

Electronic Supplementary Information (ESI)

Computational Study of the CO₂ Hydrogenation to Formic Acid Catalyzed by a P,P-Bidentate Copper(I) Complex

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S1. Global Reaction

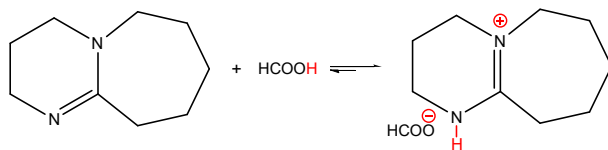


Fig. S1.: Global reaction between formic acid and LB-DBU

S2. Multiplicity

Table S1.: Relative energies of the [Cu(dtbpf)]⁺ complex in singlet and triplet states

State	Multiplicity
Singlet	0.00 kcal.mol ⁻¹
Triplet	12.99 kcal.mol ⁻¹

S3. Pairs determining Step (TDI – TDTS)

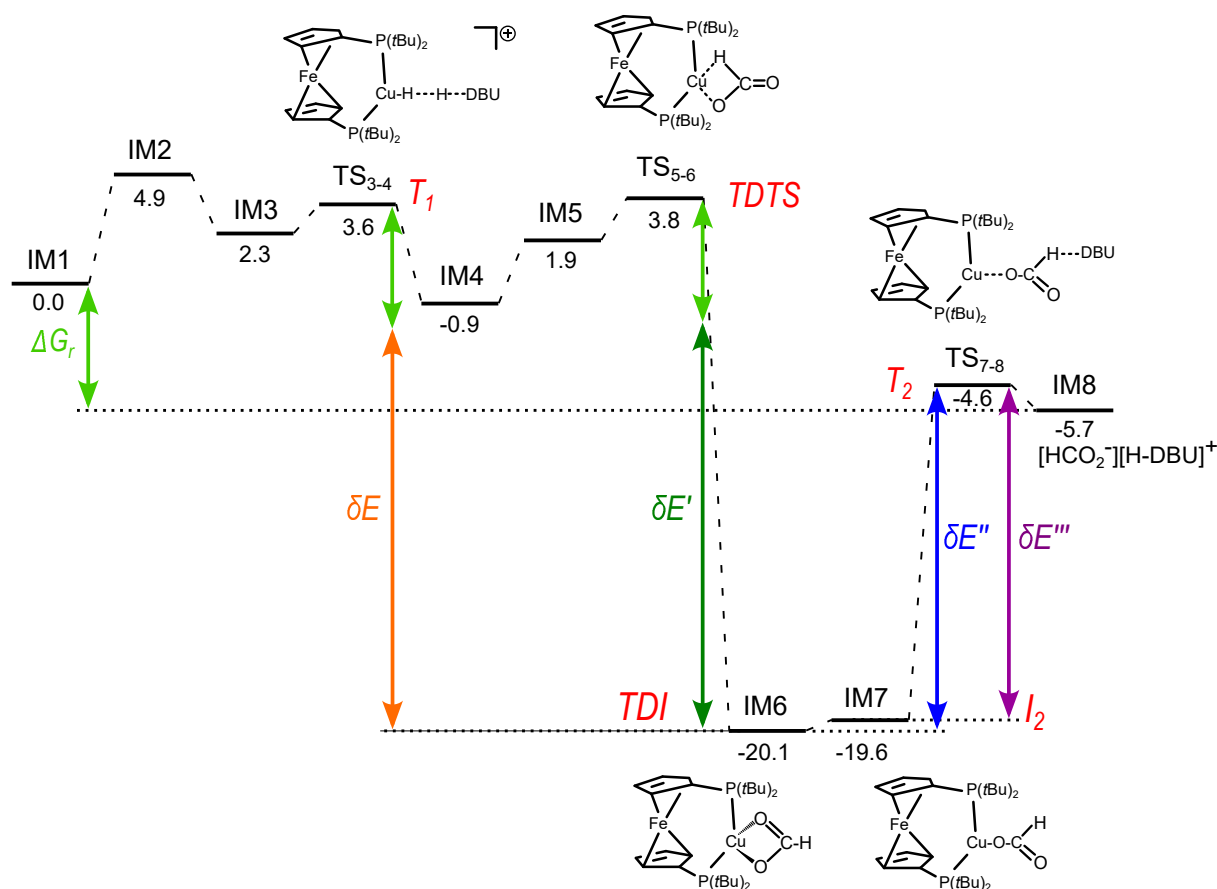


Fig. S2.: Assessment of potential TDTS and TDI Pairings. Relative free energies ΔG (in black) in kcal.mol⁻¹ at 298.15K and 1atm

S4. Coordination Mode

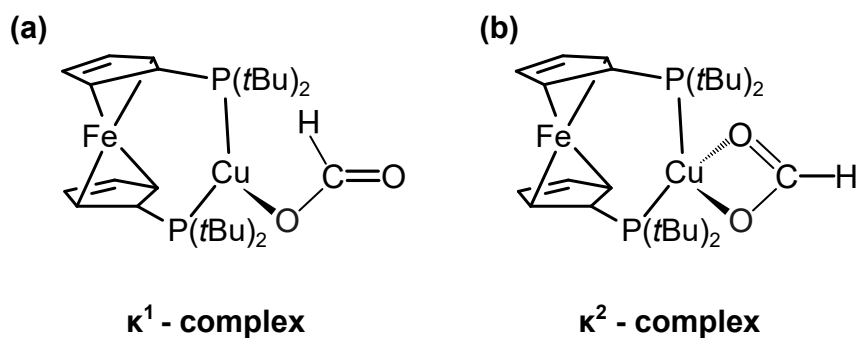


Fig. S3.: Electronic structure of κ^1 and κ^2 isomers in DMF

S5. IRI and FBO Analysis

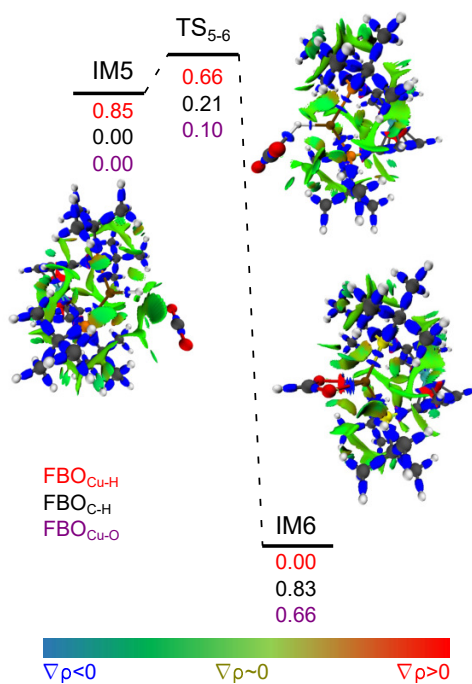


Fig. S4.: Analysis of IRI (Interaction Region Indicator) and FBO (Fuzzy Bond Order) of the interactions involved in formate formation.

S6. Bite Angle Analysis

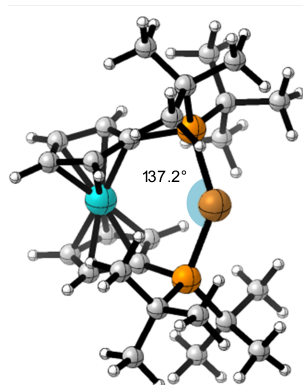


Table S2.: Influence of key bond distances and bite angle on the stability of intermediates and transition states in the catalytic cycle

System	$\Delta\theta_{\text{P1-Cu2-P3}}/^\circ$	$\Delta d_{\text{P1-Cu2}}/\text{\AA}$	$\Delta d_{\text{Cu2-P2}}/\text{\AA}$
IM1	0.0	0.000	0.000
IM2	-11.9	0.032	0.034
IM3	-11.9	0.045	0.038
TS ₃₋₄	-14.9	0.083	0.046
IM4	-23.9	0.083	0.085
IM5	-25.3	0.080	0.086
TS ₅₋₆	-23.3	0.063	0.071
IM6	-16.3	0.025	0.025
IM7	-16.3	0.020	0.032
TS ₇₋₈	0.5	-0.009	-0.009
IM1...DBU ^a	0.6	-0.002	-0.002

^avdW complex.

S7. Cartesian Coordinates

H2	1 3.346864000 -0.118506000 -0.582928000
G: -1.175546	1 1.533940000 1.527178000 1.280502000
1 0.000000000 0.000000000 0.380574000	1 1.299824000 0.923183000 -1.718670000
1 0.000000000 0.000000000 -0.380574000	1 1.436993000 -1.211762000 1.566772000
	1 0.602768000 -2.600771000 -0.484168000
CO2	1 3.550335000 0.070232000 1.160574000
G: -188.451882	1 2.700370000 2.137889000 0.096098000
6 0.000000000 0.000000000 0.000000000	1 0.604949000 2.357755000 -0.982727000
8 0.000000000 0.000000000 -1.163127000	1 2.626876000 -2.127911000 0.639812000
8 0.000000000 0.000000000 1.163127000	1 1.339212000 -1.355677000 -1.501667000
	7 -1.478310000 -1.451236000 -0.144930000
HCOO-	6 -1.464907000 1.434897000 -0.018235000
G: -189.147339	6 -2.717335000 -0.709942000 0.029979000
8 -1.130850000 -0.212080000 0.000000000	6 -2.496607000 0.620465000 0.751535000
8 1.130950000 -0.211125000 0.000000000	1 -3.435315000 -1.336337000 0.587015000
6 0.000000000 0.318934000 0.000000000	1 -3.185634000 -0.516228000 -0.957074000
1 -0.000805000 1.472035000 0.000000000	1 -2.123550000 0.417266000 1.770153000
	1 -3.431572000 1.194112000 0.849356000
DBU	1 -1.922345000 1.875246000 -0.925219000
G: -461.581871	1 -1.106647000 2.276929000 0.598328000
6 2.789088000 -0.001347000 0.364977000	
6 2.000298000 1.310313000 0.302978000	H-DBU
6 0.901170000 1.320298000 -0.769073000	G: -462.050236
6 1.945771000 -1.262255000 0.587345000	6 -2.816317000 0.015005000 0.373975000
7 -0.316608000 0.606331000 -0.391821000	6 -2.023962000 -1.295864000 0.368706000
6 0.895927000 -1.543257000 -0.507433000	6 -0.949741000 -1.371444000 -0.720753000
6 -0.398847000 -0.768883000 -0.348557000	6 -1.975076000 1.282774000 0.551479000

7 0.287800000 -0.635775000 -0.390457000	6 -6.285830000 5.645213000 0.413671000
6 -0.918429000 1.508873000 -0.551503000	6 -5.670269000 4.258847000 3.095508000
6 0.330608000 0.690879000 -0.362255000	7 -5.672328000 6.679586000 1.244567000
1 -3.374445000 0.093804000 -0.576403000	6 -6.493006000 5.552970000 3.281034000
1 -1.546986000 -1.467747000 1.348978000	6 -5.867468000 6.756645000 2.605353000
1 -1.340290000 -1.007969000 -1.684382000	1 -7.042834000 3.239617000 1.780457000
1 -1.474544000 1.281027000 1.534763000	1 -4.534245000 4.393232000 0.409784000
1 -0.625498000 2.567175000 -0.577443000	1 -7.361561000 5.570656000 0.649753000
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1 -2.721452000 -2.133514000 0.207234000	1 -5.419686000 2.544242000 1.799969000
1 -0.646014000 -2.412734000 -0.884187000	1 -5.960451000 3.663265000 -0.359480000
1 -2.644835000 2.156485000 0.545770000	1 -6.233044000 6.007824000 -0.624971000
1 -1.345781000 1.280828000 -1.541695000	1 -7.527102000 5.393787000 2.925932000
7 1.466378000 1.339618000 -0.131660000	6 -5.967495000 3.502888000 1.792909000
6 1.488390000 -1.448114000 -0.108064000	6 -4.675334000 7.527271000 0.577729000
6 2.753715000 0.689721000 0.111415000	6 -4.840527000 8.851014000 2.674302000
6 2.497014000 -0.676645000 0.731706000	6 -3.882415000 8.338317000 1.596041000
1 3.339857000 1.333973000 0.780366000	1 -4.302419000 9.464766000 3.417179000
1 3.304478000 0.598867000 -0.839581000	1 -5.593175000 9.521396000 2.206734000
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1 1.926705000 -1.769005000 -1.067885000	1 -5.186524000 8.196495000 -0.140935000
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	1 -4.595102000 4.506221000 3.147852000
	1 -0.703217000 5.899404000 1.226028000
[HCOO ⁻][DBU]	6 -1.736299000 5.426817000 1.365702000
G: -650.726382	8 -2.298150000 5.060033000 0.308451000
7 -5.496530000 7.744843000 3.354239000	8 -2.133471000 5.355606000 2.549653000
6 -5.625402000 4.263037000 0.506008000	

	1 2.787034000 1.993927000 0.495804000
	1 -1.805175000 0.737867000 -0.112245000
[HCOO ⁻][H-DBU] ⁺	8 -3.353647000 0.575823000 0.154675000
G: -651.219714	8 -3.356335000 -1.652024000 -0.212752000
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1 2.059361000 2.554062000 -1.024206000	

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6	1.696730000	1.075518000	0.267984000	1	-1.680519000	-2.271607000	-2.482411000
6	-1.752804000	1.082374000	-0.438515000	6	-2.804456000	-0.817146000	1.685531000
6	-1.659240000	3.406829000	-0.494528000	6	-2.865518000	-2.310254000	2.075916000
6	1.604881000	3.399593000	0.357364000	6	-1.807921000	-0.152849000	2.656663000
6	2.018412000	2.288706000	-0.434843000	6	-4.194486000	-0.175013000	1.815951000
6	-1.124937000	1.500491000	-1.667914000	1	-3.619077000	-2.876258000	1.518068000
6	-1.081419000	2.922573000	-1.703848000	1	-3.124477000	-2.383567000	3.144755000
1	0.683609000	0.812575000	2.266125000	1	-1.889086000	-2.800816000	1.933880000
1	-2.538041000	2.351205000	1.261359000	1	-1.661517000	0.916510000	2.470760000
1	0.592954000	3.490002000	2.363660000	1	-0.826618000	-0.648660000	2.608313000
1	-1.741477000	4.449606000	-0.192309000	1	-2.185871000	-0.268240000	3.685453000
1	1.687370000	4.446390000	0.069459000	1	-4.202967000	0.880229000	1.509456000
1	2.479097000	2.369658000	-1.414908000	1	-4.515778000	-0.219649000	2.869918000
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6	-4.330996000	-0.124380000	-1.734601000	6	4.232094000	-0.178744000	1.597190000
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1	-4.719228000	-2.380300000	-0.197552000	1	4.657268000	-2.385090000	0.003973000
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1	-4.959693000	0.116197000	-0.866317000	1	4.489731000	-2.940444000	1.676491000

1 4.872902000 0.093071000 0.746987000	6 2.938639000 0.440074000 -1.853675000
1 3.747280000 0.735724000 1.967545000	6 4.164206000 -0.149295000 -2.273657000
6 2.772498000 -0.777257000 -1.878248000	1 2.503668000 -1.641792000 2.006032000
6 4.158947000 -0.121097000 -1.973274000	1 4.912333000 0.861471000 0.832469000
6 2.855016000 -2.259727000 -2.303405000	1 4.892611000 -2.630288000 1.287889000
6 1.780780000 -0.101442000 -2.847344000	1 6.111497000 -0.418778000 -1.183294000
1 2.170384000 -0.192885000 -3.874140000	1 4.683984000 -3.554068000 -1.256596000
1 1.622089000 0.962495000 -2.641998000	1 2.168803000 -3.171092000 -2.087191000
1 0.802778000 -0.606147000 -2.818801000	1 2.032800000 0.477631000 -2.445528000
1 4.156026000 0.926147000 -1.640858000	1 4.338879000 -0.640658000 -3.229285000
1 4.909794000 -0.663230000 -1.381728000	15 1.760244000 1.877071000 0.344232000
1 4.495763000 -0.137869000 -3.023219000	15 0.035923000 -1.802188000 0.096756000
1 1.883072000 -2.765027000 -2.186851000	6 1.512044000 3.411312000 -0.780183000
1 3.128306000 -2.303571000 -3.370274000	6 0.716016000 4.492356000 -0.027105000
1 3.608305000 -2.830567000 -1.750288000	6 2.841746000 3.995660000 -1.286371000
1 -0.438020000 -3.565176000 -0.252692000	6 0.671497000 2.947912000 -1.990117000
1 0.347930000 -3.571736000 -0.249334000	1 -0.203664000 4.095937000 0.429027000
	1 0.420455000 5.276997000 -0.742658000
	1 1.313769000 4.977645000 0.755774000
	1 3.422823000 3.256513000 -1.856507000
	1 3.472052000 4.373420000 -0.470509000
	1 2.625987000 4.842561000 -1.959596000
	1 1.233608000 2.288309000 -2.662155000
	1 0.374176000 3.830572000 -2.579670000
	1 -0.245586000 2.425298000 -1.682879000
	6 2.407674000 2.355398000 2.075781000
	6 1.259380000 3.012788000 2.872256000
	6 2.738497000 1.029853000 2.795375000
	6 3.627920000 3.289601000 2.063145000
IM3	
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6 -1.093049000 7.708174000 -0.202209000	1 -4.014839000 4.623260000 -0.489361000
6 -1.965760000 6.550438000 0.245497000	1 -1.882998000 3.871700000 1.590676000
1 -0.387702000 9.700076000 1.699412000	1 -3.592649000 3.391368000 1.619180000
1 -0.559521000 7.069753000 3.288132000	1 -4.319702000 5.680102000 2.016314000
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1 -0.829177000 7.487485000 -1.244234000	1 0.910851000 8.472277000 0.004800000
1 0.974080000 8.837827000 2.420417000	1 0.649175000 6.940997000 0.833983000
1 -1.054590000 8.683977000 3.824496000	
1 -3.080312000 7.645586000 3.201205000	