1}.

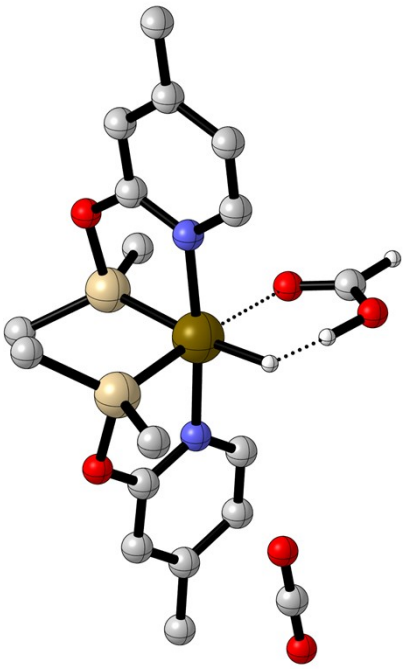
	E(DZ)	E(TZ)	G_{corr}	ΔG
A	-1756.1623	-1757.5897	0.3124	0.0
A + FA	-1945.8135	-1947.4654	0.3399	-9.8
B	-1945.8198	-1947.4656	0.3418	-8.7
TSAC	-1756.1136	-1757.5458	0.3061	23.6
TSBC	-1945.7719	-1947.4232	0.3368	14.7
C	-1945.7805	-1947.4325	0.3334	6.8
TSCA	-1945.7798	-1947.4320	0.3302	5.1
HCOOH	-189.6290	-189.8587	0.0260	
CO_2	-188.4447	-188.6740	-0.0136	
H_2	-1.1741	-1.1798	-0.0044	

Figure S22. Geometrical representation for the DFT optimized structures. Only the most relevant hydrogen atoms are shown for clarity and distances are given in Å.

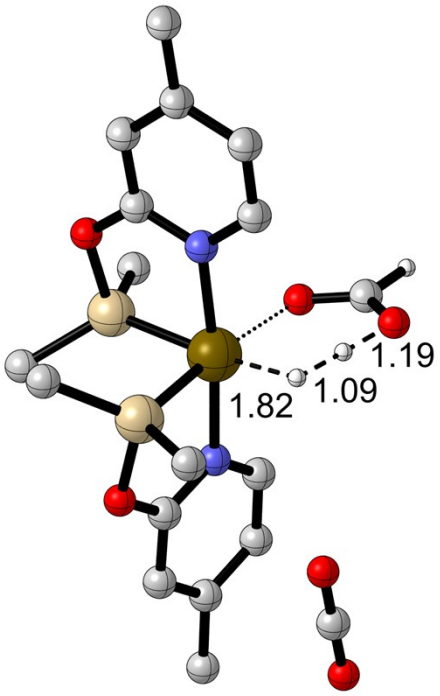




TSBC



C



TSCA

Table S2. Cartesian coordinates (XYZ data) for all DFT calculated species

51
A

77	0.000000	0.352515	-0.000003
7	-2.080661	0.328582	0.036758
6	-2.784214	1.163413	0.840753
6	-2.755177	-0.566472	-0.733808
6	-4.162184	1.141334	0.914708
1	-2.180464	1.858477	1.425185
6	-4.160037	-0.630614	-0.699480
6	-4.886371	0.220338	0.126605
1	-4.675704	1.835387	1.581623
1	-4.651035	-1.366142	-1.337496
7	2.080661	0.328582	-0.036762
6	2.755177	-0.566462	0.733815
6	2.784214	1.163405	-0.840765
6	4.160037	-0.630604	0.699488
6	4.162183	1.141326	-0.914720
1	2.180463	1.858462	-1.425205
6	4.886371	0.220338	-0.126606
1	4.651035	-1.366124	1.337514
1	4.675704	1.835373	-1.581640
8	-2.072630	-1.384300	-1.510681
8	2.072630	-1.384282	1.510697
14	-0.308537	-1.202831	-1.635441
14	0.308537	-1.202808	1.635457
6	-0.029411	-0.414006	-3.327601
1	1.054057	-0.313230	-3.509328
1	-0.455728	-1.035681	-4.132623
1	-0.474392	0.591255	-3.376839
6	0.337469	-2.967048	-1.718824
1	0.228416	-3.364612	-2.740892
1	1.407260	-2.993064	-1.454885
1	-0.201697	-3.630525	-1.029207
6	-0.337470	-2.967023	1.718862
1	0.201693	-3.630505	1.029246
1	-0.228409	-3.364580	2.740932
1	-1.407262	-2.993043	1.454930
6	0.029414	-0.413958	3.327606
1	-1.054054	-0.313174	3.509329
1	0.455726	-1.035622	4.132639
1	0.474399	0.591303	3.376828
8	-0.065937	2.485206	-1.106099
6	-0.000001	3.082773	-0.000019
1	-0.000002	4.198157	-0.000025
8	0.065936	2.485218	1.106067
6	-6.386760	0.172752	0.185330
1	-6.815839	1.146319	-0.101981
1	-6.796237	-0.598612	-0.480887
1	-6.727111	-0.035280	1.212603
6	6.386759	0.172747	-0.185336
1	6.815843	1.146341	0.101876
1	6.796241	-0.598555	0.480949
1	6.727101	-0.035385	-1.212593

56
A+FA

77	0.260001	0.002452	-0.249494
7	2.285406	-0.446546	-0.126522
6	2.715503	-1.724600	0.014248
6	3.201301	0.557435	-0.159253
6	4.050942	-2.051701	0.130584
1	1.929077	-2.480385	0.030397
6	4.575565	0.281548	-0.046452
6	5.022580	-1.027124	0.102098
1	4.340546	-3.097269	0.244229
1	5.268150	1.123148	-0.079060
7	-1.774703	0.432214	-0.330962
6	-2.441205	0.737791	0.816064
6	-2.468824	0.366314	-1.492878
6	-3.824566	0.975952	0.803236
6	-3.831053	0.578709	-1.560123
1	-1.877964	0.121116	-2.375776
6	-4.545794	0.882434	-0.382441
1	-4.310924	1.200009	1.752920
1	-4.339728	0.501045	-2.521815
8	2.779543	1.800373	-0.289915
8	-1.770700	0.784411	1.951622
14	1.057535	2.109116	-0.587408
14	-0.062793	0.302749	1.986187
6	0.950069	2.523711	-2.423666
1	1.258471	1.668382	-3.043146
1	-0.092425	2.773341	-2.683168
1	1.583170	3.392659	-2.669105
6	0.676768	3.667873	0.387370
1	-0.409062	3.755690	0.553658
1	1.176467	3.670373	1.365201
1	1.008756	4.554721	-0.176347
6	0.747251	1.541720	3.142376
1	0.554226	1.259586	4.190083
1	1.838149	1.552742	2.987183
1	0.365296	2.558696	2.980464
6	-0.038736	-1.375977	2.850716
1	-0.515886	-2.159177	2.242796
1	1.008879	-1.676690	3.020816
1	-0.544393	-1.325615	3.829330
8	-2.881251	-2.956070	-0.414228
6	-3.407745	-2.408626	0.666439
1	-2.661158	-1.949636	1.352706
8	-4.593076	-2.405605	0.898795
6	6.483851	-1.352469	0.225049
1	6.801482	-2.016235	-0.595376
1	7.105995	-0.447627	0.201753
1	6.682302	-1.890525	1.165939
6	-6.038372	1.039422	-0.400061
1	-6.394047	1.636960	0.450888
1	-6.384537	1.502190	-1.335647
1	-6.508572	0.043532	-0.329792

8	-0.375244	-2.322130	-0.775663
1	-1.891140	-2.802188	-0.466179
6	-0.125706	-2.115429	-2.006777
1	-0.294323	-2.952396	-2.720437
8	0.287078	-1.020101	-2.438262
B			
77	0.075130	0.198149	-0.051577
7	-2.014465	-0.030834	-0.012296
6	-2.841263	0.843869	0.610131
6	-2.552874	-1.166996	-0.537132
6	-4.198820	0.634382	0.743134
1	-2.373345	1.741266	1.005821
6	-3.929760	-1.433249	-0.430864
6	-4.776804	-0.538956	0.213787
1	-4.807643	1.378815	1.258078
1	-4.301590	-2.359597	-0.869836
7	2.156992	0.201979	-0.055990
6	2.819684	-0.693359	0.726648
6	2.870873	1.028070	-0.858382
6	4.224139	-0.768019	0.699181
6	4.249683	0.998372	-0.920628
1	2.272276	1.708461	-1.464903
6	4.961949	0.074535	-0.125532
1	4.706110	-1.503249	1.344376
1	4.772783	1.685298	-1.587571
8	-1.764598	-2.032848	-1.146640
8	2.131104	-1.500057	1.511980
14	-0.098015	-1.546018	-1.510000
14	0.387149	-1.212088	1.726505
6	-0.175126	-1.077925	-3.333388
1	-0.920359	-0.288438	-3.505866
1	0.803001	-0.696969	-3.667862
1	-0.432503	-1.959481	-3.944182
6	0.974609	-3.086041	-1.398096
1	1.231540	-3.379940	-0.372723
1	0.484577	-3.935014	-1.902936
1	1.915458	-2.875634	-1.933866
6	-0.420627	-2.902899	1.902199
1	0.120347	-3.511214	2.646003
1	-1.444295	-2.744327	2.281799
1	-0.495888	-3.468870	0.965363
6	0.275467	-0.407627	3.428767
1	0.868572	0.516853	3.464232
1	-0.773406	-0.144301	3.644987
1	0.625364	-1.099236	4.213232
8	-1.052460	3.793489	0.977394
6	-0.184766	3.158071	1.692142
1	0.082642	3.695598	2.625916
8	0.330526	2.071203	1.445578
6	-6.250395	-0.798641	0.344812
1	-6.829217	0.009068	-0.131650
1	-6.538140	-1.752897	-0.116822
1	-6.546153	-0.819822	1.406180
6	6.462233	0.013463	-0.176520
1	6.862535	-0.746673	0.507975
1	6.804667	-0.220958	-1.197512
1	6.898848	0.989431	0.090192
8	-1.613956	3.144555	-1.321668
1	-1.252407	3.385743	0.001170
6	-0.862281	2.522732	-2.114604
1	-1.020965	2.730585	-3.201552
8	0.042025	1.701757	-1.833348
51			
TSAC			
77	0.016697	0.356339	-0.082296
8	-0.979123	4.116454	0.359822
8	0.503915	3.443484	-1.287962
6	-0.206280	3.580410	-0.353478
7	2.101849	0.317888	-0.059468
6	2.846875	1.067865	-0.905087
6	2.727438	-0.568162	0.759883
6	4.220512	0.947698	-0.992755
1	2.286622	1.782812	-1.509614
6	4.121258	-0.735207	0.711898
6	4.891401	0.016789	-0.171033
1	4.771070	1.574477	-1.695876
1	4.571349	-1.465180	1.385627
7	-2.076535	0.219034	-0.112723
6	-2.868589	1.206678	0.383954
6	-2.675754	-0.921747	-0.565585
6	-4.242643	1.108852	0.455860
1	-2.344250	2.097282	0.725594
6	-4.075837	-1.071289	-0.513717
6	-4.882645	-0.063648	-0.001237
1	-4.817764	1.939545	0.867584
1	-4.495789	-2.004664	-0.890139
14	-0.194856	-1.639586	-1.317442
14	0.300124	-0.807206	1.831810
8	1.993064	-1.278140	1.600676
8	-1.942901	-1.900839	-1.050878
6	-0.106234	-1.312589	-3.185419
1	-0.506034	-2.162351	-3.764851
1	-0.672394	-0.407705	-3.459298
1	0.943319	-1.156319	-3.486955
6	0.590338	-3.336533	-1.063470
1	0.644070	-3.644854	-0.010454
1	0.048827	-4.110274	-1.633523
1	1.621949	-3.294349	-1.452501
6	-0.679088	-2.358597	2.232099
1	-0.151905	-2.952967	2.996802
1	-1.646520	-2.045181	2.658655
1	-0.883828	-2.996011	1.363106
6	0.341315	0.235945	3.401066
1	-0.662348	0.642539	3.606812
1	0.652127	-0.372180	4.267648
1	1.036349	1.082359	3.292464
1	-0.007088	1.987446	0.572953
6	6.383793	-0.141298	-0.247274
1	6.691748	-0.424646	-1.266753
1	6.887235	0.811068	-0.014730
1	6.747867	-0.906713	0.451492
6	-6.376601	-0.202570	0.068347

1	-6.722948	-0.125457	1.111803
1	-6.867406	0.610168	-0.491075
1	-6.716092	-1.163557	-0.341326
56			
TSBC			
77	0.014436	0.113236	-0.222998
8	-0.811855	3.861689	0.694950
8	1.476783	3.538037	0.587716
6	0.296127	3.464555	0.542347
7	2.097101	0.027776	-0.218009
6	2.840209	0.288515	-1.319366
6	2.726413	-0.387538	0.915107
6	4.213073	0.144704	-1.347436
1	2.278391	0.609008	-2.196920
6	4.122142	-0.555112	0.942239
6	4.889096	-0.293661	-0.188567
1	4.758069	0.366898	-2.266009
1	4.575078	-0.892450	1.875091
7	-2.075858	0.016034	-0.103657
6	-2.845789	1.126816	0.034359
6	-2.685713	-1.203085	-0.073398
6	-4.216625	1.079322	0.180577
1	-2.309455	2.075205	0.046417
6	-4.083043	-1.307006	0.069789
6	-4.872219	-0.170971	0.197515
1	-4.776185	2.009589	0.288558
1	-4.514970	-2.308223	0.080982
14	-0.221475	-2.200729	-0.530365
14	0.310778	-0.106946	2.026859
8	2.006098	-0.640764	1.992909
8	-1.963753	-2.300577	-0.165423
6	-0.128455	-2.817837	-2.313516
1	-0.478464	-3.861279	-2.386754
1	-0.728786	-2.185480	-2.982757
1	0.916282	-2.780856	-2.665028
6	0.608990	-3.542898	0.502140
1	0.691964	-3.302170	1.569617
1	0.079123	-4.504033	0.392384
1	1.630967	-3.678509	0.108748
6	-0.666878	-1.355625	3.040158
1	-0.094183	-1.659320	3.932290
1	-1.584414	-0.852611	3.389233
1	-0.965448	-2.253971	2.485798
6	0.384651	1.455890	3.080838
1	-0.571314	2.000361	3.020767
1	0.571668	1.201135	4.137424
1	1.183698	2.125542	2.732652
1	0.012289	1.918965	-0.149201
6	6.382067	-0.461811	-0.186385
1	6.694366	-1.164736	-0.975363
1	6.879365	0.498502	-0.399184
1	6.747863	-0.835822	0.779498
6	-6.363548	-0.256186	0.354694
1	-6.679741	0.213376	1.300238
1	-6.869597	0.290221	-0.457566
1	-6.715110	-1.296782	0.347336
8	-0.155496	0.339444	-2.656977
6	-0.578896	1.391392	-3.117710
8	-0.807335	2.472220	-2.422722
1	-0.806120	1.511408	-4.193495
1	-0.520949	2.280469	-1.467120
56			
C			
77	0.273565	-0.260216	-0.147470
1	0.014882	-1.892084	0.510735
7	2.357697	-0.423748	0.051507
6	2.966281	-1.579868	0.421508
6	3.136583	0.680084	-0.143736
6	4.326735	-1.691840	0.620725
1	2.301373	-2.430876	0.557138
6	4.531113	0.622310	0.054162
6	5.149913	-0.559110	0.441033
1	4.747896	-2.652861	0.919599
1	5.100120	1.537565	-0.112666
7	-1.770244	0.136665	-0.333003
6	-2.371672	0.915956	0.606674
6	-2.500752	-0.286934	-1.389716
6	-3.723235	1.284739	0.479357
6	-3.832654	0.037154	-1.561538
1	-1.963680	-0.896950	-2.115947
6	-4.478178	0.850916	-0.605820
1	-4.153751	1.911408	1.261151
1	-4.368365	-0.336922	-2.435007
8	2.588054	1.815143	-0.517527
8	-1.669488	1.325122	1.644915
14	0.875759	1.830846	-1.045311
14	-0.076342	0.583556	1.938546
6	1.036026	1.943546	-2.929426
1	0.031732	1.992709	-3.383831
1	1.595157	2.843471	-3.237169
1	1.538780	1.051326	-3.331796
6	0.214358	3.516224	-0.505291
1	0.901207	4.327955	-0.798930
1	-0.743381	3.684552	-1.027166
1	0.020621	3.586941	0.573488
6	1.022554	1.921625	2.678260
1	0.482901	2.480106	3.461217
1	1.883577	1.424319	3.156148
1	1.413311	2.630388	1.937248
6	-0.438971	-0.630627	3.336744
1	0.459307	-1.232931	3.551503
1	-0.729328	-0.102993	4.261251
1	-1.249361	-1.316475	3.047738
8	0.488292	-1.280340	-2.337647
6	0.506515	-2.510375	-2.371338
1	0.683446	-3.050389	-3.322301
8	0.325620	-3.292739	-1.354747
1	0.161770	-2.677263	-0.499685
6	6.633678	-0.641717	0.660610
1	7.079124	-1.414326	0.013405
1	7.129738	0.316263	0.453630
1	6.854211	-0.931216	1.700995

6	-5.933423	1.195029	-0.743211
1	-6.547993	0.302816	-0.538879
1	-6.232281	1.984265	-0.039802
1	-6.167008	1.524036	-1.767391
6	-4.451248	-1.967897	1.100399
8	-3.334943	-2.044504	1.417276
8	-5.569318	-1.899374	0.788894

56
TSCA

77	0.280144	-0.255178	-0.153194
1	0.003716	-1.910794	0.555007
7	2.361883	-0.426903	0.036122
6	2.970311	-1.590109	0.381067
6	3.138296	0.679815	-0.145333
6	4.331629	-1.703412	0.574404
1	2.307713	-2.445959	0.497933
6	4.532392	0.621757	0.048382
6	5.152679	-0.566335	0.413785
1	4.755360	-2.669315	0.853120
1	5.100646	1.539724	-0.105389
7	-1.763494	0.146270	-0.333379
6	-2.364211	0.924782	0.607536
6	-2.493504	-0.277344	-1.390810
6	-3.717240	1.289546	0.482739
6	-3.826405	0.043214	-1.559526
1	-1.953228	-0.882435	-2.118750
6	-4.472422	0.854092	-0.601406
1	-4.148117	1.914988	1.265261
1	-4.362620	-0.330321	-2.432878
8	2.582101	1.817742	-0.504061
8	-1.661539	1.337264	1.643588
14	0.879719	1.817996	-1.048673
14	-0.062232	0.607018	1.933571
6	1.043433	1.903100	-2.930654
1	0.040076	1.926721	-3.388577
1	1.587358	2.808450	-3.248916
1	1.564063	1.013942	-3.316248
6	0.179520	3.487402	-0.519999
1	0.856353	4.309341	-0.807705
1	-0.773478	3.636548	-1.055841
1	-0.029567	3.557735	0.555633
6	1.023237	1.954220	2.674999
1	0.481277	2.500365	3.464954
1	1.893460	1.464655	3.144152
1	1.400974	2.673128	1.936967
6	-0.414176	-0.617008	3.325971
1	0.488233	-1.214530	3.536672
1	-0.707656	-0.096743	4.253549
1	-1.220162	-1.306857	3.033625
8	0.449076	-1.303098	-2.287491
6	0.434120	-2.544648	-2.275206
1	0.579549	-3.097112	-3.227482
8	0.257560	-3.282206	-1.244900
1	0.108942	-2.557035	-0.313850
6	6.637050	-0.651447	0.627856
1	7.081461	-1.410717	-0.035627
1	7.131433	0.310961	0.438316
1	6.860550	-0.961086	1.661753
6	-5.928594	1.194680	-0.736388
1	-6.540150	0.300657	-0.531041
1	-6.228353	1.983097	-0.032499
1	-6.164510	1.522746	-1.760297
6	-4.439960	-1.973971	1.086510
8	-3.322197	-2.049901	1.398374
8	-5.559361	-1.905700	0.779831

5
HCOOH

6	-0.070484	0.432479	0.020809
8	-1.114535	-0.269021	-0.016950
8	1.059472	-0.116657	-0.051433
1	-0.143528	1.495878	0.114341
1	1.006941	-1.005329	0.307875

3
CO_2

6	0.000000	0.000000	0.000000
8	0.000000	0.000000	1.163049
8	0.000000	0.000000	-1.163049

2
H_2

1	0.000000	0.000000	0.380606
1	0.000000	0.000000	-0.380606