

Supporting Information

Theoretical Studies on the CuCl-Catalyzed C–H Activation/C–O Coupling

Reactions: Oxidant and Substituent Effect

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Table S1-1. Some optimized Cartesian Coordinates of stationary points for the entire catalytic cycle, involved in the discussion on TBHP (**OX-a**) as oxidant, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide with bond lengths in Å.

Species	Cartesian coordinates			
1a	6	0.246234000	0.823069000	0.160252000
	8	0.457848000	1.832221000	-0.493749000
	8	1.160290000	-0.131593000	0.396310000
	6	2.477116000	0.056246000	-0.205882000
	6	3.333809000	-1.134052000	0.184414000
	1	2.891670000	0.998960000	0.161716000
	1	2.350423000	0.134332000	-1.289221000
	1	4.330197000	-1.022525000	-0.255175000
	1	3.443736000	-1.200978000	1.270965000
	1	2.899746000	-2.069079000	-0.182219000
	6	-1.984227000	-0.323651000	-0.149066000
	8	-1.581457000	-0.723685000	-1.232626000
	6	-3.389828000	-0.586769000	0.342697000
	1	-3.377566000	-0.992794000	1.359860000
	1	-3.944689000	0.358378000	0.382577000
	1	-3.901233000	-1.277209000	-0.329995000
	6	-1.088660000	0.486941000	0.792520000
	1	-1.603146000	1.415553000	1.059604000
	1	-0.949246000	-0.090889000	1.712799000
	CuCl	29	0.000000000	0.000000000
17		0.000000000	0.000000000	-1.356359000
CAT	6	1.371842000	-0.069308000	-0.365902000
	8	0.502100000	-0.880291000	-0.072658000
	8	2.678681000	-0.290254000	-0.246095000
	6	3.086990000	-1.606694000	0.259314000
	6	4.602541000	-1.624706000	0.303478000
	1	2.681314000	-2.366163000	-0.413874000

	1	2.640882000	-1.740482000	1.248008000
	1	4.937663000	-2.596792000	0.678827000
	1	5.028213000	-1.475966000	-0.693122000
	1	4.986865000	-0.847923000	0.970923000
	6	0.144775000	2.118340000	-0.026261000
	8	-0.935483000	1.654752000	0.354621000
	6	0.562994000	3.503909000	0.363167000
	1	0.764713000	4.094060000	-0.539056000
	1	-0.207658000	3.987178000	0.964584000
	1	1.505655000	3.457142000	0.922232000
	6	1.082795000	1.319432000	-0.921404000
	1	0.565893000	1.181618000	-1.880905000
	1	2.011336000	1.860363000	-1.103753000
	29	-1.794503000	-0.099953000	0.107065000
	17	-3.291076000	-1.669052000	-0.071768000
TBHP	6	0.392997000	1.270210000	0.889315000
	6	0.390026000	-0.000003000	0.028214000
	1	0.370302000	2.162958000	0.255982000
	1	-0.474387000	1.294979000	1.553665000
	1	1.297932000	1.305997000	1.504683000
	6	0.392936000	-1.270551000	0.888819000
	6	1.567318000	0.000157000	-0.957100000
	1	0.369918000	-2.163041000	0.255134000
	1	1.298010000	-1.306757000	1.503957000
	1	-0.474295000	-1.295421000	1.553365000
	1	2.509558000	0.000157000	-0.401018000
	1	1.544098000	-0.888775000	-1.595221000
	1	1.543998000	0.889217000	-1.595038000
	8	-0.749937000	0.000202000	-0.869576000
	8	-1.975619000	-0.000038000	-0.049653000
	1	-2.640349000	0.000496000	-0.777161000
COM1-a	6	-0.682758000	-0.952760000	1.850620000
	8	-0.142515000	0.155209000	1.874683000
	6	-2.080177000	-0.635664000	-0.234633000
	8	-1.763820000	0.495257000	-0.587112000
	6	-1.166765000	-1.569179000	0.541984000
	1	-1.656095000	-2.528527000	0.711481000
	1	-0.267786000	-1.724405000	-0.069896000
	29	0.118935000	1.549456000	0.381735000
	17	0.380048000	3.714368000	-0.057819000
	8	1.636711000	0.455438000	-0.952465000
	1	1.392142000	0.584901000	-1.901873000
	8	-3.263016000	-1.193613000	-0.490823000
	6	-4.223182000	-0.392909000	-1.257910000

	1	-3.759428000	-0.132517000	-2.212805000
	1	-4.416468000	0.527369000	-0.700853000
	6	-5.474045000	-1.231864000	-1.435085000
	1	-5.914147000	-1.492745000	-0.468172000
	1	-5.256820000	-2.153064000	-1.983580000
	1	-6.212125000	-0.658523000	-2.004908000
	6	-0.859836000	-1.758392000	3.105381000
	1	-0.385247000	-2.739742000	2.985562000
	1	-0.433016000	-1.237377000	3.963276000
	1	-1.927716000	-1.946053000	3.271699000
	8	1.828703000	-0.997811000	-0.894072000
	6	3.241669000	-1.290484000	-0.637777000
	6	3.665030000	-0.677198000	0.700644000
	1	3.031454000	-1.045962000	1.513431000
	1	4.702844000	-0.944096000	0.924632000
	1	3.592097000	0.412988000	0.669729000
	6	4.105729000	-0.786430000	-1.798073000
	1	4.079454000	0.304826000	-1.862197000
	1	5.146750000	-1.090867000	-1.650326000
	1	3.758331000	-1.203429000	-2.749090000
	6	3.230480000	-2.823259000	-0.576456000
	1	2.888901000	-3.252055000	-1.523567000
	1	4.243743000	-3.186256000	-0.380218000
	1	2.577841000	-3.179947000	0.226427000
TS1-a	6	-0.482825000	-0.743827000	1.979215000
	8	-0.123346000	0.437023000	1.992819000
	6	-2.018551000	-0.632283000	-0.025749000
	8	-1.979573000	0.580027000	-0.222412000
	6	-0.935203000	-1.418033000	0.693456000
	1	-1.266634000	-2.441438000	0.872080000
	1	-0.056315000	-1.436615000	0.026621000
	29	-0.020430000	1.679873000	0.288410000
	17	0.186774000	3.747366000	-0.433139000
	8	1.233986000	0.590345000	-0.675150000
	1	1.337209000	0.921338000	-1.594787000
	8	-3.012377000	-1.414632000	-0.433425000
	6	-4.100719000	-0.776717000	-1.184985000
	1	-3.664638000	-0.286976000	-2.059251000
	1	-4.549877000	-0.014376000	-0.543589000
	6	-5.086425000	-1.864544000	-1.564578000
	1	-5.499239000	-2.350626000	-0.675846000
	1	-4.613136000	-2.623466000	-2.194317000
	1	-5.912491000	-1.417744000	-2.126832000
	6	-0.463167000	-1.570554000	3.231393000

	1	0.136615000	-2.473913000	3.068769000
	1	-0.063150000	-0.997661000	4.068746000
	1	-1.481590000	-1.909615000	3.458104000
	8	1.854639000	-1.180164000	-1.171698000
	6	3.170636000	-1.338722000	-0.673923000
	6	3.200544000	-1.251444000	0.860220000
	1	2.545326000	-2.011012000	1.300828000
	1	4.213853000	-1.413179000	1.243747000
	1	2.860417000	-0.263632000	1.182544000
	6	4.136909000	-0.326486000	-1.310908000
	1	3.874009000	0.689374000	-1.002107000
	1	5.169949000	-0.523362000	-1.004300000
	1	4.083672000	-0.383039000	-2.403223000
	6	3.522883000	-2.777797000	-1.137445000
	1	3.495024000	-2.853320000	-2.228348000
	1	4.533617000	-3.025407000	-0.795602000
	1	2.823569000	-3.505230000	-0.715027000
INT1-a	6	-1.452325000	0.248693000	-0.297437000
	8	-0.564592000	-0.607982000	-0.245724000
	8	-2.734857000	-0.044095000	-0.191426000
	6	-3.100377000	-1.461159000	-0.023476000
	6	-4.612043000	-1.527947000	0.060386000
	1	-2.614186000	-1.823440000	0.885235000
	1	-2.703520000	-2.010411000	-0.880509000
	1	-4.914210000	-2.572285000	0.186838000
	1	-4.985660000	-0.956346000	0.914725000
	1	-5.075591000	-1.144217000	-0.852884000
	6	-0.061477000	2.314928000	0.293580000
	8	0.981206000	1.689356000	0.473139000
	6	-0.245579000	3.708644000	0.823052000
	1	-0.571539000	4.376927000	0.017528000
	1	-1.045896000	3.705985000	1.573427000
	1	0.679892000	4.074930000	1.268694000
	6	-1.220201000	1.730300000	-0.511609000
	1	-2.145079000	2.281559000	-0.336788000
	1	-0.956552000	1.866712000	-1.571413000
	29	1.514618000	-0.349558000	-0.249506000
	17	2.090423000	-2.240380000	0.828612000
	8	3.003566000	0.158964000	-1.217091000
	1	3.540644000	0.773527000	-0.673756000
'BuO•	6	1.268352000	-0.811643000	-0.312448000
	6	-0.000674000	-0.029292000	0.081095000
	1	2.165787000	-0.252874000	-0.030774000
	1	1.288036000	-1.778920000	0.200362000

	1	1.292911000	-0.997203000	-1.391264000
	6	-1.289089000	-0.778348000	-0.312268000
	6	0.018221000	1.388325000	-0.585480000
	1	-2.171955000	-0.197223000	-0.029534000
	1	-1.319576000	-0.962381000	-1.391200000
	1	-1.333491000	-1.745291000	0.199692000
	1	0.015506000	1.245142000	-1.670704000
	1	-0.865663000	1.962772000	-0.297600000
	1	0.917704000	1.938496000	-0.298615000
	8	0.003735000	0.271653000	1.435530000
DMF	6	-0.860602000	-0.646490000	-0.000341000
	8	-1.967627000	-0.091532000	0.000615000
	7	0.340560000	-0.020553000	-0.001706000
	1	-0.765612000	-1.746767000	-0.000575000
	6	0.435085000	1.435304000	0.000142000
	1	0.971005000	1.780742000	0.891943000
	1	0.975311000	1.782488000	-0.888323000
	1	-0.570852000	1.854614000	-0.001839000
	6	1.591480000	-0.770795000	0.000604000
	1	2.187146000	-0.528612000	-0.887204000
	1	2.182450000	-0.531566000	0.892399000
	1	1.381866000	-1.842889000	-0.001814000
INT2-a	6	-1.749307000	0.848127000	0.057390000
	8	-1.296882000	-0.071376000	-0.625072000
	8	-2.853921000	1.507669000	-0.269596000
	6	-3.532036000	1.115701000	-1.511994000
	6	-4.743305000	2.014230000	-1.667700000
	1	-3.804134000	0.060806000	-1.427494000
	1	-2.820640000	1.229858000	-2.333702000
	1	-5.271457000	1.744947000	-2.587822000
	1	-5.433840000	1.894632000	-0.827847000
	1	-4.448743000	3.065462000	-1.735798000
	6	-0.843542000	0.276372000	2.372510000
	8	-0.357685000	-0.799484000	2.046140000
	6	-1.155152000	0.618135000	3.805927000
	1	-0.674971000	1.565057000	4.079328000
	1	-2.235782000	0.768942000	3.918270000
	1	-0.820575000	-0.179148000	4.471029000
	6	-1.131306000	1.368766000	1.336156000
	1	-1.749072000	2.164163000	1.754362000
	1	-0.154837000	1.792093000	1.067377000
	29	0.393738000	-1.318660000	-0.238089000
	17	-0.797938000	-3.198658000	-0.857472000
	8	1.998587000	-2.241367000	0.099528000

	1	1.823718000	-3.191049000	-0.046477000
	8	1.449590000	0.499045000	-0.388090000
	6	2.707220000	0.475916000	-0.362185000
	1	3.226977000	-0.472086000	-0.181327000
	7	3.477960000	1.550126000	-0.549871000
	6	2.911216000	2.871728000	-0.818751000
	1	3.325579000	3.267043000	-1.751898000
	1	1.829217000	2.788501000	-0.908966000
	1	3.159036000	3.560010000	-0.003419000
	6	4.936535000	1.454392000	-0.486160000
	1	5.376138000	1.766982000	-1.439100000
	1	5.321873000	2.100748000	0.309453000
	1	5.232879000	0.424403000	-0.279717000
TS2-a	6	-2.138332000	0.803217000	-1.270645000
	6	-2.070477000	-0.063457000	0.000015000
	1	-1.312545000	1.521589000	-1.294751000
	1	-2.073446000	0.172599000	-2.163414000
	1	-3.077185000	1.366534000	-1.312529000
	6	-3.219539000	-1.097089000	-0.000294000
	6	-2.138408000	0.802575000	1.271106000
	1	-3.165354000	-1.733387000	0.888278000
	1	-4.184073000	-0.577606000	-0.000080000
	1	-3.165417000	-1.732783000	-0.889302000
	1	-3.077195000	1.365984000	1.313168000
	1	-2.073704000	0.171494000	2.163564000
	1	-1.312534000	1.520833000	1.295686000
	8	-0.889822000	-0.868273000	-0.000139000
	6	1.255636000	0.542744000	-0.000044000
	8	1.219288000	1.768866000	-0.000068000
	7	2.332770000	-0.253547000	0.000063000
	1	0.168026000	-0.117051000	-0.000052000
	6	3.687143000	0.312134000	0.000060000
	1	4.229495000	-0.023102000	0.890701000
	1	4.229097000	-0.021937000	-0.891265000
	1	3.624476000	1.399751000	0.000785000
	6	2.226103000	-1.714204000	-0.000075000
	1	2.716898000	-2.122881000	-0.890139000
	1	2.716912000	-2.123031000	0.889914000
	1	1.178673000	-2.012443000	-0.000092000
BuOH	6	0.597655000	1.309498000	-0.519537000
	6	-0.004497000	-0.000626000	0.014271000
	1	0.066243000	2.171505000	-0.103173000
	1	1.655873000	1.393706000	-0.243083000
	1	0.533185000	1.357952000	-1.612138000

	6	0.757637000	-1.217436000	-0.535165000
	6	-1.494404000	-0.090346000	-0.331233000
	1	0.338469000	-2.144190000	-0.129699000
	1	0.700593000	-1.261099000	-1.628299000
	1	1.817736000	-1.171447000	-0.256938000
	1	-1.641728000	-0.093264000	-1.415723000
	1	-1.928348000	-1.008025000	0.079386000
	1	-2.035979000	0.763415000	0.089347000
	8	0.046595000	-0.008481000	1.463548000
	1	0.982849000	0.052757000	1.741917000
(CH3)2N(O)C•	6	-0.866784000	-0.657189000	0.000035000
	8	-1.999088000	-0.204362000	-0.000022000
	7	0.316820000	-0.046052000	0.000005000
	6	1.557404000	-0.821603000	-0.000013000
	6	0.435735000	1.420976000	0.000002000
	1	0.979306000	1.752357000	-0.891459000
	1	-0.561960000	1.860148000	0.000500000
	1	0.980154000	1.752233000	0.890984000
	1	2.151709000	-0.587505000	0.890304000
	1	1.316031000	-1.885369000	0.000122000
	1	2.151600000	-0.587704000	-0.890456000
TS3-a	6	0.869889000	1.634918000	-0.272443000
	8	-0.245525000	1.385116000	-0.734158000
	8	1.817877000	2.235227000	-1.004798000
	6	1.471895000	2.599882000	-2.380993000
	6	2.680546000	3.287716000	-2.986443000
	1	0.597820000	3.254978000	-2.348176000
	1	1.202549000	1.686359000	-2.917769000
	1	2.448804000	3.576523000	-4.016516000
	1	2.941566000	4.190749000	-2.426993000
	1	3.548297000	2.621705000	-3.005059000
	6	0.429746000	1.068820000	2.205140000
	8	-0.738479000	0.703668000	2.037868000
	6	0.995181000	1.256544000	3.594420000
	1	1.950117000	0.729725000	3.699819000
	1	1.195868000	2.320537000	3.768688000
	1	0.285982000	0.894413000	4.340073000
	6	1.377014000	1.305002000	1.083114000
	1	2.247717000	1.904086000	1.354116000
	1	1.967338000	0.081919000	0.957960000
	29	-2.047246000	0.615607000	0.090995000
	17	-3.034345000	2.718312000	-0.005945000
	8	-3.599772000	-0.264576000	0.698438000
	1	-4.286903000	0.418444000	0.819623000

	6	2.498074000	-1.214762000	1.030855000
	8	1.831306000	-1.978792000	1.706654000
	7	3.648786000	-1.403427000	0.389256000
	6	4.321075000	-2.713730000	0.438977000
	1	4.430152000	-3.108156000	-0.576259000
	1	5.312920000	-2.599353000	0.887913000
	1	3.726210000	-3.402641000	1.037336000
	6	4.321392000	-0.352776000	-0.379164000
	1	5.309036000	-0.154768000	0.049749000
	1	4.444407000	-0.677960000	-1.417248000
	1	3.737644000	0.566306000	-0.366700000
	6	-1.996249000	-2.239944000	-0.582185000
	8	-1.282373000	-1.208225000	-0.639471000
	7	-1.629163000	-3.431539000	-1.065553000
	1	-2.987285000	-2.189259000	-0.115683000
	6	-0.338159000	-3.632826000	-1.722156000
	1	0.244466000	-4.384037000	-1.178151000
	1	-0.493119000	-3.982832000	-2.748386000
	1	0.206768000	-2.690206000	-1.737347000
	6	-2.509258000	-4.594522000	-0.959637000
	1	-2.749274000	-4.978587000	-1.956846000
	1	-2.019256000	-5.387839000	-0.385056000
	1	-3.436324000	-4.314541000	-0.455952000
INT3	6	1.370023000	0.571039000	-0.000244000
	8	0.611423000	-0.455421000	-0.001363000
	8	2.687980000	0.375730000	0.000080000
	6	3.193702000	-0.998341000	-0.000514000
	6	4.708144000	-0.912600000	0.000799000
	1	2.810404000	-1.505732000	-0.889430000
	1	2.808956000	-1.507029000	0.887029000
	1	5.124921000	-1.924734000	0.000348000
	1	5.073866000	-0.389849000	-0.887846000
	1	5.072390000	-0.391252000	0.890877000
	6	-0.373346000	2.292563000	0.000352000
	8	-1.393359000	1.486236000	0.000604000
	6	-0.776163000	3.751766000	-0.000355000
	6	0.960873000	1.928360000	0.000403000
	1	1.732995000	2.687987000	0.000669000
	29	-1.293105000	-0.413234000	-0.000113000
	17	-1.403058000	-2.609768000	0.000112000
	8	-3.105897000	-0.343172000	0.000550000
	1	-3.490626000	-1.247565000	0.000184000
	1	-1.391439000	3.958475000	0.880875000
	1	0.096314000	4.407072000	0.002156000

	1	-1.386303000	3.958761000	-0.885126000
TS4	6	1.988573000	-0.585628000	0.420671000
	8	1.397592000	0.031869000	-0.494751000
	8	3.067350000	-1.342028000	0.143923000
	6	3.509860000	-1.395743000	-1.244113000
	6	4.749846000	-2.269931000	-1.290627000
	1	3.714505000	-0.376765000	-1.584441000
	1	2.698720000	-1.805451000	-1.852480000
	1	5.108747000	-2.333826000	-2.322893000
	1	5.550669000	-1.851004000	-0.673905000
	1	4.531174000	-3.283082000	-0.940039000
	6	0.519695000	0.032096000	2.331259000
	8	-0.403869000	0.673241000	1.670442000
	6	0.256230000	0.003098000	3.824682000
	6	1.639147000	-0.592330000	1.814440000
	1	2.302132000	-1.122423000	2.488090000
	29	-0.225268000	1.333977000	-0.101391000
	17	-0.203022000	2.263190000	-2.103832000
	8	-0.280133000	3.022470000	0.648655000
	1	-0.232848000	3.687473000	-0.071906000
	1	0.988217000	-0.612988000	4.350046000
	1	0.292740000	1.024409000	4.217870000
	1	-0.748812000	-0.386792000	4.012784000
	6	-2.374826000	-0.780943000	-0.032815000
	8	-1.555015000	-0.235188000	-0.807692000
	7	-3.257772000	-1.715018000	-0.403588000
	1	-2.408164000	-0.511552000	1.031055000
	6	-4.190517000	-2.303201000	0.557615000
	1	-4.030867000	-1.868661000	1.546250000
	1	-5.222874000	-2.109488000	0.247856000
1	-4.036848000	-3.385823000	0.617213000	
6	-3.338559000	-2.189254000	-1.785190000	
1	-2.588248000	-1.676637000	-2.385295000	
1	-3.159029000	-3.269097000	-1.818028000	
1	-4.334748000	-1.984642000	-2.191721000	
INT4	6	2.017572000	-0.558337000	0.272085000
	8	1.035850000	-0.695286000	-0.469754000
	8	3.229419000	-1.081673000	-0.033343000
	6	3.327032000	-1.821002000	-1.282064000
	6	4.759957000	-2.304226000	-1.418695000
	1	3.039771000	-1.158385000	-2.103841000
	1	2.617431000	-2.653273000	-1.251988000
	1	4.866384000	-2.866545000	-2.352015000
	1	5.458767000	-1.462545000	-1.443602000

	1	5.034833000	-2.962089000	-0.588597000
	6	0.935294000	0.745053000	2.119848000
	8	-0.252640000	0.719870000	1.588716000
	6	1.053579000	1.488441000	3.430556000
	6	2.046252000	0.139444000	1.549204000
	1	3.003239000	0.198793000	2.056724000
	29	-0.531663000	1.240033000	-0.260982000
	17	-1.072332000	2.104384000	-2.256173000
	8	0.904709000	2.357897000	-0.125238000
	1	0.929829000	2.960356000	-0.901245000
	1	0.279217000	1.141754000	4.122148000
	1	2.034234000	1.357494000	3.893574000
	1	0.880990000	2.555536000	3.252348000
	6	-2.049695000	-1.088524000	0.203797000
	8	-2.118982000	0.069021000	-0.298799000
	7	-3.073829000	-1.934340000	0.228956000
	1	-1.114529000	-1.444144000	0.644919000
	6	-2.939469000	-3.269383000	0.817063000
	1	-1.925314000	-3.410660000	1.194331000
	1	-3.647421000	-3.384429000	1.643811000
	1	-3.148754000	-4.032021000	0.060384000
	6	-4.383277000	-1.581630000	-0.326345000
	1	-4.347034000	-0.569703000	-0.726007000
	1	-4.644371000	-2.282996000	-1.125202000
	1	-5.142918000	-1.639892000	0.459634000
TS5	6	-2.517400000	0.581724000	0.005816000
	8	-1.781840000	-0.453072000	-0.070353000
	8	-3.837936000	0.403881000	0.147397000
	6	-4.346882000	-0.963720000	0.221557000
	6	-5.850255000	-0.871838000	0.404960000
	1	-3.861702000	-1.469839000	1.060395000
	1	-4.078214000	-1.484454000	-0.701311000
	1	-6.267713000	-1.882115000	0.463609000
	1	-6.103197000	-0.341478000	1.327807000
	1	-6.319303000	-0.354896000	-0.437485000
	6	-0.786314000	2.318466000	-0.250215000
	8	0.223937000	1.525106000	-0.404522000
	6	-0.422342000	3.788454000	-0.311818000
	6	-2.105839000	1.938635000	-0.047236000
	1	-2.874529000	2.695264000	0.052894000
	29	0.146990000	-0.401362000	-0.249172000
	17	0.235829000	-2.634172000	-0.593499000
	8	0.897563000	-0.344399000	1.880727000
	1	0.893785000	-1.268399000	2.215188000

	1	0.057938000	4.003882000	-1.271528000
	1	-1.298671000	4.428030000	-0.193150000
	1	0.302316000	4.014425000	0.477036000
	6	2.805423000	-0.180636000	0.211568000
	8	2.096367000	-0.308111000	-0.814574000
	7	4.114960000	-0.004022000	0.220354000
	1	2.131199000	-0.232648000	1.233993000
	6	4.845260000	0.139448000	1.483938000
	1	4.150757000	0.067796000	2.321516000
	1	5.596705000	-0.651725000	1.569476000
	1	5.347060000	1.111738000	1.514144000
	6	4.903797000	0.073776000	-1.018165000
	1	4.248548000	-0.069497000	-1.876300000
	1	5.387421000	1.053433000	-1.085207000
	1	5.673648000	-0.704038000	-1.009912000
INT5	6	-2.020419000	0.782445000	0.006746000
	8	-1.513763000	-0.295094000	0.360068000
	8	-3.352074000	0.944351000	-0.012370000
	6	-4.171472000	-0.205043000	0.362495000
	6	-5.624673000	0.213625000	0.238889000
	1	-3.912298000	-0.493123000	1.384871000
	1	-3.924130000	-1.035859000	-0.303929000
	1	-6.266662000	-0.628792000	0.515370000
	1	-5.851732000	1.051284000	0.904984000
	1	-5.864837000	0.505981000	-0.787630000
	6	-0.007281000	2.258532000	-0.355671000
	8	0.817308000	1.344067000	0.247917000
	6	0.577039000	3.568902000	-0.799422000
	6	-1.337326000	2.002154000	-0.416185000
	1	-1.983344000	2.791392000	-0.784774000
	29	-0.027463000	-1.496271000	-0.240300000
	17	1.167355000	-2.528759000	-1.771055000
	8	0.151735000	-2.356367000	1.845867000
	1	-0.686724000	-2.262313000	2.342997000
	1	1.176953000	3.443165000	-1.703243000
	1	-0.222633000	4.285186000	-0.994857000
	1	1.233901000	3.973181000	-0.021512000
	6	2.153644000	1.197901000	-0.147232000
	8	2.532414000	1.462690000	-1.281447000
	7	2.891048000	0.698539000	0.865898000
	1	0.325724000	-3.319450000	1.816156000
	6	2.350308000	0.402531000	2.199416000
	1	1.596715000	1.137447000	2.479845000
	1	1.904848000	-0.597552000	2.235436000

	1	3.172770000	0.457298000	2.917044000
	6	4.263141000	0.265646000	0.599536000
	1	4.519558000	0.484575000	-0.435378000
	1	4.956090000	0.793305000	1.263371000
	1	4.357136000	-0.812063000	0.774892000
TS6	6	-0.563184000	1.750509000	0.331236000
	8	-0.362390000	0.668632000	0.883319000
	8	-1.785705000	2.314185000	0.245900000
	6	-2.893715000	1.579305000	0.844492000
	6	-4.154817000	2.394506000	0.622917000
	1	-2.679716000	1.437044000	1.907735000
	1	-2.953418000	0.596137000	0.368542000
	1	-5.007969000	1.868379000	1.063151000
	1	-4.077072000	3.378128000	1.095887000
	1	-4.351150000	2.533562000	-0.444446000
	6	1.762990000	2.335952000	-0.409417000
	8	2.342742000	1.209332000	0.149799000
	6	2.766533000	3.242839000	-1.049875000
	6	0.446521000	2.606958000	-0.309530000
	1	0.086283000	3.539803000	-0.731716000
	29	-1.147396000	-1.774231000	0.074192000
	17	-2.255821000	-1.834009000	-1.781706000
	8	-0.218448000	-1.970529000	1.808169000
	1	-0.211451000	-1.099512000	2.262056000
	1	3.239775000	2.729162000	-1.895170000
	1	2.306295000	4.166877000	-1.404369000
	1	3.559315000	3.487434000	-0.333999000
	6	2.170610000	-0.017422000	-0.476183000
	8	1.633442000	-0.120580000	-1.574742000
	7	2.710524000	-1.023725000	0.247845000
	1	-0.624665000	-2.608656000	2.434613000
	6	3.256148000	-0.880412000	1.597055000
	1	3.284639000	0.165338000	1.891688000
	1	2.636861000	-1.437287000	2.309877000
	1	4.273583000	-1.286405000	1.626695000
	6	2.622313000	-2.390414000	-0.263320000
	1	2.326346000	-2.371523000	-1.310762000
	1	3.599301000	-2.876959000	-0.172423000
	1	1.885280000	-2.963844000	0.311336000
INT6	6	-2.501453000	-0.200117000	0.080437000
	8	-1.893085000	0.055164000	-0.963559000
	8	-3.786285000	0.154643000	0.257941000
	6	-4.434522000	0.872719000	-0.834518000
	6	-5.855078000	1.179995000	-0.397579000

	1	-4.406685000	0.240945000	-1.726578000
	1	-3.861140000	1.781372000	-1.037817000
	1	-6.370295000	1.719579000	-1.198662000
	1	-6.411229000	0.260977000	-0.189927000
	1	-5.864719000	1.806157000	0.499555000
	6	-0.831131000	-1.572675000	1.377638000
	8	-0.074814000	-1.804706000	0.245971000
	6	-0.383518000	-2.251390000	2.638620000
	6	-1.988527000	-0.884425000	1.276033000
	1	-2.630637000	-0.845437000	2.149744000
	29	1.567041000	1.761725000	-0.328698000
	17	2.557845000	3.182277000	0.963666000
	8	0.663873000	0.602895000	-1.615076000
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	1	0.558168000	-1.824372000	2.992886000
	1	-1.138052000	-2.145024000	3.419721000
	1	-0.217230000	-3.317685000	2.447295000
	6	1.299428000	-1.597407000	0.286079000
	8	1.812853000	-0.824636000	1.091943000
	7	1.937017000	-2.309442000	-0.666846000
	1	0.613990000	0.984104000	-2.518251000
	6	1.246175000	-3.131524000	-1.662616000
	1	1.891461000	-3.974197000	-1.925707000
	1	0.311412000	-3.517811000	-1.261579000
	1	1.036033000	-2.551260000	-2.569515000
	6	3.345399000	-2.017704000	-0.935192000
	1	3.760026000	-1.433051000	-0.116257000
	1	3.900681000	-2.956082000	-1.027801000
	1	3.446335000	-1.452277000	-1.869680000
3a	6	1.623880000	0.015014000	-0.097296000
	8	1.051714000	-1.062346000	-0.210207000
	8	2.970145000	0.129385000	0.018499000
	6	3.731368000	-1.110565000	0.005443000
	6	5.198949000	-0.750499000	0.153593000
	1	3.532003000	-1.632108000	-0.935341000
	1	3.381164000	-1.742951000	0.826604000
	1	5.799999000	-1.665556000	0.147434000
	1	5.533853000	-0.114518000	-0.671466000
	1	5.382609000	-0.225832000	1.096128000
	6	-0.303365000	1.625405000	-0.221193000
	8	-1.203526000	0.631246000	-0.588007000
	6	-0.908073000	2.993275000	-0.151855000
	6	1.003790000	1.355435000	-0.052142000
	1	1.674064000	2.187736000	0.139197000

	1	-1.677659000	3.018592000	0.627683000
	1	-0.154793000	3.752321000	0.067530000
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	6	-1.945208000	0.033599000	0.412865000
	8	-1.789512000	0.315072000	1.598913000
	7	-2.831948000	-0.860238000	-0.085916000
	6	-2.991085000	-1.172541000	-1.505784000
	1	-2.349504000	-0.539407000	-2.112948000
	1	-2.733736000	-2.222313000	-1.690677000
	1	-4.033987000	-1.013554000	-1.803305000
	6	-3.685558000	-1.608841000	0.833710000
	1	-3.468291000	-1.311576000	1.857937000
	1	-4.741060000	-1.408488000	0.615229000
	1	-3.504773000	-2.684558000	0.723162000
CAT-H₂O	6	0.249558000	2.122985000	-0.261430000
	8	-0.815102000	1.724619000	0.213511000
	6	1.478004000	-0.076207000	-0.376813000
	8	0.656046000	-0.832434000	0.128697000
	6	1.109708000	1.199126000	-1.121003000
	1	2.006167000	1.702160000	-1.483857000
	1	0.495419000	0.900341000	-1.980960000
	29	-1.609602000	-0.246183000	0.144847000
	17	-3.022267000	-1.415490000	-1.128329000
	8	2.794569000	-0.273127000	-0.344055000
	6	3.269281000	-1.487880000	0.328212000
	1	2.803706000	-2.347773000	-0.160027000
	1	2.933001000	-1.451100000	1.367536000
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	1	5.095815000	-1.531443000	-0.835270000
	1	5.166013000	-2.405933000	0.706473000
	6	0.739403000	3.524905000	-0.036159000
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	1	1.724918000	3.500198000	0.444550000
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	1	-1.874496000	0.636284000	2.717141000
	1	-2.677806000	-0.687815000	2.603408000
TS7	6	-0.709002000	-0.449034000	2.168446000
	8	-0.886969000	0.731977000	1.856328000
	6	-1.307523000	-1.494679000	-0.062757000
	8	-1.583858000	-0.492577000	-0.714769000
	6	-0.365879000	-1.507323000	1.129578000
	1	-0.334209000	-2.502088000	1.574928000

	1	0.635157000	-1.263746000	0.743289000
	29	-0.880091000	1.585912000	0.020991000
	17	-0.607485000	3.233602000	-1.438516000
	8	1.808640000	0.751513000	-0.373407000
	1	1.626039000	0.974404000	-1.317300000
	8	-1.787400000	-2.707775000	-0.328272000
	6	-2.678904000	-2.833236000	-1.486990000
	1	-2.138375000	-2.479685000	-2.368709000
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	6	-3.072541000	-4.293368000	-1.599458000
	1	-3.599630000	-4.630082000	-0.702005000
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	1	-3.740444000	-4.418901000	-2.457545000
	6	-0.798299000	-0.887154000	3.601438000
	1	0.130324000	-1.391834000	3.893709000
	1	-0.985072000	-0.034824000	4.255783000
	1	-1.602164000	-1.626033000	3.707340000
	8	2.399649000	-0.580632000	-0.495494000
	6	3.838935000	-0.518837000	-0.231035000
	6	4.090032000	-0.001957000	1.189242000
	1	3.582215000	-0.633465000	1.925630000
	1	5.162377000	-0.011930000	1.409976000
	1	3.727681000	1.023293000	1.299742000
	6	4.534548000	0.348712000	-1.285620000
	1	4.218914000	1.392817000	-1.206143000
	1	5.619665000	0.313437000	-1.145473000
	1	4.307740000	-0.011953000	-2.294430000
	6	4.240739000	-1.992862000	-0.369540000
	1	4.029038000	-2.364503000	-1.376881000
	1	5.313432000	-2.098627000	-0.181964000
	1	3.702998000	-2.614445000	0.353122000
	8	-3.509840000	2.781492000	0.270493000
	1	-3.314231000	3.207328000	1.127214000
	1	-2.910221000	3.225070000	-0.360426000
COM2-a	6	-0.733325000	-0.373143000	2.031941000
	8	-0.108497000	0.611320000	1.632130000
	6	-2.145322000	-0.772335000	-0.035991000
	8	-1.755415000	0.124893000	-0.776703000
	6	-1.298117000	-1.401542000	1.056881000
	1	-1.862376000	-2.175744000	1.577223000
	1	-0.429750000	-1.859200000	0.563562000
	29	0.175826000	1.297722000	-0.309655000
	17	0.533049000	3.216958000	-1.413587000
	8	1.529645000	-0.277955000	-1.197951000

	1	1.188402000	-0.524959000	-2.093056000
	8	-3.358183000	-1.317056000	-0.103310000
	6	-4.258445000	-0.813030000	-1.146673000
	1	-3.766228000	-0.950929000	-2.112741000
	1	-4.404360000	0.256886000	-0.977854000
	6	-5.553830000	-1.594613000	-1.043296000
	1	-6.022436000	-1.453978000	-0.064912000
	1	-5.383342000	-2.663372000	-1.202356000
	1	-6.248387000	-1.239365000	-1.811115000
	6	-0.939229000	-0.622702000	3.498308000
	1	-0.550031000	-1.612814000	3.764287000
	1	-0.447052000	0.146754000	4.094404000
	1	-2.013699000	-0.639635000	3.718593000
	8	1.634890000	-1.590478000	-0.551585000
	6	3.047486000	-1.901691000	-0.315375000
	6	3.665101000	-0.842690000	0.603001000
	1	3.104802000	-0.770543000	1.540484000
	1	4.700528000	-1.108176000	0.839298000
	1	3.666185000	0.138485000	0.121306000
	6	3.792756000	-2.013236000	-1.649080000
	1	3.825673000	-1.048438000	-2.162607000
	1	4.823557000	-2.338653000	-1.476532000
	1	3.307448000	-2.744533000	-2.303757000
	6	2.947052000	-3.263380000	0.383945000
	1	2.465792000	-4.003297000	-0.262941000
	1	3.951924000	-3.621186000	0.627174000
	1	2.376880000	-3.185982000	1.314892000
	8	0.911127000	4.133173000	1.748352000
	1	0.773251000	3.284564000	2.207952000
	1	0.809121000	3.910888000	0.800217000
DMF-H₂O	8	3.700722000	-0.216506000	-0.073348000
	1	2.757148000	0.060188000	-0.074240000
	1	3.920243000	-0.348050000	0.866861000
	6	0.107678000	-0.300023000	-0.031164000
	8	0.985270000	0.582319000	-0.040486000
	7	-1.220596000	-0.077278000	0.000201000
	1	0.370166000	-1.370647000	-0.048746000
	6	-1.762646000	1.278754000	0.027321000
	1	-2.402870000	1.446065000	-0.846111000
	1	-2.360030000	1.427680000	0.933836000
	1	-0.938541000	1.991188000	0.014796000
	6	-2.179443000	-1.178543000	0.008813000
	1	-2.797868000	-1.139059000	0.912508000
	1	-2.835245000	-1.120432000	-0.867110000

	1	-1.650299000	-2.133617000	-0.012352000
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Table S1-2. Some optimized Cartesian Coordinates of stationary points for the entire catalytic cycle, involved in the discussion on m-CPBA (**OX-b**) as oxidant, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide with bond lengths in Å.

Species	Cartesian coordinates			
m-CPBA	6	-1.988159000	0.241958000	0.000170000
	8	-2.868705000	1.079518000	-0.000037000
	6	-0.520885000	0.524725000	0.000095000
	6	-0.120964000	1.869907000	0.000104000
	6	0.440265000	-0.501081000	0.000009000
	6	1.237638000	2.189913000	0.000038000
	6	1.790651000	-0.155833000	-0.000061000
	6	2.205442000	1.179423000	-0.000046000
	1	-0.875314000	2.651054000	0.000167000
	1	0.144121000	-1.544916000	-0.000009000
	1	1.552215000	3.230671000	0.000050000
	1	3.264050000	1.425465000	-0.000102000
	8	-2.214399000	-1.102909000	0.000156000
	8	-3.638395000	-1.367069000	-0.000011000
	1	-3.599062000	-2.358304000	0.000165000
	17	3.001297000	-1.433786000	-0.000175000
	COM1-b1	6	-2.969466000	-1.263195000
8		-2.793568000	-0.348963000	-0.736654000
8		-3.942212000	-2.166398000	-0.043912000
6		-4.836444000	-2.049225000	-1.201145000
6		-5.841096000	-3.181810000	-1.113998000
1		-4.226158000	-2.104366000	-2.106207000
1		-5.313696000	-1.066825000	-1.160421000
1		-6.524711000	-3.120312000	-1.966665000
1		-5.342090000	-4.154824000	-1.143363000
1		-6.431298000	-3.115744000	-0.195343000
6		-2.090805000	-0.290749000	2.231115000
8		-1.840228000	0.838431000	1.814297000
6		-2.368626000	-0.554227000	3.684636000
1		-1.669929000	-1.309163000	4.064800000
1		-2.281829000	0.364204000	4.266599000
1		-3.375372000	-0.975555000	3.794792000
6		-2.104032000	-1.497376000	1.288211000
1		-1.072945000	-1.628276000	0.936025000
1		-2.415180000	-2.404049000	1.807421000
29		-1.491075000	1.467455000	-0.248481000

	17	-2.003860000	3.422359000	-1.212529000
	6	2.696928000	-0.069072000	-0.573198000
	6	3.790511000	-0.239894000	0.293109000
	6	2.672449000	-0.715765000	-1.820660000
	6	4.842641000	-1.059086000	-0.111017000
	6	3.752712000	-1.506892000	-2.213569000
	6	4.845582000	-1.688147000	-1.359769000
	1	3.814853000	0.233572000	1.268115000
	1	1.815658000	-0.588647000	-2.476281000
	1	3.745561000	-1.993712000	-3.185544000
	1	5.684372000	-2.311732000	-1.658032000
	6	1.483347000	0.695714000	-0.191316000
	8	0.350665000	0.340866000	-0.511983000
	8	1.531411000	1.837719000	0.546650000
	8	2.856830000	2.429983000	0.618568000
	1	2.904549000	2.624386000	1.591709000
	17	6.202918000	-1.301177000	0.978532000
TS1-b1	6	-3.189467000	-1.016426000	-0.088825000
	8	-2.896745000	0.049623000	-0.626588000
	8	-4.354211000	-1.630708000	-0.267049000
	6	-5.320933000	-0.989088000	-1.167067000
	6	-6.551098000	-1.874230000	-1.214180000
	1	-4.848366000	-0.881147000	-2.146561000
	1	-5.539217000	0.005934000	-0.771397000
	1	-7.292531000	-1.420183000	-1.879172000
	1	-6.307237000	-2.868490000	-1.599532000
	1	-6.999078000	-1.980250000	-0.221910000
	6	-1.817963000	-0.954910000	2.049983000
	8	-1.353355000	0.171425000	1.905632000
	6	-1.939891000	-1.601699000	3.402698000
	1	-1.415675000	-2.564851000	3.402570000
	1	-1.531671000	-0.951986000	4.177930000
	1	-2.994737000	-1.818614000	3.610828000
	6	-2.274164000	-1.786045000	0.844481000
	1	-1.366534000	-2.032709000	0.279153000
	1	-2.751609000	-2.714322000	1.158896000
	29	-1.092747000	1.266024000	-0.146609000
	17	-1.875040000	3.359626000	-0.000368000
	6	2.604788000	-0.329305000	-0.712356000
	6	3.720777000	-0.035346000	0.089403000
	6	2.649487000	-1.390217000	-1.633996000
	6	4.866841000	-0.814846000	-0.050140000
	6	3.818561000	-2.138414000	-1.772162000
	6	4.935836000	-1.859102000	-0.977416000

	1	3.688713000	0.774092000	0.808941000
	1	1.776384000	-1.615653000	-2.239664000
	1	3.864631000	-2.949121000	-2.494920000
	1	5.845269000	-2.446317000	-1.075498000
	6	1.319376000	0.385731000	-0.562954000
	8	0.225132000	-0.178596000	-0.783138000
	8	1.200144000	1.647033000	-0.154874000
	17	6.262983000	-0.471050000	0.964684000
	8	2.660034000	2.525254000	-0.328639000
	1	2.185418000	3.394250000	-0.358946000
INT1-b1	6	-3.155646000	-0.760760000	-0.179559000
	8	-2.640714000	0.254233000	-0.664861000
	8	-4.330999000	-1.213809000	-0.571979000
	6	-5.027140000	-0.477390000	-1.641200000
	6	-6.329990000	-1.202935000	-1.910820000
	1	-4.369912000	-0.458490000	-2.513764000
	1	-5.182128000	0.546137000	-1.292168000
	1	-6.871249000	-0.676694000	-2.703308000
	1	-6.149071000	-2.229634000	-2.241498000
	1	-6.962131000	-1.224026000	-1.018551000
	6	-2.068379000	-0.820655000	2.123643000
	8	-1.444947000	0.228567000	1.999435000
	6	-2.386452000	-1.409222000	3.469757000
	1	-2.024091000	-2.442851000	3.520024000
	1	-1.937103000	-0.812955000	4.264817000
	1	-3.474667000	-1.450778000	3.601144000
	6	-2.529614000	-1.618081000	0.897896000
	1	-1.622482000	-2.065140000	0.468986000
	1	-3.211971000	-2.422050000	1.175002000
	29	-0.836761000	1.084545000	-0.086325000
	17	-1.556429000	3.209563000	0.012597000
	6	2.683664000	-0.530337000	-0.369082000
	6	3.821423000	0.262169000	-0.147084000
	6	2.814138000	-1.892117000	-0.681597000
	6	5.079897000	-0.327732000	-0.241811000
	6	4.085940000	-2.461494000	-0.771221000
	6	5.228622000	-1.683568000	-0.551911000
	1	3.713783000	1.315406000	0.093858000
	1	1.924860000	-2.492118000	-0.851173000
	1	4.196958000	-3.515779000	-1.012654000
	1	6.219647000	-2.124625000	-0.621121000
	6	1.336812000	0.084837000	-0.271299000
	8	0.274807000	-0.602769000	-0.470903000
	8	1.192278000	1.324435000	0.017793000

	17	6.514817000	0.655158000	0.034679000
•OH	8	0.000000000	0.000000000	0.110774000
	1	0.000000000	0.000000000	-0.886189000
TS2-b1	6	2.937242000	-0.698853000	-0.201290000
	8	1.971134000	-1.265083000	-0.732870000
	8	4.112138000	-0.605301000	-0.822857000
	6	4.228438000	-1.217114000	-2.153205000
	6	5.652889000	-1.002638000	-2.626052000
	1	3.495388000	-0.740461000	-2.808989000
	1	3.977945000	-2.276337000	-2.058175000
	1	5.770283000	-1.453618000	-3.616424000
	1	5.888811000	0.062615000	-2.705064000
	1	6.369132000	-1.473694000	-1.946791000
	6	2.001439000	-0.396129000	2.181793000
	8	0.902020000	-0.914869000	1.950775000
	6	2.418598000	-0.069268000	3.594855000
	1	2.775178000	0.964391000	3.663953000
	1	1.582219000	-0.222477000	4.278028000
	1	3.253918000	-0.716238000	3.888882000
	6	2.962333000	-0.014891000	1.113127000
	1	2.588706000	1.273076000	0.855400000
	1	3.980405000	0.149943000	1.468954000
	29	0.098512000	-1.703748000	-0.001275000
	17	0.440165000	-3.922169000	0.241012000
	6	-3.149959000	0.385610000	-0.460226000
	6	-4.387877000	-0.206567000	-0.162987000
	6	-3.085835000	1.715164000	-0.904029000
	6	-5.548502000	0.548757000	-0.316226000
	6	-4.262399000	2.452965000	-1.049967000
	6	-5.503212000	1.875339000	-0.757031000
	1	-4.431224000	-1.235856000	0.179909000
	1	-2.120932000	2.159388000	-1.130073000
	1	-4.222103000	3.484031000	-1.392719000
	1	-6.420485000	2.447485000	-0.869676000
	6	-1.903767000	-0.407222000	-0.300623000
	8	-0.758802000	0.090927000	-0.572705000
8	-1.940948000	-1.618114000	0.119308000	
6	2.090325000	2.582825000	0.781537000	
8	1.052694000	2.737353000	1.399962000	
7	2.821689000	3.440222000	0.076267000	
6	4.071201000	3.070074000	-0.593859000	
1	4.302123000	2.019515000	-0.424015000	
1	3.978218000	3.243152000	-1.670774000	
1	4.892196000	3.680820000	-0.205201000	

	6	2.395004000	4.844962000	-0.057047000
	1	1.454912000	4.989139000	0.473860000
	1	3.161330000	5.501640000	0.366830000
	1	2.260074000	5.086102000	-1.116069000
	17	-7.107587000	-0.183294000	0.053443000
INT2-b1	6	3.690318000	-0.544250000	-0.129030000
	8	2.893446000	0.454992000	-0.073447000
	8	4.994000000	-0.296863000	-0.079451000
	6	5.444832000	1.094439000	0.042348000
	6	6.959675000	1.065590000	0.097651000
	1	5.005584000	1.517140000	0.949294000
	1	5.073020000	1.649904000	-0.822047000
	1	7.332152000	2.090899000	0.187720000
	1	7.312092000	0.494654000	0.961511000
	1	7.379362000	0.626144000	-0.811854000
	6	2.011698000	-2.313874000	-0.306822000
	8	0.967208000	-1.536774000	-0.331264000
	6	1.647253000	-3.781592000	-0.371434000
	1	1.028837000	-4.038050000	0.494400000
	1	1.054280000	-3.969990000	-1.271428000
	1	2.539681000	-4.409235000	-0.381823000
	6	3.330147000	-1.911196000	-0.231725000
	1	4.127861000	-2.643899000	-0.240244000
	29	1.013136000	0.344523000	-0.195960000
	17	0.881434000	2.545975000	-0.181726000
	6	-2.901901000	0.036456000	0.795516000
	6	-3.609802000	0.173760000	-0.409269000
	6	-3.585970000	-0.212543000	1.994702000
	6	-4.999264000	0.061289000	-0.389876000
	6	-4.978028000	-0.322675000	1.988621000
	6	-5.697141000	-0.186380000	0.795673000
	1	-3.083084000	0.367194000	-1.337987000
	1	-3.023712000	-0.315723000	2.917856000
	1	-5.513394000	-0.514625000	2.915438000
	1	-6.780724000	-0.270590000	0.788470000
	6	-1.403088000	0.153894000	0.835924000
	8	-0.758936000	0.120628000	1.888341000
	8	-0.851231000	0.289070000	-0.354463000
	17	-5.895621000	0.236325000	-1.896973000
INT3-b1	6	3.251359000	1.302159000	0.468124000
	8	2.512230000	0.901530000	-0.490347000
	8	4.541655000	1.514677000	0.211439000
	6	5.033900000	1.272913000	-1.147133000
	6	6.518525000	1.582506000	-1.143649000

	1	4.479873000	1.919136000	-1.832686000
	1	4.830816000	0.230678000	-1.405713000
	1	6.921415000	1.412185000	-2.147084000
	1	6.703270000	2.625836000	-0.871737000
	1	7.054733000	0.935141000	-0.443622000
	6	1.537621000	1.434938000	2.214229000
	8	0.536212000	1.025587000	1.495951000
	6	1.133870000	1.786185000	3.632052000
	6	2.849743000	1.567701000	1.801981000
	1	3.605967000	1.915713000	2.494886000
	29	0.669497000	0.443839000	-0.305275000
	17	0.588039000	-0.039978000	-2.470096000
	8	-1.187237000	0.148064000	-0.227217000
	1	0.686133000	0.909167000	4.109326000
	1	1.992149000	2.122508000	4.215876000
	1	0.375866000	2.575138000	3.608070000
	6	1.721874000	-2.593815000	-0.207729000
	8	1.194025000	-1.698338000	0.479000000
	7	2.051625000	-3.818084000	0.241069000
	1	1.958063000	-2.430946000	-1.269983000
	6	2.666393000	-4.811299000	-0.636162000
	1	2.794352000	-4.395344000	-1.637686000
	1	3.648032000	-5.105638000	-0.248716000
	1	2.033864000	-5.703350000	-0.703339000
	6	1.807050000	-4.213184000	1.626211000
	1	1.350731000	-3.379789000	2.158927000
	1	1.135122000	-5.078096000	1.657445000
	1	2.751009000	-4.484214000	2.111961000
	6	-1.877516000	1.245847000	-0.449151000
	8	-1.381820000	2.340789000	-0.729903000
	6	-3.367617000	1.049427000	-0.322481000
	6	-3.917673000	-0.220565000	-0.086541000
	6	-4.203786000	2.168685000	-0.447821000
	6	-5.302347000	-0.346714000	0.017385000
	6	-5.587932000	2.018027000	-0.338215000
	6	-6.150077000	0.757789000	-0.104691000
	1	-3.273841000	-1.088426000	0.010563000
	1	-3.763440000	3.144130000	-0.630754000
	1	-6.239568000	2.883202000	-0.435264000
	1	-7.226889000	0.637206000	-0.019905000
	17	-5.999526000	-1.939496000	0.309808000
TS3-b1	6	2.313574000	1.902556000	0.584806000
	8	2.071543000	1.275091000	-0.463686000
	8	3.110457000	2.984744000	0.581540000

	6	3.671747000	3.396442000	-0.701102000
	6	4.484831000	4.654385000	-0.457713000
	1	2.848073000	3.567498000	-1.399865000
	1	4.287348000	2.579194000	-1.087057000
	1	4.922207000	4.989618000	-1.403590000
	1	3.856830000	5.459688000	-0.065160000
	1	5.298467000	4.467312000	0.249421000
	6	1.074116000	0.459362000	2.198542000
	8	0.813334000	-0.526984000	1.382436000
	6	0.492167000	0.258146000	3.582936000
	6	1.809733000	1.591336000	1.905062000
	1	2.008107000	2.309343000	2.692775000
	29	0.691516000	-0.399574000	-0.501596000
	17	0.459483000	-0.451232000	-2.715439000
	8	-1.205705000	-0.327585000	-0.313588000
	1	0.781082000	-0.725956000	3.963618000
	1	0.831333000	1.030248000	4.275990000
	1	-0.600932000	0.281684000	3.521750000
	6	2.675634000	-2.442973000	0.263330000
	8	2.315767000	-1.704439000	-0.689775000
	7	3.680534000	-3.314048000	0.186671000
	1	2.161328000	-2.396918000	1.231038000
	6	4.049849000	-4.151114000	1.330111000
	1	3.398750000	-3.933043000	2.178464000
	1	3.949391000	-5.208813000	1.066473000
	1	5.087516000	-3.953455000	1.617321000
	6	4.461383000	-3.483167000	-1.040941000
	1	4.087694000	-2.802263000	-1.803821000
	1	5.515466000	-3.266670000	-0.839556000
	1	4.372957000	-4.515318000	-1.395225000
	6	-1.782363000	0.849953000	-0.349515000
	8	-1.206833000	1.930060000	-0.501813000
	6	-3.283674000	0.773266000	-0.169753000
	6	-4.011508000	1.969574000	-0.088436000
	6	-3.946529000	-0.461508000	-0.087782000
	6	-5.398418000	1.931451000	0.073550000
	6	-5.331686000	-0.475018000	0.071768000
	6	-6.072020000	0.707368000	0.154943000
	1	-3.485241000	2.916934000	-0.154223000
	1	-3.387203000	-1.388876000	-0.150292000
	1	-5.965311000	2.857385000	0.136586000
	1	-7.151144000	0.674049000	0.279870000
	17	-6.169128000	-2.024244000	0.171046000
INT4-b1	6	1.503168000	1.985524000	0.671002000

8	1.929709000	1.235599000	-0.220497000
8	1.649270000	3.323441000	0.615917000
6	2.336859000	3.864477000	-0.549741000
6	2.345128000	5.376217000	-0.414344000
1	1.806929000	3.534823000	-1.447591000
1	3.349268000	3.451121000	-0.577270000
1	2.857553000	5.813809000	-1.277127000
1	1.326481000	5.774273000	-0.381852000
1	2.872275000	5.688207000	0.492277000
6	0.604099000	0.231690000	2.206518000
8	1.042211000	-0.775620000	1.500903000
6	-0.168489000	-0.147576000	3.449585000
6	0.821160000	1.561498000	1.883729000
1	0.443895000	2.337715000	2.540915000
29	0.854083000	-0.885264000	-0.411685000
17	0.632255000	-1.302766000	-2.603719000
8	-0.995601000	-0.604575000	-0.225440000
1	-0.395267000	0.721557000	4.070641000
1	-1.103865000	-0.635962000	3.156289000
1	0.409990000	-0.869315000	4.034426000
6	3.599873000	-1.307706000	0.119090000
8	2.592432000	-1.810200000	-0.458364000
7	4.776138000	-1.916770000	0.183472000
1	3.532880000	-0.322264000	0.587839000
6	5.918762000	-1.290271000	0.855001000
1	5.630423000	-0.315626000	1.251898000
1	6.258343000	-1.926040000	1.678384000
1	6.739558000	-1.158658000	0.143316000
6	4.996639000	-3.240602000	-0.407211000
1	4.077604000	-3.587838000	-0.875884000
1	5.791051000	-3.178015000	-1.157382000
1	5.299888000	-3.943924000	0.374606000
6	-1.594855000	0.458585000	-0.716717000
8	-1.051865000	1.410619000	-1.277043000
6	-3.094393000	0.421681000	-0.505501000
6	-3.730971000	-0.714757000	0.017930000
6	-3.848614000	1.552320000	-0.852998000
6	-5.115795000	-0.698680000	0.180833000
6	-5.234387000	1.546833000	-0.678120000
6	-5.881707000	0.419501000	-0.159411000
1	-3.151526000	-1.591121000	0.287647000
1	-3.343056000	2.423446000	-1.258384000
1	-5.821222000	2.422070000	-0.947012000
1	-6.959992000	0.410957000	-0.023571000

	17	-5.919942000	-2.126980000	0.833172000
TS4-b1	6	3.325633000	-1.131239000	-0.450209000
	8	3.094603000	0.029448000	0.021641000
	8	4.484935000	-1.714912000	-0.138159000
	6	5.420894000	-0.987512000	0.720276000
	6	6.640716000	-1.871006000	0.899826000
	1	4.923533000	-0.775762000	1.670245000
	1	5.667408000	-0.039292000	0.235704000
	1	7.364466000	-1.356321000	1.539787000
	1	6.374328000	-2.819125000	1.376108000
	1	7.120132000	-2.081609000	-0.060666000
	6	1.221052000	-1.466068000	-1.678776000
	8	0.660618000	-0.339169000	-1.348039000
	6	0.361423000	-2.329082000	-2.576912000
	6	2.475684000	-1.899467000	-1.288136000
	1	2.840161000	-2.865234000	-1.616595000
	29	1.509792000	1.054036000	-0.342547000
	17	2.328530000	2.798957000	0.802195000
	8	-0.459059000	0.479720000	1.730991000
	1	0.130167000	-1.778040000	-3.494040000
	1	0.862182000	-3.264686000	-2.831430000
	1	-0.587860000	-2.549595000	-2.079620000
	6	-1.041436000	2.044823000	-0.223074000
	8	0.019704000	2.159833000	-0.892338000
	7	-2.140209000	2.714464000	-0.521293000
	1	-0.921703000	1.138981000	0.872569000
	6	-3.351072000	2.597490000	0.297559000
	1	-3.164112000	1.945542000	1.149670000
	1	-3.641250000	3.588099000	0.661344000
	1	-4.168470000	2.184306000	-0.301415000
	6	-2.223308000	3.621826000	-1.680457000
	1	-1.276033000	3.617921000	-2.217354000
	1	-3.024893000	3.287890000	-2.346272000
	1	-2.446012000	4.635687000	-1.333990000
	6	-1.195144000	-0.438494000	2.342598000
	8	-0.863249000	-0.871206000	3.447713000
	6	-2.433983000	-0.945489000	1.655808000
	6	-2.514120000	-1.022077000	0.255999000
	6	-3.510535000	-1.381571000	2.443945000
	6	-3.674962000	-1.530986000	-0.328860000
6	-4.670010000	-1.867901000	1.836875000	
6	-4.761457000	-1.949624000	0.442480000	
1	-1.677188000	-0.721354000	-0.366365000	
1	-3.433934000	-1.328687000	3.526233000	

	1	-5.510773000	-2.190839000	2.446225000
	1	-5.658835000	-2.335344000	-0.034061000
	17	-3.769147000	-1.650269000	-2.084624000
INT5-b1	6	-3.155052000	-0.568051000	-1.044894000
	8	-1.949641000	-0.479071000	-0.794057000
	8	-3.723118000	-1.697316000	-1.504402000
	6	-2.848754000	-2.850437000	-1.695356000
	6	-3.705641000	-3.991849000	-2.211068000
	1	-2.382826000	-3.089463000	-0.735186000
	1	-2.063875000	-2.572960000	-2.404728000
	1	-3.076629000	-4.874439000	-2.365330000
	1	-4.489895000	-4.250680000	-1.493425000
	1	-4.174587000	-3.733623000	-3.165282000
	6	-3.956154000	1.688316000	-0.307466000
	8	-2.785637000	1.927861000	0.398548000
	6	-4.982158000	2.773563000	-0.204652000
	6	-4.152778000	0.505265000	-0.921117000
	1	-5.127783000	0.307493000	-1.355478000
	29	-0.806851000	-1.252360000	0.968742000
	17	-2.152980000	-2.216594000	2.408725000
	8	2.406637000	-1.285071000	1.788787000
	1	-4.593682000	3.696221000	-0.648321000
	1	-5.906176000	2.495302000	-0.714799000
	1	-5.201911000	2.978954000	0.849260000
	6	-1.861384000	2.796168000	-0.153869000
	8	-1.985604000	3.247454000	-1.289428000
	7	-0.853794000	3.057852000	0.711887000
	1	1.574063000	-1.552332000	2.267315000
	6	-0.736566000	2.432275000	2.030038000
	1	-1.718940000	2.190186000	2.430879000
	1	-0.135337000	1.515023000	1.982639000
	1	-0.244827000	3.136523000	2.707116000
	6	0.293343000	3.839398000	0.252435000
	1	0.084041000	4.245693000	-0.735498000
	1	0.483484000	4.662933000	0.948869000
	1	1.189928000	3.209749000	0.200350000
	6	2.096166000	-0.767890000	0.604195000
	8	0.929595000	-0.650384000	0.194571000
	6	3.257028000	-0.332031000	-0.206153000
	6	4.566492000	-0.471409000	0.286006000
	6	3.028385000	0.220771000	-1.477002000
	6	5.629814000	-0.050999000	-0.509789000
	6	4.110190000	0.634346000	-2.254688000
	6	5.419102000	0.501619000	-1.777229000

	1	4.746054000	-0.898718000	1.267143000
	1	2.011319000	0.320530000	-1.843794000
	1	3.941784000	1.062985000	-3.239451000
	1	6.263290000	0.822958000	-2.381913000
	17	7.273432000	-0.219934000	0.093888000
CAT-ROH	6	-3.648700000	0.614644000	-0.338900000
	8	-2.543130000	0.411230000	-0.836167000
	8	-4.378152000	1.698872000	-0.575929000
	6	-3.819867000	2.692664000	-1.502248000
	6	-4.832105000	3.814718000	-1.625247000
	1	-3.632816000	2.194485000	-2.456820000
	1	-2.866538000	3.035309000	-1.092267000
	1	-4.442466000	4.573464000	-2.311230000
	1	-5.782145000	3.446933000	-2.023563000
	1	-5.015134000	4.288948000	-0.656686000
	6	-3.462941000	-0.669883000	1.829025000
	8	-2.310183000	-1.077786000	1.683824000
	6	-4.072740000	-0.491287000	3.189514000
	1	-4.989787000	-1.088208000	3.264411000
	1	-3.369422000	-0.785985000	3.969346000
	1	-4.368998000	0.556033000	3.325455000
	6	-4.335597000	-0.347672000	0.614876000
	1	-4.479830000	-1.291512000	0.071600000
	1	-5.310845000	0.039022000	0.910910000
	29	-1.259507000	-1.255391000	-0.155499000
	17	-0.676563000	-3.069673000	-1.406348000
	6	2.931876000	0.330111000	0.227715000
	6	4.207693000	-0.064200000	-0.209214000
	6	2.773282000	1.498447000	0.989470000
	6	5.306765000	0.723915000	0.126811000
	6	3.888994000	2.271644000	1.313796000
	6	5.165596000	1.890394000	0.884678000
	1	4.333307000	-0.966752000	-0.798115000
	1	1.780818000	1.789911000	1.319827000
	1	3.772806000	3.177628000	1.903509000
	1	6.036372000	2.490604000	1.135544000
	6	1.728858000	-0.480404000	-0.108293000
	8	0.591554000	-0.157815000	0.258105000
	8	1.985830000	-1.569032000	-0.829532000
	1	1.135315000	-2.064507000	-1.021165000
	17	6.910153000	0.238417000	-0.416334000
COM1-b2	6	-2.095557000	-2.225142000	0.891389000
	8	-1.654831000	-1.123398000	1.224203000
	6	-3.184244000	-1.189678000	-1.158010000

	8	-2.442989000	-0.602651000	-1.931818000
	6	-2.803188000	-2.467098000	-0.434233000
	1	-3.679774000	-3.097730000	-0.256177000
	1	-2.111130000	-3.036211000	-1.066563000
	29	-1.457123000	0.803160000	0.589524000
	17	-2.350875000	2.823396000	0.491483000
	8	0.605994000	0.709822000	2.338645000
	8	-4.415119000	-0.786057000	-0.823766000
	6	-4.882168000	0.471081000	-1.415815000
	1	-4.859422000	0.361055000	-2.503490000
	1	-4.184429000	1.258910000	-1.121316000
	6	-6.285146000	0.722974000	-0.896807000
	1	-6.290486000	0.818000000	0.193137000
	1	-6.965737000	-0.084637000	-1.182870000
	1	-6.663589000	1.657480000	-1.323489000
	6	-1.948547000	-3.415479000	1.799290000
	1	-1.646038000	-4.303482000	1.235104000
	1	-1.230827000	-3.203878000	2.593104000
	1	-2.925376000	-3.638452000	2.247084000
	1	0.417953000	-0.164189000	2.774414000
	8	1.839077000	0.411960000	1.650608000
	6	1.669706000	0.378484000	0.296063000
	8	0.592556000	0.504607000	-0.264878000
	6	2.965970000	0.168223000	-0.400574000
	6	4.183676000	0.104771000	0.299935000
	6	2.940182000	0.033720000	-1.798189000
	6	5.359959000	-0.094505000	-0.419814000
	6	4.132299000	-0.165667000	-2.495019000
	6	5.351466000	-0.231342000	-1.811589000
	1	4.214784000	0.211708000	1.379271000
	1	1.991833000	0.086106000	-2.324426000
	1	4.119579000	-0.270980000	-3.576957000
	1	6.281435000	-0.385650000	-2.352711000
	17	6.889924000	-0.173750000	0.444162000
TS1-b2	6	2.663411000	-0.172070000	2.183853000
	8	2.380966000	-1.231546000	1.633488000
	6	2.681714000	1.225541000	0.049755000
	8	2.319861000	0.388091000	-0.784781000
	6	2.356104000	1.175959000	1.525394000
	1	2.851378000	1.997892000	2.043271000
	1	1.269582000	1.310491000	1.615125000
	29	1.287661000	-1.350093000	-0.407740000
	17	2.384510000	-2.785923000	-1.729572000
	8	-0.061282000	-2.547724000	-0.117024000

	8	3.398747000	2.285836000	-0.276449000
	6	3.750916000	2.462870000	-1.694899000
	1	2.820690000	2.502958000	-2.266616000
	1	4.320888000	1.584987000	-2.008023000
	6	4.553429000	3.744095000	-1.801953000
	1	5.470059000	3.686501000	-1.208034000
	1	3.968311000	4.605577000	-1.467684000
	1	4.831386000	3.902412000	-2.848678000
	6	3.288700000	-0.124615000	3.550877000
	1	2.694281000	0.516841000	4.212098000
	1	3.368700000	-1.128073000	3.970743000
	1	4.283530000	0.332015000	3.480226000
	1	-0.337566000	-3.163095000	-0.846177000
	8	-1.792202000	-1.842815000	0.567722000
	6	-1.536126000	-0.574590000	0.489974000
	8	-0.385334000	-0.066536000	0.544535000
	6	-2.740058000	0.318558000	0.332084000
	6	-3.989729000	-0.225293000	-0.006031000
	6	-2.605505000	1.700310000	0.535461000
	6	-5.082800000	0.628469000	-0.145740000
	6	-3.715858000	2.536227000	0.396645000
	6	-4.965556000	2.007140000	0.052609000
	1	-4.096038000	-1.294336000	-0.161104000
	1	-1.634105000	2.108213000	0.798847000
	1	-3.616064000	3.607608000	0.554323000
	1	-5.831155000	2.654932000	-0.058598000
	17	-6.651800000	-0.047622000	-0.584156000
INT1-b2	6	2.578915000	-0.340101000	2.211610000
	8	2.629013000	-1.279595000	1.428764000
	6	2.027438000	1.392977000	0.418470000
	8	1.870130000	0.680332000	-0.589336000
	6	1.839650000	0.954674000	1.848786000
	1	2.108679000	1.773605000	2.517012000
	1	0.771368000	0.737216000	1.983275000
	29	1.384836000	-1.237104000	-0.662917000
	17	3.097960000	-1.688617000	-1.966584000
	8	0.824039000	-2.955374000	-0.814828000
	1	1.442580000	-3.438598000	-1.407277000
	8	2.377103000	2.654593000	0.309552000
	6	2.558008000	3.216581000	-1.043931000
	1	1.618677000	3.081675000	-1.584895000
	1	3.341118000	2.637388000	-1.538094000
	6	2.929371000	4.675355000	-0.873970000
	1	3.861262000	4.782912000	-0.311853000

	1	2.137800000	5.226926000	-0.359022000
	1	3.071179000	5.120704000	-1.863603000
	6	3.192719000	-0.393374000	3.583999000
	1	2.449898000	-0.114495000	4.340428000
	1	3.583458000	-1.391036000	3.788167000
	1	4.001898000	0.344377000	3.648837000
	8	-0.217583000	-0.881248000	0.329392000
	6	-1.189958000	-0.541274000	-0.484528000
	8	-1.044837000	-0.379429000	-1.703671000
	6	-2.523255000	-0.350240000	0.190357000
	6	-3.584927000	0.157200000	-0.574683000
	6	-2.719719000	-0.671694000	1.542019000
	6	-4.828329000	0.335631000	0.027932000
	6	-3.976580000	-0.488008000	2.124867000
	6	-5.042225000	0.018577000	1.372893000
	1	-3.426843000	0.401246000	-1.620568000
	1	-1.895311000	-1.066902000	2.127200000
	1	-4.134919000	-0.739571000	3.170884000
	1	-6.020628000	0.163076000	1.823574000
	17	-6.165020000	0.973642000	-0.929380000
INT2-b2	6	1.583633000	-2.979888000	-1.445677000
	8	1.877238000	-1.970021000	-2.067041000
	6	1.882462000	-1.882160000	0.856303000
	8	2.028199000	-0.684321000	0.573459000
	6	1.170098000	-2.923365000	0.031339000
	1	1.281158000	-3.897536000	0.510272000
	1	0.102337000	-2.671466000	0.044504000
	29	1.457772000	0.377412000	-0.990723000
	17	3.570325000	0.916777000	-1.418935000
	8	0.992228000	1.333030000	-2.475421000
	1	1.786125000	1.778069000	-2.846105000
	8	2.365604000	-2.375322000	1.979819000
	6	3.049998000	-1.454670000	2.904052000
	1	2.351968000	-0.651262000	3.149930000
	1	3.906929000	-1.030874000	2.375474000
	6	3.458319000	-2.263412000	4.118854000
	1	4.141265000	-3.072189000	3.843797000
	1	2.585283000	-2.691465000	4.619647000
	1	3.972195000	-1.605170000	4.826366000
	6	1.563953000	-4.348983000	-2.076543000
	1	0.609144000	-4.847890000	-1.874279000
	1	1.729314000	-4.273583000	-3.152194000
	1	2.347582000	-4.969197000	-1.624387000
	8	-0.416277000	-0.138320000	-0.984271000

	6	-1.196460000	-0.291509000	0.052598000
	8	-0.851092000	-0.452049000	1.229860000
	6	-2.668085000	-0.299510000	-0.323738000
	6	-3.600370000	-0.666044000	0.659263000
	6	-3.107285000	0.053220000	-1.608620000
	6	-4.956568000	-0.673201000	0.339187000
	6	-4.473099000	0.044594000	-1.906477000
	6	-5.411373000	-0.320749000	-0.934956000
	1	-3.255889000	-0.935033000	1.652800000
	1	-2.380692000	0.334601000	-2.363806000
	1	-4.816542000	0.322271000	-2.900343000
	1	-6.473852000	-0.330806000	-1.163578000
	17	-6.129951000	-1.135243000	1.574339000
	6	0.642466000	3.279110000	0.076365000
	8	1.138977000	2.235761000	0.535196000
	7	0.427284000	4.410446000	0.778255000
	1	0.336810000	3.341786000	-0.979013000
	6	0.774765000	4.504607000	2.193294000
	1	1.504928000	5.306622000	2.350649000
	1	-0.119216000	4.723437000	2.788317000
	1	1.202466000	3.556492000	2.517455000
	6	-0.162064000	5.592340000	0.156433000
	1	-1.098031000	5.862563000	0.658443000
	1	0.526858000	6.442277000	0.220426000
	1	-0.374264000	5.391871000	-0.895946000
TS2-b2	6	1.412770000	-2.802256000	-1.480145000
	8	1.645002000	-1.738782000	-2.080003000
	6	1.905681000	-1.941187000	0.843346000
	8	2.106831000	-0.716240000	0.626156000
	6	1.226650000	-2.881831000	-0.027108000
	1	1.203958000	-3.891557000	0.381147000
	1	-0.058163000	-2.371399000	0.055027000
	29	1.629522000	0.280628000	-0.957813000
	17	3.782605000	0.703162000	-1.466063000
	8	1.175467000	1.314397000	-2.367685000
	1	1.971843000	1.641428000	-2.842533000
	8	2.270611000	-2.449239000	2.017786000
	6	2.843984000	-1.543023000	3.018645000
	1	2.128272000	-0.737224000	3.199989000
	1	3.759139000	-1.113219000	2.604404000
	6	3.110392000	-2.365971000	4.264350000
	1	3.817708000	-3.174773000	4.059005000
	1	2.185267000	-2.797660000	4.657289000
	1	3.542343000	-1.719052000	5.034499000

	6	1.238787000	-4.090313000	-2.256943000
	1	0.346312000	-4.629877000	-1.923455000
	1	1.171109000	-3.879688000	-3.325554000
	1	2.098916000	-4.744307000	-2.070848000
	8	-0.445205000	0.095106000	-0.664570000
	6	-1.352677000	-0.682932000	-0.270653000
	8	-1.208870000	-1.903979000	0.116770000
	6	-2.760971000	-0.151314000	-0.247736000
	6	-3.806742000	-0.968480000	0.210459000
	6	-3.027620000	1.154482000	-0.685477000
	6	-5.104652000	-0.460623000	0.223572000
	6	-4.336333000	1.641912000	-0.665336000
	6	-5.387361000	0.837982000	-0.209575000
	1	-3.599549000	-1.978636000	0.547492000
	1	-2.210592000	1.775117000	-1.039223000
	1	-4.547522000	2.653002000	-1.005260000
	1	-6.406898000	1.214242000	-0.192159000
	17	-6.421350000	-1.482352000	0.799499000
	6	0.887047000	3.142639000	0.122076000
	8	1.396812000	2.090700000	0.551097000
	7	0.686680000	4.256773000	0.850165000
	1	0.560527000	3.216851000	-0.925510000
	6	1.068076000	4.325331000	2.258667000
	1	1.808651000	5.118576000	2.410802000
	1	0.189425000	4.542879000	2.876160000
	1	1.494634000	3.368945000	2.558888000
	6	0.086616000	5.451880000	0.263187000
	1	-0.835188000	5.715414000	0.793678000
	1	0.780689000	6.297514000	0.325637000
	1	-0.152190000	5.270551000	-0.786805000
m-CBA	6	-0.946333000	0.190243000	-0.000082000
	6	0.203065000	-0.618286000	-0.000114000
	6	-0.826866000	1.588242000	-0.000003000
	6	1.456238000	-0.007510000	0.000027000
	6	0.438704000	2.178262000	0.000158000
	6	1.590757000	1.383837000	0.000197000
	1	0.115800000	-1.699623000	-0.000218000
	1	-1.724413000	2.199835000	-0.000066000
	1	0.536621000	3.260989000	0.000232000
	1	2.577769000	1.839487000	0.000285000
	6	-2.312808000	-0.409905000	-0.000181000
	8	-3.348624000	0.242619000	0.000003000
	8	-2.302648000	-1.759575000	-0.000075000
	1	-3.243280000	-2.070310000	0.000012000

	17	2.901831000	-1.013178000	0.000019000
TS2-b2'	6	-2.692919000	0.626518000	2.036736000
	8	-2.450082000	1.401064000	1.119811000
	6	-2.742807000	-1.459667000	0.573688000
	8	-2.372821000	-1.021530000	-0.523679000
	6	-2.379802000	-0.870724000	1.915605000
	1	-2.853578000	-1.445718000	2.711861000
	1	-1.290155000	-0.956957000	2.020950000
	29	-1.299608000	0.683979000	-0.889968000
	17	-2.802739000	1.396805000	-2.386011000
	8	-0.275792000	2.233575000	-1.296359000
	1	-0.742255000	2.821349000	-1.938643000
	8	-3.511747000	-2.527553000	0.674535000
	6	-3.915920000	-3.202862000	-0.570738000
	1	-3.006298000	-3.513680000	-1.090107000
	1	-4.444120000	-2.472631000	-1.188045000
	6	-4.792239000	-4.376132000	-0.180918000
	1	-5.686423000	-4.040867000	0.352233000
	1	-4.247396000	-5.083808000	0.450342000
	1	-5.109121000	-4.898601000	-1.088984000
	6	-3.272840000	1.082832000	3.348223000
	1	-2.647436000	0.732695000	4.177785000
	1	-3.356420000	2.170149000	3.371775000
	1	-4.262008000	0.629205000	3.485894000
	8	0.164280000	0.000485000	0.207147000
	6	0.934231000	-0.754442000	-0.526917000
	8	0.721563000	-0.995116000	-1.729217000
	6	2.127255000	-1.341228000	0.185487000
	6	2.980827000	-2.195533000	-0.529592000
	6	2.393591000	-1.052976000	1.532547000
	6	4.085306000	-2.747957000	0.115748000
	6	3.507359000	-1.617213000	2.160864000
	6	4.364104000	-2.471292000	1.457417000
	1	2.770972000	-2.414957000	-1.571775000
	1	1.730626000	-0.389824000	2.079468000
	1	3.716303000	-1.395295000	3.204801000
	1	5.230812000	-2.912488000	1.942613000
	17	5.158611000	-3.823495000	-0.782281000
	1	1.071417000	3.086668000	-0.992466000
	6	1.952767000	3.779089000	-0.745616000
8	2.899083000	3.863357000	-1.533503000	
7	1.815246000	4.417968000	0.426021000	
6	2.853690000	5.330392000	0.911693000	
1	2.426092000	6.325409000	1.074610000	

	1	3.261645000	4.961634000	1.859074000
	1	3.651940000	5.393882000	0.172921000
	6	0.643895000	4.225525000	1.281832000
	1	0.955291000	3.836895000	2.257607000
	1	0.130630000	5.181585000	1.432093000
	1	-0.043278000	3.517733000	0.817629000

Table S1-3. Some optimized Cartesian Coordinates of stationary points for the entire catalytic cycle, involved in the discussion on TBPB (**OX-d**) and BP (**OX-e**) as oxidants, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide with bond lengths in Å.

Species	Cartesian coordinates			
TBPB	6	-0.342994000	0.928640000	-0.209081000
	8	-0.131294000	2.126291000	-0.162315000
	6	-1.685315000	0.284612000	-0.095540000
	6	-2.792372000	1.127362000	0.103750000
	6	-1.871603000	-1.107382000	-0.177925000
	6	-4.073134000	0.584230000	0.221005000
	6	-3.155574000	-1.645046000	-0.060294000
	6	-4.256644000	-0.802307000	0.139193000
	1	-2.638442000	2.201009000	0.165368000
	1	-1.022517000	-1.765752000	-0.333622000
	1	-4.927050000	1.239774000	0.375547000
	1	-3.297705000	-2.721326000	-0.124561000
	1	-5.254921000	-1.225065000	0.230277000
	8	0.627374000	-0.017834000	-0.385371000
	8	1.936917000	0.603069000	-0.535766000
	6	2.928066000	-0.268492000	0.106358000
	6	2.951734000	-1.639846000	-0.576937000
	1	3.768201000	-2.244025000	-0.168639000
	1	2.016363000	-2.181482000	-0.413298000
	1	3.108775000	-1.530692000	-1.654482000
	6	2.646725000	-0.372239000	1.608280000
	1	1.704304000	-0.892413000	1.799944000
	1	3.447701000	-0.934358000	2.099009000
	1	2.596954000	0.622728000	2.061432000
	6	4.218054000	0.515499000	-0.170020000
	1	4.178880000	1.509763000	0.284765000
	1	5.066133000	-0.026479000	0.258359000
	1	4.387687000	0.625928000	-1.245214000
COM1-d	6	1.868069000	-0.574896000	-2.015245000
	8	1.380099000	0.356697000	-1.365691000
	6	2.992861000	-2.000970000	-0.225711000
	8	2.911247000	-2.798255000	0.691438000
	6	2.002544000	-1.953516000	-1.389044000
	1	2.325749000	-2.695783000	-2.126821000

	1	1.026907000	-2.263155000	-1.003808000
	29	0.877240000	0.446516000	0.623377000
	17	1.861432000	0.851171000	2.565937000
	8	-1.305697000	1.896454000	0.437870000
	8	3.970605000	-1.097771000	-0.374210000
	6	4.972422000	-1.023127000	0.690598000
	1	5.429565000	-2.010098000	0.799352000
	1	4.450315000	-0.766364000	1.615556000
	6	5.983347000	0.034778000	0.290767000
	1	5.505165000	1.011922000	0.175508000
	1	6.480335000	-0.227284000	-0.648110000
	1	6.746407000	0.116051000	1.071575000
	6	2.321216000	-0.377172000	-3.431062000
	1	1.758921000	-1.046572000	-4.093851000
	1	2.184865000	0.658612000	-3.744384000
	1	3.376167000	-0.663189000	-3.518840000
	6	-1.460011000	3.054142000	-0.467551000
	6	-2.705637000	3.852991000	-0.075847000
	1	-2.755998000	4.769594000	-0.671910000
	1	-3.619425000	3.281570000	-0.258350000
	1	-2.670035000	4.130595000	0.981935000
	6	-0.174128000	3.830905000	-0.157141000
	1	-0.159777000	4.743172000	-0.760849000
	1	-0.128728000	4.113498000	0.898287000
	1	0.713973000	3.241491000	-0.403864000
	6	-1.496313000	2.580033000	-1.921564000
	1	-0.614669000	1.975271000	-2.151486000
	1	-2.394804000	1.990635000	-2.124615000
	1	-1.506195000	3.446701000	-2.590185000
	8	-2.479318000	1.043384000	0.291152000
	6	-2.145827000	-0.271710000	0.336962000
	8	-0.996867000	-0.685290000	0.451712000
	6	-3.344918000	-1.141003000	0.239979000
	6	-4.648112000	-0.618297000	0.143402000
	6	-3.143507000	-2.532899000	0.246959000
	6	-5.737080000	-1.487141000	0.053237000
	6	-4.237191000	-3.394650000	0.156094000
	6	-5.534178000	-2.873399000	0.059112000
	1	-4.811121000	0.455141000	0.140979000
	1	-2.133793000	-2.925956000	0.323410000
	1	-6.744158000	-1.083756000	-0.020601000
	1	-4.079926000	-4.470616000	0.161374000
	1	-6.385948000	-3.546500000	-0.010988000
TS1-d	6	1.219087000	0.279016000	2.297078000

8	0.919773000	-0.798021000	1.789243000
6	2.468967000	1.194174000	0.284226000
8	2.321099000	0.265373000	-0.509945000
6	1.533653000	1.501820000	1.434213000
1	1.925417000	2.326482000	2.030355000
1	0.581106000	1.812891000	0.984471000
29	0.691814000	-1.161339000	-0.490987000
17	1.913880000	-2.735884000	-1.529706000
8	-1.015637000	-1.973127000	-0.441375000
8	3.478343000	2.051860000	0.213420000
6	4.435555000	1.878926000	-0.888197000
1	3.879226000	1.929856000	-1.827378000
1	4.877374000	0.883892000	-0.794761000
6	5.467211000	2.983173000	-0.766680000
1	6.000617000	2.921847000	0.186295000
1	5.001074000	3.969356000	-0.847991000
1	6.196758000	2.880029000	-1.576124000
6	1.260981000	0.471456000	3.788002000
1	0.618299000	1.312852000	4.073084000
1	0.943201000	-0.436410000	4.302191000
1	2.280520000	0.737871000	4.092464000
8	-2.452304000	-0.560951000	-0.930943000
6	-1.776594000	0.525895000	-0.819979000
8	-0.515339000	0.600094000	-0.917471000
6	-2.570529000	1.779086000	-0.568661000
6	-3.900548000	1.711201000	-0.120222000
6	-1.975915000	3.031482000	-0.796646000
6	-4.622262000	2.885401000	0.112395000
6	-2.702516000	4.203716000	-0.571142000
6	-4.025592000	4.132640000	-0.114145000
1	-4.358622000	0.741144000	0.051090000
1	-0.949966000	3.077759000	-1.151939000
1	-2.239438000	5.171545000	-0.750817000
1	-4.589522000	5.046018000	0.063350000
1	-5.648325000	2.829484000	0.469326000
6	-1.598809000	-3.032675000	0.305141000
6	-2.285535000	-2.464473000	1.560628000
1	-2.714158000	-3.276451000	2.157366000
1	-1.564560000	-1.920573000	2.177073000
1	-3.087172000	-1.780457000	1.271349000
6	-0.446129000	-3.984465000	0.739789000
1	-0.892111000	-4.800786000	1.317463000
1	0.070489000	-4.388070000	-0.131330000
1	0.273718000	-3.456735000	1.369565000

	6	-2.582746000	-3.788665000	-0.602900000
	1	-3.375694000	-3.114386000	-0.937183000
	1	-2.066074000	-4.181791000	-1.483548000
	1	-3.037847000	-4.624549000	-0.061585000
INT1-d	6	1.818721000	0.312737000	2.324903000
	8	1.775376000	-0.712402000	1.656718000
	6	1.672136000	1.907223000	0.343747000
	8	1.523748000	1.124257000	-0.603926000
	6	1.277302000	1.637893000	1.775632000
	1	1.567321000	2.482717000	2.401112000
	1	0.183359000	1.546640000	1.795084000
	29	0.762969000	-0.770596000	-0.583835000
	17	2.605497000	-1.490068000	-1.591807000
	8	-0.102930000	-2.372570000	-0.957193000
	8	2.203303000	3.103799000	0.178005000
	6	2.601747000	3.498122000	-1.184528000
	1	1.714755000	3.440393000	-1.819805000
	1	3.338451000	2.772931000	-1.537585000
	6	3.163988000	4.902688000	-1.097843000
	1	4.039120000	4.937938000	-0.442791000
	1	2.413793000	5.606118000	-0.725596000
	1	3.470212000	5.223992000	-2.098309000
	6	2.361953000	0.341311000	3.728027000
	1	1.622144000	0.780150000	4.407852000
	1	2.625505000	-0.664821000	4.056665000
	1	3.245973000	0.989711000	3.763565000
	8	-0.853059000	-0.073044000	0.186517000
	6	-1.653218000	0.366188000	-0.755160000
	8	-1.352984000	0.383779000	-1.960066000
	6	-2.983708000	0.868248000	-0.262614000
	6	-3.860206000	1.477400000	-1.175754000
	6	-3.364457000	0.738894000	1.083701000
	6	-5.102909000	1.951743000	-0.747802000
	6	-4.609375000	1.212063000	1.509510000
	6	-5.479811000	1.819734000	0.595530000
	1	-3.558412000	1.572651000	-2.215032000
	1	-2.687113000	0.265656000	1.788248000
	1	-5.777740000	2.422738000	-1.459322000
	1	-4.901246000	1.107130000	2.552204000
	1	-6.447988000	2.188397000	0.928074000
	6	-0.171438000	-3.415184000	-0.005938000
	6	1.201123000	-4.034074000	0.302886000
	1	1.083740000	-4.911615000	0.947564000
	1	1.707458000	-4.334060000	-0.617817000

	1	1.835524000	-3.309628000	0.821717000
	6	-0.904172000	-3.007095000	1.282176000
	1	-1.050015000	-3.881687000	1.925208000
	1	-0.320168000	-2.269564000	1.838980000
	1	-1.879285000	-2.569489000	1.053678000
	6	-1.042827000	-4.451208000	-0.793899000
	1	-2.021119000	-4.027478000	-1.032920000
	1	-0.542988000	-4.749480000	-1.718449000
	1	-1.177580000	-5.331562000	-0.156277000
TS2-d	6	1.626474000	-2.139689000	2.203871000
	8	0.448752000	-1.855384000	2.016245000
	6	2.372834000	-2.008619000	-0.221029000
	8	1.329403000	-1.679179000	-0.785815000
	6	2.713718000	-1.697681000	1.220218000
	1	3.684396000	-2.123578000	1.475053000
	1	2.768380000	-0.604426000	1.300745000
	29	-0.351025000	-0.650844000	0.109179000
	17	-1.697253000	-2.307736000	-0.681438000
	8	3.339370000	-2.680087000	-0.834443000
	6	3.136516000	-3.013506000	-2.250994000
	1	2.979192000	-2.079800000	-2.796617000
	1	2.231459000	-3.621125000	-2.326039000
	6	4.371980000	-3.756075000	-2.720936000
	1	4.518328000	-4.678590000	-2.151711000
	1	5.266891000	-3.134757000	-2.623059000
	1	4.249964000	-4.019175000	-3.776385000
	6	2.082777000	-2.903036000	3.417939000
	1	2.853132000	-2.331338000	3.949069000
	1	1.241918000	-3.107341000	4.082056000
	1	2.550604000	-3.844124000	3.104047000
	8	0.373604000	1.379473000	-1.592130000
	6	0.998067000	1.581610000	-0.529605000
	8	0.905006000	0.802432000	0.508491000
	6	1.918708000	2.763824000	-0.381510000
	6	2.121933000	3.621929000	-1.474767000
	6	2.577034000	3.025152000	0.831867000
	6	2.972940000	4.724613000	-1.357999000
	6	3.427099000	4.129321000	0.949102000
	6	3.627346000	4.980489000	-0.145487000
	1	1.608706000	3.414913000	-2.409730000
	1	2.415780000	2.362716000	1.677176000
	1	3.932834000	4.327034000	1.891884000
	1	4.289344000	5.839216000	-0.054139000
	1	3.126504000	5.384460000	-2.209298000

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	7	-4.013458000	0.413873000	-1.973584000
	6	-2.812762000	1.026238000	-2.544382000
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	1	-2.030612000	1.128765000	-1.794752000
	1	-2.433657000	0.403126000	-3.361327000
	6	-5.151587000	0.221597000	-2.881092000
	1	-4.870648000	-0.460206000	-3.691272000
	1	-5.992401000	-0.196567000	-2.328968000
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	1	-0.316204000	0.558767000	2.851381000
	1	-0.724943000	2.212596000	2.364588000
	6	-2.852316000	-0.531664000	2.683723000
	1	-3.170474000	-0.353976000	3.716937000
	1	-3.704983000	-0.928754000	2.126910000
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	6	-3.435694000	1.863099000	2.044170000
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	1	-3.707640000	2.131192000	3.070222000
	1	-3.050586000	0.183671000	-0.071298000
INT2-d	6	-2.522456000	-0.848243000	-0.194325000
	8	-2.073286000	0.205528000	-0.661116000
	8	-3.669330000	-1.366273000	-0.592307000
	6	-4.413286000	-0.654402000	-1.645409000
	6	-5.668507000	-1.455255000	-1.927845000
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	1	-6.244222000	-0.948424000	-2.708622000
	1	-5.423995000	-2.461576000	-2.279609000
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	17	-1.165043000	3.213819000	0.049639000
	6	3.288802000	-0.266185000	-0.358764000
	6	4.387258000	0.577227000	-0.118500000
	6	3.496562000	-1.614936000	-0.695112000
	6	5.685572000	0.071930000	-0.213668000
	6	4.796788000	-2.115559000	-0.789432000
	6	5.890992000	-1.273393000	-0.548845000
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	1	6.903281000	-1.665246000	-0.622683000
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BP	6	-1.423008000	-0.109797000	-0.570481000
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	6	-4.741035000	0.962819000	0.954096000
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COMI-e	6	-1.154657000	-1.681756000	1.560192000
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	6	0.116531000	-2.089963000	2.278265000
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	1	0.579402000	-1.170573000	2.653175000
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	6	2.484204000	2.472591000	0.454330000
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	6	3.489363000	1.576517000	0.860627000
	6	4.177366000	4.045585000	-0.275930000
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	6	5.177192000	3.151347000	0.128085000
	1	2.060423000	4.409687000	-0.428313000
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TS1-e	6	-0.131137000	-2.319106000	1.669832000
	8	-0.735151000	-1.981315000	0.657354000
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	8	1.993388000	-1.687213000	-0.423195000
	6	1.322245000	-1.894005000	1.906813000
	1	1.742074000	-2.382524000	2.786484000
	1	1.300519000	-0.811221000	2.084153000
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	17	0.008674000	-1.659554000	-3.110019000
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	1	3.104463000	1.739077000	-0.574076000
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INT1-e	6	2.187705000	-1.124091000	2.363378000
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	17	0.137052000	-3.130085000	-0.832476000
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	1	-6.894035000	-0.639775000	1.475951000
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TS2-e	6	2.643797000	-0.846731000	2.717859000
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	6	-5.701316000	0.897209000	2.192921000
	6	-6.178079000	1.361381000	0.959217000
	1	-3.341498000	1.013866000	-0.897517000
	1	-3.995639000	0.119354000	3.269456000
	1	-5.693139000	1.772705000	-1.106996000
	1	-6.362259000	0.866173000	3.056077000
	1	-7.209541000	1.694409000	0.865856000
	8	-3.776083000	-2.723536000	-0.471478000
	6	-2.932810000	-2.123307000	-1.136080000
	7	-2.667305000	-2.198048000	-2.430021000
	6	-1.582837000	-1.435806000	-3.059734000
	1	-1.985796000	-0.886115000	-3.915859000
	1	-1.137867000	-0.730991000	-2.358887000
	1	-0.807921000	-2.125942000	-3.407076000
	6	-3.390472000	-3.153874000	-3.285032000
	1	-2.698407000	-3.924114000	-3.640258000
	1	-4.195440000	-3.618739000	-2.716779000
	1	-3.808016000	-2.621758000	-4.144619000
INT2-e	6	-2.522456000	-0.848243000	-0.194325000
	8	-2.073286000	0.205528000	-0.661116000
	8	-3.669330000	-1.366273000	-0.592307000
	6	-4.413286000	-0.654402000	-1.645409000
	6	-5.668507000	-1.455255000	-1.927845000
	1	-3.761126000	-0.576455000	-2.518511000
	1	-4.631867000	0.350209000	-1.275961000
	1	-6.244222000	-0.948424000	-2.708622000
	1	-5.423995000	-2.461576000	-2.279609000
	1	-6.295550000	-1.534384000	-1.035227000
	6	-1.432494000	-0.884553000	2.107652000

	8	-0.887769000	0.209824000	2.006747000
	6	-1.701126000	-1.526692000	3.440274000
	1	-1.265653000	-2.532674000	3.464286000
	1	-1.291546000	-0.919143000	4.248189000
	1	-2.782917000	-1.648986000	3.574249000
	6	-1.840234000	-1.684881000	0.864787000
	1	-0.905166000	-2.060326000	0.427386000
	1	-2.466916000	-2.538520000	1.124388000
	29	-0.317622000	1.134977000	-0.070194000
	17	-1.165043000	3.213819000	0.049639000
	6	3.288802000	-0.266185000	-0.358764000
	6	4.387258000	0.577227000	-0.118500000
	6	3.496562000	-1.614936000	-0.695112000
	6	5.685572000	0.071930000	-0.213668000
	6	4.796788000	-2.115559000	-0.789432000
	6	5.890992000	-1.273393000	-0.548845000
	1	4.216763000	1.618658000	0.140362000
	1	2.641057000	-2.258852000	-0.879771000
	1	4.959105000	-3.158960000	-1.049699000
	1	6.903281000	-1.665246000	-0.622683000
	6	1.911381000	0.265842000	-0.258473000
	8	0.886451000	-0.476008000	-0.472491000
	8	1.688129000	1.491526000	0.048745000
	1	6.536446000	0.723222000	-0.027669000

Table S1-4. Some optimized Cartesian Coordinates of stationary points for the reduction process, involved in the discussion on Cu(OAc)₂ as catalyst, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide with bond lengths in Å.

Species	Cartesian coordinates			
pre-CAT-OAc	1	1.153542000	2.604429000	3.638785000
	6	0.264235000	2.786455000	3.033058000
	6	0.177542000	1.779963000	1.904410000
	1	-0.636170000	2.753868000	3.647909000
	1	0.349001000	3.786962000	2.594706000
	8	-0.985126000	1.443562000	1.513526000
	8	1.276113000	1.358758000	1.421229000
	29	1.565818000	0.082869000	-0.027778000
	8	2.204020000	-1.495778000	1.079627000
	6	2.421831000	-2.140579000	-0.004977000
	8	2.153180000	-1.537956000	-1.102426000
	6	2.988819000	-3.528740000	0.008158000
	1	2.644026000	-4.089113000	-0.863046000
	1	4.081385000	-3.460963000	-0.038187000
	1	2.715578000	-4.043991000	0.930891000
	1	1.093182000	3.229162000	-3.151381000

	6	0.136560000	2.707234000	-3.100573000
	6	0.103617000	1.768786000	-1.911926000
	1	-0.690195000	3.417568000	-3.049660000
	1	0.019464000	2.110514000	-4.011842000
	8	-1.038347000	1.489763000	-1.426379000
	8	1.217387000	1.306820000	-1.507245000
	29	-1.517709000	0.283753000	0.034373000
	8	-2.376339000	-1.203925000	1.117792000
	6	-2.741880000	-1.759690000	0.023668000
	8	-2.408890000	-1.172569000	-1.064559000
	6	-3.546448000	-3.024907000	0.016958000
	1	-3.343759000	-3.600787000	-0.888044000
	1	-3.332696000	-3.618096000	0.908030000
	1	-4.610143000	-2.762096000	0.025427000
H₂O...H₂O	8	-1.491076000	-0.003500000	0.118977000
	1	-1.802737000	0.024131000	-0.803628000
	1	-0.510635000	-0.001770000	0.053447000
	8	1.338926000	0.002640000	-0.103708000
	1	1.765347000	-0.781681000	0.294718000
	1	1.765225000	0.766195000	0.333315000
LE-INT1	1	-2.830542000	3.387189000	1.936646000
	6	-3.478926000	3.145846000	1.089913000
	6	-2.887672000	1.998936000	0.280763000
	1	-4.446350000	2.835429000	1.498843000
	1	-3.620692000	4.026688000	0.461857000
	8	-2.819899000	2.088329000	-0.965308000
	8	-2.500013000	0.991128000	0.995529000
	29	-2.077438000	-0.796219000	0.360617000
	8	-3.559735000	-1.154815000	-1.010449000
	6	-3.227952000	-2.391127000	-1.026215000
	8	-2.262064000	-2.755699000	-0.273774000
	6	-3.933312000	-3.368213000	-1.924770000
	1	-3.826866000	-4.385934000	-1.544964000
	1	-4.988485000	-3.103641000	-2.021844000
	1	-3.479498000	-3.319754000	-2.920841000
	1	-0.111631000	-2.594060000	3.918079000
	6	0.645233000	-1.883170000	3.584337000
	6	0.217553000	-1.202399000	2.296580000
	1	0.776490000	-1.116915000	4.356062000
	1	1.606505000	-2.383188000	3.446299000
	8	1.145006000	-0.621326000	1.638296000
	8	-1.009177000	-1.245253000	1.990117000
	29	1.051813000	0.619488000	0.128426000
	8	1.000481000	2.308502000	-0.984257000

	6	1.421412000	2.985318000	0.020733000
	8	1.609451000	2.354588000	1.114556000
	6	1.707010000	4.454001000	-0.102358000
	1	1.659135000	4.937375000	0.875065000
	1	2.717563000	4.582988000	-0.505449000
	1	1.004382000	4.920652000	-0.796219000
	8	-0.202804000	-0.496854000	-1.046961000
	8	2.967273000	-0.089812000	-0.741257000
	6	3.709433000	-0.923091000	-0.176863000
	1	3.426931000	-1.366941000	0.787764000
	7	4.882776000	-1.351776000	-0.663943000
	6	5.406965000	-0.860754000	-1.937352000
	1	4.705402000	-0.142773000	-2.359716000
	1	6.376507000	-0.375796000	-1.780178000
	1	5.539822000	-1.695747000	-2.633792000
	6	5.694850000	-2.330092000	0.057403000
	1	5.840740000	-3.226221000	-0.555252000
	1	6.675021000	-1.904592000	0.298092000
	1	5.196780000	-2.615325000	0.986191000
	1	0.190817000	-1.342084000	-1.358125000
	1	-0.528988000	0.023914000	-1.867962000
	8	-1.288412000	0.952261000	-2.880943000
	1	-0.696663000	1.670063000	-3.184506000
	1	-1.911104000	1.376388000	-2.228133000
LE-TS1	1	-4.180989000	2.546850000	2.060500000
	6	-4.443639000	2.502970000	1.002110000
	6	-3.394639000	1.733740000	0.223810000
	1	-5.398129000	1.971940000	0.911440000
	1	-4.571699000	3.506850000	0.593380000
	8	-3.255659000	2.038840000	-1.009800000
	8	-2.746169000	0.839330000	0.849200000
	29	-1.897129000	-0.889410000	0.284630000
	8	-3.200069000	-1.388690000	-1.200000000
	6	-2.854819000	-2.619280000	-1.096660000
	8	-1.984869000	-2.920580000	-0.214030000
	6	-3.440509000	-3.658520000	-2.011650000
	1	-3.358339000	-4.651960000	-1.567040000
	1	-4.483659000	-3.424300000	-2.235430000
	1	-2.882989000	-3.651640000	-2.954780000
	1	-0.116199000	-2.264430000	4.102210000
	6	0.581981000	-1.493220000	3.773900000
	6	0.199591000	-0.962320000	2.403340000
	1	0.549601000	-0.663430000	4.488490000
	1	1.602911000	-1.880630000	3.758450000

	8	1.117821000	-0.371660000	1.749860000
	8	-1.004539000	-1.127550000	2.035250000
	29	1.049001000	0.745190000	0.113090000
	8	0.986261000	2.462580000	-1.040030000
	6	1.578291000	3.094600000	-0.095030000
	8	1.863171000	2.446260000	0.966170000
	6	1.942541000	4.544800000	-0.252360000
	1	2.168581000	4.994160000	0.715910000
	1	2.828201000	4.619770000	-0.892650000
	1	1.130241000	5.085860000	-0.743770000
	8	-0.216629000	-0.286920000	-0.962680000
	8	2.958961000	-0.082670000	-0.749320000
	6	3.671711000	-0.908290000	-0.141120000
	1	3.384001000	-1.278700000	0.853200000
	7	4.821911000	-1.418800000	-0.608970000
	6	5.352441000	-1.033980000	-1.915490000
	1	4.674211000	-0.319250000	-2.379660000
	1	6.341111000	-0.576790000	-1.798560000
	1	5.447111000	-1.917520000	-2.556180000
	6	5.599911000	-2.381010000	0.168500000
	1	5.701781000	-3.321350000	-0.384050000
	1	6.599891000	-1.983270000	0.373070000
	1	5.100511000	-2.583100000	1.118220000
	1	0.229821000	-1.040200000	-1.398970000
	1	-0.810499000	0.589770000	-1.847880000
	8	-1.371979000	1.350760000	-2.386450000
	1	-0.777369000	2.132480000	-2.438040000
	1	-2.263309000	1.628370000	-1.710420000
LE-INT2	1	-4.709644000	1.482796000	2.134255000
	6	-4.631491000	2.164314000	1.287521000
	6	-3.467988000	1.773714000	0.409525000
	1	-5.558113000	2.148983000	0.706244000
	1	-4.490001000	3.187922000	1.648448000
	8	-3.365398000	2.523087000	-0.681987000
	8	-2.690497000	0.856438000	0.686722000
	29	-1.607064000	-1.082927000	-0.073573000
	8	-2.763235000	-1.381433000	-1.750572000
	6	-3.556560000	-2.103670000	-1.051929000
	8	-3.278276000	-2.266339000	0.184094000
	6	-4.759803000	-2.752187000	-1.678053000
	1	-5.476916000	-3.056133000	-0.913795000
	1	-5.227981000	-2.069877000	-2.391472000
	1	-4.434569000	-3.641030000	-2.229604000
	1	-0.286077000	-2.160157000	4.103529000

	6	0.616267000	-2.045918000	3.499016000
	6	0.297786000	-1.298460000	2.216593000
	1	1.395446000	-1.533888000	4.065221000
	1	0.972456000	-3.048410000	3.237572000
	8	1.175275000	-0.483902000	1.790343000
	8	-0.819071000	-1.563432000	1.669938000
	29	1.177842000	0.731556000	0.226379000
	8	1.260283000	2.555190000	-0.782252000
	6	1.901759000	3.040155000	0.213613000
	8	2.128074000	2.270244000	1.207230000
	6	2.394836000	4.460594000	0.197139000
	1	2.591872000	4.812797000	1.211112000
	1	3.328013000	4.502931000	-0.375292000
	1	1.668128000	5.108282000	-0.298526000
	8	-0.122891000	-0.154692000	-0.926004000
	8	2.998850000	-0.157288000	-0.770744000
	6	3.693300000	-1.053776000	-0.248064000
	1	3.439176000	-1.463738000	0.740243000
	7	4.784939000	-1.600772000	-0.806179000
	6	5.265718000	-1.173763000	-2.118830000
	1	4.609061000	-0.394575000	-2.503426000
	1	6.285958000	-0.783610000	-2.035124000
	1	5.269593000	-2.023139000	-2.810675000
	6	5.545595000	-2.647529000	-0.126876000
	1	5.562225000	-3.558986000	-0.734238000
	1	6.576681000	-2.318369000	0.041818000
	1	5.086638000	-2.875446000	0.837324000
	1	0.352099000	-0.783868000	-1.513240000
	1	-0.843255000	1.162607000	-1.812777000
	8	-1.253421000	1.998626000	-2.161754000
	1	-0.570127000	2.675523000	-1.984635000
	1	-2.541877000	2.271705000	-1.229129000
LE-TS2	1	6.275720000	-0.269282000	-0.117319000
	6	5.981100000	-1.218442000	-0.564469000
	6	4.490690000	-1.242201000	-0.802849000
	1	6.508279000	-1.361892000	-1.512679000
	1	6.264399000	-2.045092000	0.094011000
	8	4.069479000	-2.390101000	-1.324929000
	8	3.749540000	-0.292651000	-0.544209000
	29	1.670670000	0.643049000	0.183461000
	8	2.018600000	2.414619000	-0.782369000
	6	2.612330000	2.851049000	0.266021000
	8	2.675040000	2.078899000	1.280641000
	6	3.237861000	4.218239000	0.284011000

	1	3.281921000	4.605989000	1.303561000
	1	4.261301000	4.141429000	-0.099639000
	1	2.683351000	4.901489000	-0.362549000
	1	1.599449000	-1.985361000	3.787941000
	6	0.695769000	-2.256211000	3.240501000
	6	0.481930000	-1.341281000	2.048111000
	1	0.799789000	-3.284231000	2.876131000
	1	-0.175341000	-2.225040000	3.898911000
	8	-0.679660000	-1.324270000	1.535831000
	8	1.491610000	-0.676501000	1.645031000
	29	-1.325190000	-0.375500000	-0.098589000
	8	-4.626210000	-1.253990000	0.043871000
	6	-3.814751000	-2.221720000	-0.331759000
	8	-2.609251000	-2.045430000	-0.580149000
	6	-4.467161000	-3.575320000	-0.436869000
	1	-3.740241000	-4.322330000	-0.755419000
	1	-4.886851000	-3.854560000	0.534541000
	1	-5.296091000	-3.530040000	-1.149509000
	8	0.418410000	-0.164441000	-1.063729000
	8	-2.220290000	1.171740000	-0.854839000
	6	-3.367590000	1.166800000	-0.292909000
	1	-4.116480000	-0.317720000	0.017241000
	7	-4.079770000	2.292830000	-0.222609000
	6	-3.613750000	3.575250000	-0.771039000
	1	-2.614170000	3.449870000	-1.184659000
	1	-4.295390000	3.914300000	-1.558679000
	1	-3.590089000	4.330280000	0.021981000
	6	-5.400440000	2.303681000	0.406281000
	1	-5.416430000	3.021831000	1.233511000
	1	-6.166480000	2.592691000	-0.322009000
	1	-5.632550000	1.311601000	0.794311000
	1	0.304460000	0.454709000	-1.817429000
	1	1.047859000	-1.636421000	-1.601879000
	8	1.503949000	-2.477181000	-1.893539000
	1	1.031509000	-3.209131000	-1.450009000
	1	3.065899000	-2.376441000	-1.496399000
LE-INT3	1	6.148108000	-0.637115000	0.164654000
	6	5.773539000	-1.659187000	0.111991000
	6	4.280048000	-1.656681000	-0.109969000
	1	6.266227000	-2.192893000	-0.706644000
	1	6.010685000	-2.192177000	1.037606000
	8	3.762743000	-2.881247000	-0.145227000
	8	3.619330000	-0.626413000	-0.248771000
	29	1.568141000	0.627860000	-0.076333000

	8	2.136260000	1.891068000	-1.591363000
	6	2.703757000	2.644628000	-0.724995000
	8	2.632430000	2.304304000	0.503594000
	6	3.454617000	3.876468000	-1.151072000
	1	3.471611000	4.613101000	-0.345533000
	1	4.488186000	3.595617000	-1.382176000
	1	3.009665000	4.303894000	-2.052016000
	1	1.135095000	-1.172026000	3.997607000
	6	0.133750000	-0.835626000	3.724428000
	6	0.081276000	-0.393538000	2.271329000
	1	-0.598880000	-1.624536000	3.907707000
	1	-0.130055000	0.019809000	4.356301000
	8	-1.056114000	-0.360922000	1.712460000
	8	1.192917000	-0.060210000	1.738791000
	29	-1.471776000	0.031005000	-0.263549000
	8	-3.865855000	-2.564841000	0.455367000
	6	-3.387161000	-2.555441000	-0.795086000
	8	-2.551650000	-1.744469000	-1.189878000
	6	-3.980280000	-3.640157000	-1.652419000
	1	-3.565436000	-3.588196000	-2.658271000
	1	-3.766620000	-4.617434000	-1.209259000
	1	-5.067912000	-3.527312000	-1.689074000
	8	0.333783000	-0.521460000	-1.026951000
	8	-2.800997000	1.592167000	-1.735690000
	6	-2.782825000	1.453901000	-0.496279000
	1	-3.438659000	-1.833374000	0.972908000
	7	-3.507602000	2.182229000	0.365586000
	6	-4.409246000	3.242827000	-0.100339000
	1	-4.378705000	3.291680000	-1.188339000
	1	-5.433774000	3.032711000	0.226478000
	1	-4.099583000	4.207928000	0.316319000
	6	-3.432263000	1.981002000	1.811020000
	1	-3.083907000	2.898277000	2.300533000
	1	-4.424000000	1.732445000	2.206889000
	1	-2.740238000	1.170141000	2.034823000
	1	0.391508000	-0.317885000	-1.984579000
	1	0.806687000	-2.101130000	-0.786850000
	8	1.186213000	-3.018471000	-0.639660000
	1	0.677012000	-3.407328000	0.098381000
	1	2.757836000	-2.862122000	-0.313007000
LE-INT4a	1	3.309328000	-3.584921000	0.467213000
	6	3.530199000	-2.519165000	0.390824000
	6	2.263028000	-1.722020000	0.203119000
	1	4.065453000	-2.177060000	1.279996000

	1	4.184119000	-2.354448000	-0.472446000
	8	2.281573000	-0.452088000	0.390245000
	8	1.176930000	-2.278366000	-0.154535000
	29	0.260683000	-0.348928000	-0.097304000
	8	-3.062269000	-0.106053000	0.747018000
	6	-2.718712000	-1.043219000	-0.105388000
	8	-1.581009000	-1.146415000	-0.605112000
	6	-3.822729000	-2.000313000	-0.462489000
	1	-3.419435000	-2.868653000	-0.982814000
	1	-4.359931000	-2.307088000	0.438392000
	1	-4.537329000	-1.486664000	-1.114516000
	8	-1.276634000	1.718255000	0.898619000
	6	-0.226939000	1.546187000	0.215067000
	1	-2.306187000	0.588914000	0.864276000
	7	0.520954000	2.591384000	-0.177579000
	6	0.149581000	3.971272000	0.159996000
	1	-0.746057000	3.962848000	0.778786000
	1	0.968912000	4.452019000	0.705750000
	1	-0.043182000	4.541509000	-0.755801000
	6	1.710724000	2.447765000	-1.013513000
	1	1.555445000	2.949737000	-1.975638000
	1	2.575317000	2.902774000	-0.517529000
	1	1.927418000	1.394564000	-1.186371000
LE-INT4b	1	-2.391783000	3.062036000	-0.616739000
	6	-3.079352000	2.298412000	-0.254082000
	6	-2.344110000	1.009237000	0.008265000
	1	-3.585432000	2.634959000	0.653866000
	1	-3.848071000	2.115443000	-1.012620000
	8	-3.024214000	0.137121000	0.705340000
	8	-1.192498000	0.837121000	-0.438751000
	29	0.483619000	-0.306890000	-0.320758000
	8	2.465500000	-0.761568000	-0.106554000
	6	2.683229000	0.458139000	0.223370000
	8	1.682245000	1.251528000	0.249266000
	6	4.063298000	0.921735000	0.593709000
	1	4.171564000	1.990641000	0.400956000
	1	4.214539000	0.747241000	1.664790000
	1	4.818303000	0.353557000	0.046830000
	8	-0.248245000	-1.950938000	-0.861074000
	1	0.470676000	-2.616257000	-0.839095000
	1	-1.345275000	-2.256880000	0.217747000
	8	-2.073866000	-2.210987000	0.935088000
	1	-2.758397000	-2.867100000	0.693470000
	1	-2.580844000	-0.807188000	0.798686000

CAT-OAc	29	-0.095745000	0.069984000	-0.058271000
	8	-2.600833000	-1.392571000	0.171894000
	6	-2.801517000	-0.170072000	0.034231000
	8	-1.859342000	0.724113000	-0.088386000
	6	-4.213186000	0.400051000	-0.001422000
	1	-4.339705000	1.127212000	0.807092000
	1	-4.955809000	-0.392646000	0.101093000
	1	-4.374630000	0.934734000	-0.942829000
	8	1.707468000	-0.562220000	-0.056298000
	6	2.812178000	-0.001962000	0.031228000
	8	2.967171000	1.305560000	0.167236000
	6	4.100306000	-0.766328000	-0.032224000
	1	4.533769000	-0.634638000	-1.029864000
	1	3.914110000	-1.826031000	0.138666000
	1	4.813632000	-0.373879000	0.695581000
	1	2.082848000	1.766532000	0.173680000
	N...H₂O	6	-0.462641000	0.816078000
8		-1.076711000	1.818594000	0.236027000
7		-0.921565000	-0.457876000	-0.094239000
6		-2.203162000	-0.740034000	0.547771000
1		-2.867306000	-1.259439000	-0.152175000
1		-2.055572000	-1.377730000	1.427831000
1		-2.667478000	0.194756000	0.856694000
6		-0.147170000	-1.616258000	-0.540701000
1		0.326419000	-2.126970000	0.307037000
1		-0.821427000	-2.320519000	-1.037694000
1		0.621612000	-1.313943000	-1.249072000
8		0.801054000	0.908883000	-0.665420000
1		1.007345000	1.873630000	-0.716856000
8		3.233160000	-0.291703000	0.657823000
1		3.680815000	-0.796331000	-0.046648000
1		2.444363000	0.086777000	0.227878000

Table S2-1. Frequencies of some stationary points for the entire catalytic cycle, involved in the discussion on TBHP (**OX-a**) as oxidant, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide at 343K.

Species	Frequencies (cm⁻¹)												
1a	31	42	79	95	102	187	191	269	317	367	416	473	
	538	626	745	815	830	862	887	951	998	1035	1058	1136	1176
	1177	1199	1303	1304	1347	1400	1402	1434	1457	1474	1484	1498	1504
	1522	1752	1777	3045	3052	3070	3084	3122	3132	3133	3141	3155	3174
CAT	18	25	49	57	66	71	126	140	156	179	194	248	
	270	333	351	376	415	501	579	615	760	814	840	856	
	930	959	1020	1031	1047	1135	1169	1175	1222	1292	1304	1365	1400
	1407	1435	1460	1469	1474	1497	1503	1520	1700	1750	3041	3053	3054

	3091 3114 3140 3144 3163 3168 3183
TBHP	-221 117 181 236 243 260 341 357 410 461 520 743 860 921 928 947 967 1044 1049 1219 1263 1268 1381 1406 1409 1430 1483 1497 1499 1508 1509 1533 3047 3048 3055 3130 3133 3137 3143 3148 3151 3526
COM1-a	14 19 26 31 36 46 49 56 65 75 80 97 112 130 152 158 167 191 199 241 242 249 269 271 292 339 355 360 363 408 418 420 466 503 525 569 620 746 758 814 841 851 858 892 925 932 933 961 967 1020 1033 1044 1051 1052 1135 1170 1175 1208 1234 1268 1282 1292 1304 1341 1364 1400 1407 1407 1409 1431 1436 1466 1472 1476 1485 1498 1498 1499 1503 1509 1511 1520 1532 1704 1750 3040 3046 3047 3049 3054 3054 3089 3114 3132 3135 3139 3139 3143 3143 3144 3149 3161 3164 3180 3468
TS1-a	-218 17 33 35 40 45 60 63 66 89 98 104 126 139 144 156 165 194 194 214 251 254 264 270 296 322 326 339 356 370 377 417 420 475 498 514 574 618 747 758 814 839 863 876 916 920 935 954 963 963 1019 1032 1033 1042 1052 1136 1174 1181 1194 1249 1250 1254 1298 1304 1373 1388 1397 1400 1410 1417 1437 1463 1469 1476 1482 1495 1498 1499 1503 1506 1508 1519 1531 1693 1745 2984 3039 3041 3041 3047 3054 3091 3115 3120 3126 3135 3139 3140 3144 3144 3145 3156 3163 3181 3577
INT1-a	16 32 36 62 71 85 102 120 124 144 149 161 177 190 253 271 286 336 382 424 484 535 571 607 762 769 814 833 853 918 969 1014 1026 1051 1136 1174 1187 1212 1305 1313 1382 1401 1419 1438 1452 1469 1477 1497 1502 1518 1684 1755 3035 3042 3056 3096 3117 3144 3146 3156 3168 3182 3600
'BuO•	178 246 249 323 329 408 413 428 734 868 906 927 964 1004 1012 1154 1172 1247 1379 1388 1420 1475 1490 1496 1501 1504 1527 3040 3046 3052 3129 3134 3139 3141 3150 3162
DMF	108 157 239 319 338 399 655 869 1013 1080 1105 1128 1176 1276 1425 1441 1446 1474 1491 1510 1513 1546 1713 3016 3034 3040 3106 3109 3153 3183
INT2-a	16 21 25 33 49 60 72 78 83 86 105 109 131 140 146 151 161 169 180 192 221 236 258 263 270 273 340 371 375 382 412 420 487 499 558 610 675 759 814 835 840 853 872 919 966 1014 1032 1041 1051 1077 1125 1129 1136 1174 1175 1178 1217 1272 1299 1305 1373 1397 1399 1412 1436 1446 1454 1456 1471 1471 1479 1491 1498 1502 1509 1511 1519 1539 1672 1700 1771 3041 3047 3052 3054 3063 3092 3117 3117 3125 3127 3141 3144 3161 3164 3167 3178 3194 3659
TS2-a	-1492 32 48 78 91 99 148 150 200 252 252 264 270 321 336 377 406 435 438 472 551 677 750 880

	913 915 931 962 1036 1041 1050 1079 1122 1126 1173 1207 1238 1252 1263 1392 1403 1423 1430 1444 1468 1484 1491 1495 1497 1498 1509 1510 1510 1522 1529 1546 1747 3037 3039 3045 3045 3049 3118 3122 3123 3125 3130 3132 3134 3140 3189 3193
BuOH	197 257 270 340 341 362 419 461 463 746 914 920 929 962 1034 1047 1172 1228 1261 1369 1407 1414 1432 1487 1494 1497 1510 1517 1528 3030 3034 3046 3110 3116 3127 3129 3131 3138 3604
(CH3)2N(O)C•	100 151 244 282 379 395 641 845 1067 1112 1114 1169 1256 1414 1442 1467 1491 1503 1509 1535 1781 3041 3046 3116 3123 3172 3183
TS3-a	-1414 12 18 24 30 35 38 39 61 68 72 80 86 91 95 99 106 109 113 133 137 140 142 149 157 162 176 192 216 249 255 258 260 265 266 295 317 366 370 376 382 404 411 427 477 497 571 595 660 675 722 764 815 838 851 866 873 921 942 980 1021 1042 1048 1054 1074 1079 1117 1119 1123 1130 1136 1170 1174 1178 1184 1246 1268 1270 1273 1304 1382 1396 1399 1403 1422 1432 1445 1446 1449 1456 1471 1474 1482 1483 1491 1493 1498 1503 1507 1510 1510 1511 1520 1539 1540 1666 1672 1729 1785 3043 3045 3050 3053 3053 3056 3088 3113 3119 3122 3124 3130 3135 3137 3142 3143 3160 3166 3175 3194 3194 3196 3662
INT3	13 22 26 45 58 75 82 84 95 105 108 113 126 148 158 161 188 215 228 240 247 257 266 298 300 324 343 356 390 403 452 479 564 598 641 662 748 783 785 817 869 871 973 994 1010 1029 1034 1050 1077 1080 1114 1129 1136 1174 1177 1197 1274 1304 1305 1398 1400 1412 1430 1444 1445 1449 1474 1480 1491 1494 1497 1504 1510 1512 1520 1533 1545 1601 1693 3039 3044 3053 3054 3070 3086 3113 3116 3136 3137 3142 3158 3159 3169 3188 3236 3592
TS4	-94 16 22 41 50 61 82 91 95 103 124 125 127 144 157 161 179 197 213 231 254 268 269 281 292 326 364 369 387 407 429 450 527 582 632 672 746 774 794 816 871 872 955 974 1004 1022 1035 1051 1074 1079 1126 1128 1136 1175 1177 1194 1271 1272 1302 1395 1401 1410 1427 1439 1448 1455 1472 1479 1491 1496 1498 1504 1509 1510 1522 1541 1547 1613 1679 3046 3051 3051 3053 3080 3093 3124 3126 3131 3135 3140 3153 3165 3167 3195 3230 3598
INT4	19 24 32 40 54 75 80 89 93 96 126 129 139 153 164 184 188 202 212 238 253 265 269 278 304 316 355 373 407 409 419 429 548 576 615 694 728 764 812 824 871 874 963 975 992 1009 1032 1051 1071 1077 1128 1135 1136 1175 1178 1187 1262 1269 1301 1393 1398 1402 1410 1433 1449 1458 1468 1483 1490 1493 1498 1504 1507 1509 1522

	1537 1552 1659 1677 3048 3050 3053 3057 3075 3126 3129 3134 3136 3139 3149 3149 3157 3172 3200 3221 3575
TS5	-678 21 27 42 56 64 84 89 92 100 113 119 139 144 150 158 188 195 203 208 232 266 277 281 294 309 371 388 415 430 445 475 497 536 598 620 670 683 748 780 783 816 868 936 980 1007 1033 1049 1071 1076 1119 1135 1161 1173 1174 1198 1260 1299 1303 1311 1398 1400 1422 1429 1440 1448 1468 1480 1491 1493 1497 1504 1504 1507 1519 1525 1531 1593 1674 1730 3052 3053 3054 3057 3084 3135 3135 3135 3137 3142 3156 3168 3181 3194 3234 3580
INT5	20 26 34 42 46 50 62 77 81 89 97 101 104 109 130 135 149 154 181 206 225 235 254 274 309 312 330 333 361 406 416 427 492 536 553 632 732 749 764 813 817 845 870 920 997 1028 1042 1061 1080 1085 1132 1137 1148 1174 1175 1201 1259 1286 1303 1378 1407 1418 1432 1438 1451 1480 1485 1498 1498 1503 1507 1509 1519 1521 1543 1623 1653 1695 1770 3045 3053 3056 3058 3083 3117 3134 3141 3142 3143 3156 3172 3183 3197 3223 3599 3688
TS6	-7 14 28 31 45 51 52 70 76 88 95 102 112 120 132 135 157 179 209 225 232 252 272 285 304 321 363 396 412 421 484 503 513 551 634 663 725 745 766 818 833 868 873 920 985 1023 1052 1062 1074 1085 1129 1136 1159 1175 1177 1180 1245 1284 1307 1366 1404 1417 1435 1441 1447 1478 1480 1491 1498 1500 1505 1512 1517 1523 1544 1608 1690 1723 1755 3040 3042 3045 3051 3075 3108 3114 3115 3128 3140 3150 3165 3193 3211 3214 3564 3635
INT6	15 19 22 30 39 51 60 77 81 95 99 106 119 121 125 152 176 195 220 225 243 273 289 316 327 355 370 402 424 451 484 517 552 621 634 724 745 768 819 831 837 867 870 923 991 1023 1051 1061 1075 1084 1128 1138 1155 1176 1177 1182 1254 1284 1306 1369 1407 1417 1434 1439 1449 1478 1480 1490 1498 1500 1506 1513 1514 1523 1543 1643 1679 1715 1759 3036 3041 3043 3053 3072 3113 3115 3116 3128 3143 3152 3166 3193 3206 3217 3367 3604
3a	20 31 50 59 80 101 102 117 132 146 183 204 223 238 273 285 320 363 393 413 491 515 545 633 731 747 767 813 836 868 883 917 979 1026 1051 1066 1071 1085 1130 1135 1159 1176 1177 1179 1232 1283 1302 1361 1400 1416 1433 1441 1449 1480 1482 1494 1497 1503 1504 1512 1516 1523 1545 1707 1741 1746 3037 3042 3045 3051 3077 3104 3107 3119 3128 3139 3150 3164 3197 3212 3214
CAT-H₂O	21 24 37 40 58 60 71 80 86 103 129 143 152 182 212 239 270 281 354 360 373 416 453 502 561 615 754 814 838 857 930 959 1018 1032 1048 1135 1162

	1175 1226 1290 1304 1357 1400 1406 1436 1462 1471 1476 1498 1503 1520 1628 1705 1749 3040 3053 3054 3089 3114 3139 3143 3161 3166 3179 3600 3686
TS7	-47 14 23 27 30 38 41 44 49 55 58 74 80 95 101 123 133 152 153 168 171 176 192 194 246 248 250 266 271 307 339 354 355 369 403 410 417 420 467 504 524 575 618 747 761 814 840 853 859 915 924 931 935 963 966 1019 1033 1043 1051 1052 1135 1174 1178 1209 1240 1268 1284 1294 1304 1359 1372 1400 1407 1407 1410 1430 1436 1466 1472 1476 1485 1498 1498 1500 1503 1509 1511 1520 1533 1650 1698 1748 3028 3041 3045 3046 3053 3054 3090 3115 3130 3133 3138 3139 3141 3143 3143 3149 3159 3162 3180 3499
COM2-a	13 17 19 26 34 41 46 54 55 67 70 79 83 84 105 110 130 145 152 158 169 189 203 243 245 250 269 273 279 300 340 355 361 364 411 418 434 458 471 501 528 568 617 747 758 814 839 851 858 893 925 931 933 962 968 1019 1033 1044 1051 1052 1135 1171 1175 1208 1233 1269 1282 1294 1304 1341 1366 1400 1407 1408 1409 1431 1436 1464 1470 1476 1485 1498 1498 1499 1503 1509 1511 1520 1533 1678 1701 1749 3040 3047 3048 3049 3054 3054 3090 3115 3133 3135 3139 3139 3143 3143 3144 3149 3162 3164 3180 3461 3607 3731
DMF-H₂O	34 43 78 110 158 161 247 336 349 361 400 655 666 871 1017 1080 1115 1128 1177 1275 1426 1446 1449 1474 1492 1510 1511 1546 1681 1700 3038 3041 3047 3114 3117 3158 3189 3536 3725

Table S2-2. Frequencies of some stationary points for the entire catalytic cycle, involved in the discussion on m-CPBA (**OX-b**) as oxidant, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide at 343K.

Species	Frequencies (cm⁻¹)																																																																																																								
COM1-b1	7	11	14	18	32	34	37	47	58	68	75	80	84	99	117	132	140	142	153	172	186	199	210	235	270	274	276	330	352	359	382	417	422	435	490	498	560	593	616	623	680	682	736	756	808	814	815	838	854	902	926	936	960	975	996	1011	1017	1032	1050	1091	1106	1136	1138	1165	1175	1186	1221	1278	1292	1304	1315	1354	1362	1399	1407	1411	1436	1445	1464	1471	1477	1498	1503	1503	1520	1612	1638	1706	1708	1756	3040	3054	3063	3089	3115	3139	3143	3161	3166	3179	3197	3210	3216	3233	3410
TS1-b1	-661	11	14	23	32	42	50	53	62	72	86	90	99	100	112	118	132	138	153	154	170	185	188	202	234	247	270	291	336	348	367	400	418	420	430	484	497	557	576	616	663	682	712	749	757	811	814	836	845	854	911	923	939	963	998	1011	1016	1031	1051	1059	1100	1121	1136	1163	1169	1175	1186	1220	1291	1296	1305	1325	1355	1366																															

	1399 1408 1436 1445 1464 1471 1477 1498 1503 1503 1519 1593 1623 1639 1702 1763 3041 3054 3065 3091 3116 3140 3144 3163 3165 3179 3197 3209 3217 3244 3468
INT1-b1	13 18 25 44 49 59 68 79 83 98 112 124 133 146 153 159 185 188 200 212 242 264 271 300 343 345 387 401 425 434 455 493 507 536 562 615 668 684 749 760 763 814 822 834 853 888 916 921 942 970 1000 1011 1015 1026 1053 1092 1112 1136 1170 1173 1179 1182 1220 1296 1305 1315 1353 1375 1400 1415 1427 1438 1454 1457 1470 1477 1497 1501 1502 1516 1518 1621 1641 1674 1762 3041 3056 3056 3095 3117 3144 3146 3163 3168 3180 3195 3210 3218 3219
TS2-b1	-1329 11 16 20 25 35 37 48 61 68 72 77 85 91 99 102 107 115 128 132 147 147 156 162 178 186 201 210 252 256 262 274 284 291 318 339 372 391 399 408 434 439 453 471 507 536 571 606 660 668 684 723 748 763 768 815 822 850 870 887 913 916 941 941 986 999 1011 1021 1046 1059 1074 1092 1111 1115 1122 1136 1168 1169 1174 1182 1191 1251 1283 1296 1299 1304 1352 1365 1396 1403 1419 1431 1432 1446 1448 1449 1473 1478 1482 1495 1498 1502 1507 1509 1509 1514 1519 1535 1621 1632 1641 1709 1792 3045 3053 3055 3059 3090 3123 3136 3140 3140 3145 3150 3163 3177 3189 3193 3195 3209 3218 3219
INT2-b1	12 14 22 43 54 66 72 86 91 108 110 117 146 166 187 196 219 228 231 256 266 295 304 317 337 393 408 435 455 465 495 504 593 595 648 670 682 743 746 752 786 792 814 817 863 870 913 939 983 999 1010 1012 1030 1049 1073 1092 1108 1135 1153 1173 1179 1193 1261 1305 1307 1311 1350 1394 1398 1427 1444 1446 1475 1488 1497 1500 1502 1515 1526 1588 1613 1635 1664 3054 3057 3091 3141 3141 3144 3163 3174 3194 3210 3220 3225 3239
INT3-b1	9 12 16 21 26 28 49 54 69 75 81 85 89 102 106 110 110 123 136 148 161 168 186 197 214 224 231 249 251 266 291 301 318 330 345 352 392 401 403 436 453 462 486 505 591 594 644 666 669 682 742 746 752 783 787 814 817 865 869 871 914 939 982 999 1010 1011 1019 1031 1049 1073 1079 1092 1108 1117 1128 1135 1153 1173 1177 1178 1193 1261 1273 1303 1305 1309 1349 1395 1398 1420 1428 1443 1444 1446 1450 1474 1477 1491 1491 1497 1499 1503 1510 1511 1516 1527 1546 1597 1613 1635 1664 1699 3041 3046 3054 3056 3066 3088 3116 3118 3139 3141 3143 3160 3161 3173 3190 3193 3210 3221 3226 3238
TS3-b1	-24 11 17 21 23 29 46 51 55 69 75 93 95 100 114 127 132 132 143 149 159 171 177 195 199 201 226 248 257 267 269 289 317 320 373 374

	389 394 412 422 435 444 454 503 566 583 628 664 678 681 730 736 752 772 805 814 817 864 869 872 914 938 965 998 1002 1010 1020 1033 1051 1070 1078 1091 1107 1128 1133 1136 1154 1174 1177 1178 1192 1255 1269 1270 1303 1305 1348 1387 1400 1401 1406 1434 1443 1449 1457 1470 1478 1490 1494 1498 1498 1503 1508 1509 1520 1537 1545 1613 1620 1634 1664 1676 3051 3052 3054 3055 3081 3103 3131 3132 3133 3137 3141 3154 3168 3170 3192 3198 3209 3221 3227 3228
INT4-b1	11 19 20 26 29 43 49 56 64 70 90 92 95 102 120 130 135 140 146 152 165 171 192 197 200 205 226 241 265 268 273 299 317 323 362 375 390 408 410 418 434 436 459 504 547 602 617 666 682 693 724 737 752 766 811 815 821 866 870 872 915 938 964 996 998 1006 1010 1031 1051 1069 1077 1091 1107 1128 1136 1139 1153 1174 1178 1178 1190 1253 1266 1269 1302 1304 1348 1381 1392 1400 1404 1433 1443 1450 1458 1467 1480 1490 1493 1497 1498 1503 1507 1509 1520 1534 1545 1613 1634 1647 1670 1683 3051 3051 3055 3059 3080 3131 3133 3137 3139 3140 3148 3152 3162 3174 3192 3202 3209 3220 3223 3229
TS4-b1	-1278 9 17 20 26 36 41 43 48 65 72 81 82 92 98 111 115 120 132 140 155 162 173 191 198 208 214 229 266 274 290 297 306 310 321 378 395 405 429 429 446 449 465 485 489 575 597 626 664 691 692 730 750 761 783 790 816 820 850 867 906 931 940 980 998 1010 1011 1032 1049 1065 1076 1095 1111 1116 1135 1137 1158 1170 1173 1181 1198 1222 1254 1297 1304 1305 1333 1353 1392 1398 1403 1429 1442 1445 1446 1465 1481 1489 1493 1497 1503 1503 1505 1506 1515 1520 1531 1553 1596 1613 1639 1644 1697 3053 3056 3057 3060 3087 3137 3137 3138 3140 3143 3159 3170 3193 3193 3197 3209 3215 3219 3235
INT5-b1	8 14 17 19 24 25 32 39 51 54 65 72 84 96 99 103 110 122 133 136 150 164 165 171 199 203 207 223 227 275 292 312 322 346 363 395 406 418 421 425 493 494 518 544 550 582 634 654 683 702 735 749 756 766 818 819 832 849 867 876 912 917 946 988 1003 1011 1026 1048 1065 1070 1085 1096 1114 1127 1136 1158 1162 1175 1176 1182 1182 1211 1249 1287 1308 1308 1356 1365 1405 1409 1415 1433 1438 1447 1449 1478 1481 1495 1498 1502 1505 1508 1510 1515 1521 1542 1614 1640 1677 1688 1720 1749 3034 3040 3047 3052 3078 3111 3119 3123 3131 3141 3152 3165 3193 3196 3197 3211 3214 3222 3226 3318
CAT-b1	11 13 18 36 41 44 54 68 77 78 86 88 104 117 138 149 153 159 186 199 206 241 256 272 335 354 364 392 414 419 431 500 501 537 563 615 656

	680 706 749 756 796 814 821 838 848 856 915 928 944 961 1001 1011 1018 1030 1048 1094 1111 1136 1156 1166 1175 1181 1223 1254 1297 1304 1310 1354 1363 1400 1408 1419 1436 1446 1462 1470 1476 1497 1503 1507 1519 1614 1641 1691 1699 1746 3040 3051 3054 3091 3114 3140 3144 3163 3166 3180 3189 3196 3210 3220 3227
COM1-b2	8 12 18 25 34 36 42 53 60 64 70 80 86 100 109 114 130 137 165 179 191 208 212 272 283 291 302 342 357 365 374 401 416 432 471 498 508 554 626 665 680 742 750 758 813 820 827 865 891 893 907 943 944 960 1002 1011 1013 1029 1052 1085 1102 1134 1134 1179 1183 1185 1208 1255 1303 1313 1316 1356 1362 1399 1402 1406 1435 1447 1453 1469 1482 1498 1504 1506 1523 1615 1638 1723 1746 1761 3044 3051 3064 3085 3122 3129 3136 3140 3159 3179 3197 3211 3221 3225 3393
TS1-b2	-173 12 17 18 36 44 60 63 70 88 95 99 118 124 129 149 152 161 169 190 197 199 245 254 271 286 290 342 358 384 394 412 428 430 488 491 524 546 564 613 660 682 720 762 764 814 820 834 853 860 914 921 933 937 969 997 1010 1015 1028 1053 1090 1108 1136 1157 1174 1179 1181 1222 1287 1305 1313 1336 1351 1377 1400 1415 1436 1438 1454 1470 1478 1497 1499 1502 1514 1518 1617 1635 1680 1761 3041 3054 3055 3095 3117 3143 3145 3161 3167 3180 3192 3209 3217 3220 3435
INT1-b2	14 18 24 36 39 59 67 73 90 91 101 125 135 146 149 158 170 186 194 197 222 239 242 267 270 284 329 338 355 403 405 432 432 453 485 510 559 567 584 613 669 683 740 758 762 814 817 833 848 869 915 919 937 973 997 998 1011 1013 1022 1053 1092 1109 1137 1155 1173 1180 1183 1218 1293 1301 1305 1326 1350 1378 1400 1418 1436 1449 1458 1470 1478 1497 1497 1501 1516 1613 1636 1647 1653 1771 3041 3055 3057 3098 3118 3146 3147 3160 3172 3180 3193 3210 3221 3222 3574
INT2-b2	9 13 14 20 22 27 31 50 57 67 74 76 83 87 96 97 106 111 120 140 143 148 157 162 170 187 193 207 216 233 246 258 270 279 304 315 335 339 353 355 399 402 406 428 432 439 474 507 550 559 581 604 661 666 682 734 758 761 814 817 830 844 863 870 911 919 937 972 979 997 1010 1012 1026 1026 1051 1080 1090 1106 1112 1128 1137 1154 1173 1177 1178 1181 1202 1274 1288 1295 1305 1317 1348 1380 1399 1413 1418 1437 1444 1445 1448 1461 1472 1474 1480 1491 1494 1497 1502 1510 1512 1518 1546 1612 1633 1656 1668 1702 1782 3037 3041 3043 3056 3064 3070 3097 3110 3114 3118 3144 3146 3154 3157 3170 3177 3187 3191 3209 3221 3226

	3585
TS2-b2	-1286 14 18 19 30 33 44 53 56 63 77 81 87 89 96 99 105 116 127 133 135 141 154 160 176 193 195 198 214 232 247 255 262 264 278 295 300 344 347 360 378 400 404 421 434 459 488 507 573 583 597 629 662 664 682 715 749 759 782 816 819 860 866 871 907 919 942 953 968 991 1000 1011 1023 1028 1046 1063 1079 1092 1110 1115 1129 1136 1164 1173 1177 1181 1196 1273 1276 1295 1304 1332 1350 1387 1392 1404 1405 1432 1444 1445 1449 1463 1474 1477 1484 1489 1491 1497 1503 1504 1510 1511 1519 1545 1567 1603 1636 1640 1688 1701 3039 3044 3046 3054 3072 3090 3114 3117 3125 3139 3143 3159 3160 3162 3172 3188 3193 3210 3225 3228 3575
TS2-b2'	-85 9 11 15 17 19 30 45 48 57 65 68 72 85 91 95 99 121 124 135 144 150 152 161 167 179 190 194 195 213 221 242 255 258 270 297 318 340 347 352 400 403 405 425 432 435 445 488 510 559 561 612 649 668 685 739 761 761 814 820 835 851 862 870 918 921 925 937 970 997 1011 1015 1026 1052 1080 1090 1105 1108 1117 1137 1139 1158 1173 1174 1178 1179 1220 1255 1293 1305 1314 1336 1349 1375 1386 1399 1415 1431 1437 1448 1449 1456 1471 1477 1478 1497 1497 1497 1502 1510 1511 1518 1544 1607 1635 1639 1668 1704 1769 2205 3041 3044 3049 3056 3058 3095 3117 3118 3124 3144 3145 3162 3168 3179 3179 3189 3191 3209 3221 3221 3511

Table S2-3. Frequencies of some stationary points for the entire catalytic cycle, involved in the discussion on TBPB (**OX-d**) and BP (**OX-e**) as oxidant, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide at 343K.

Species	Frequencies (cm⁻¹)																																																																																																				
TBPB	9	28	42	67	142	174	187	233	243	253	255	307	347	372	408	425	447	460	469	553	626	674	694	706	751	804	836	856	887	925	933	934	953	971	995	1012	1013	1041	1046	1055	1084	1109	1174	1190	1206	1258	1269	1291	1339	1362	1409	1411	1433	1476	1485	1497	1499	1510	1510	1519	1532	1628	1647	1763	3049	3050	3056	3135	3138	3143	3145	3147	3148	3183	3193	3203	3214	3218																							
COM1-d	8	11	18	21	31	34	41	43	46	50	59	63	70	74	80	97	108	123	152	154	162	173	181	197	231	236	249	258	263	267	296	318	350	353	366	379	407	414	432	446	466	481	498	557	589	597	625	676	688	691	706	749	802	818	827	829	854	874	878	924	925	931	936	952	955	975	996	1013	1014	1020	1029	1042	1049	1053	1057	1094	1116	1135	1176	1177	1188	1191	1200	1249	1271	1274	1279	1293	1308	1341	1341	1364	1401	1403	1411	1413	1435	1436	1462	1471	1477

	1477 1486 1497 1498 1500 1504 1511 1512 1519 1520 1533 1626 1646 1715 1724 1765 3040 3051 3051 3052 3058 3072 3089 3114 3137 3138 3139 3140 3141 3143 3149 3149 3152 3161 3179 3186 3196 3204 3216 3218
TS1-d	-63 8 19 24 31 32 41 47 58 66 73 86 95 103 112 133 138 148 150 159 164 177 187 192 209 238 248 262 270 289 294 300 344 348 366 379 405 412 421 432 451 481 495 532 561 572 610 625 672 697 721 758 759 814 817 828 835 855 858 862 920 924 924 951 965 971 994 1009 1012 1016 1030 1038 1041 1047 1051 1094 1136 1154 1165 1172 1174 1176 1185 1222 1224 1236 1300 1305 1325 1358 1369 1374 1388 1394 1399 1412 1420 1436 1449 1464 1470 1477 1479 1493 1497 1498 1498 1502 1504 1506 1516 1519 1529 1628 1643 1694 1760 3041 3048 3052 3055 3056 3057 3092 3116 3136 3140 3141 3144 3149 3150 3156 3162 3164 3180 3180 3183 3189 3199 3208 3211
INT1-d	16 22 26 29 35 37 53 65 68 79 89 99 104 121 132 143 147 153 160 176 181 193 200 209 241 245 269 270 271 276 296 329 342 347 378 393 413 426 436 453 456 476 489 559 565 596 612 626 690 697 717 750 760 814 819 834 838 846 851 859 917 919 923 953 965 970 995 1008 1013 1015 1025 1027 1042 1044 1052 1093 1136 1147 1166 1171 1173 1179 1183 1220 1236 1241 1305 1307 1319 1336 1358 1374 1376 1399 1403 1415 1425 1437 1455 1471 1472 1473 1478 1488 1494 1497 1500 1501 1508 1515 1518 1524 1617 1644 1645 1668 1771 3041 3046 3048 3055 3056 3060 3096 3117 3133 3138 3144 3145 3146 3152 3154 3162 3163 3169 3179 3179 3188 3199 3212 3216
TS2-d	-679 16 20 22 25 29 32 34 48 55 60 64 69 74 80 85 96 98 106 109 120 126 132 135 149 153 154 160 164 176 187 204 213 236 241 259 261 269 270 278 300 305 324 347 358 377 395 405 413 420 436 451 452 477 496 514 554 559 612 617 627 688 698 718 723 758 760 814 824 836 841 855 860 867 923 924 925 953 966 970 979 995 1007 1013 1016 1030 1041 1048 1051 1052 1076 1091 1103 1121 1136 1142 1152 1170 1173 1174 1175 1183 1191 1226 1240 1252 1260 1299 1305 1324 1356 1368 1373 1399 1400 1408 1411 1427 1433 1436 1439 1454 1454 1471 1472 1478 1480 1486 1494 1497 1497 1498 1502 1506 1512 1513 1516 1517 1519 1528 1542 1608 1641 1646 1693 1733 1768 3041 3047 3048 3051 3052 3054 3056 3061 3092 3116 3122 3128 3133 3136 3141 3143 3144 3145 3154 3164 3164 3173 3177 3179 3187 3190 3198 3204 3210 3215
BP	19 24 31 37 70 129 153 166 191 272 340 344

	406 407 409 443 444 457 506 625 625 673 691 692 699 704 707 798 803 852 854 855 856 941 955 955 996 996 1004 1013 1014 1014 1015 1041 1051 1059 1106 1109 1176 1176 1191 1193 1242 1251 1340 1341 1364 1364 1477 1477 1519 1519 1627 1627 1646 1646 1779 1803 3186 3186 3196 3196 3204 3204 3214 3214 3219 3219
COM1-e	12 13 19 21 25 27 28 29 31 36 47 50 58 65 68 84 89 116 129 138 158 168 172 177 183 203 241 271 274 333 339 343 353 376 406 407 413 418 437 439 466 479 510 585 609 625 625 673 690 692 700 704 708 718 798 802 816 822 853 855 856 858 877 909 936 954 956 956 994 996 1006 1012 1013 1014 1015 1016 1031 1041 1051 1054 1060 1107 1109 1135 1176 1176 1176 1191 1193 1202 1227 1243 1254 1292 1309 1340 1341 1364 1364 1371 1402 1408 1435 1438 1468 1477 1477 1479 1498 1504 1518 1519 1521 1626 1627 1646 1646 1723 1762 1766 1796 3041 3052 3067 3087 3116 3126 3136 3141 3159 3183 3186 3186 3196 3196 3204 3204 3215 3215 3218 3218
TS1-e	-228 12 16 20 23 31 34 39 44 53 61 68 80 81 102 104 111 119 132 140 144 151 162 187 194 207 233 258 267 270 271 297 347 362 369 396 410 410 418 433 440 495 508 517 557 614 623 624 671 681 692 692 716 720 757 799 801 814 836 851 852 852 854 855 922 950 951 962 993 993 1011 1011 1012 1012 1015 1032 1042 1042 1051 1095 1100 1117 1136 1147 1169 1174 1175 1175 1183 1187 1218 1219 1263 1292 1304 1335 1335 1360 1361 1368 1399 1408 1436 1461 1471 1474 1474 1478 1498 1503 1510 1511 1519 1571 1594 1624 1626 1637 1637 1705 1766 3041 3054 3064 3090 3116 3139 3143 3162 3164 3179 3185 3185 3194 3195 3204 3204 3215 3216 3218 3218
INT1-e	13 14 19 20 25 29 37 47 59 66 70 74 86 93 109 118 131 141 149 152 161 164 180 187 220 235 254 271 272 276 306 337 345 396 408 409 419 428 430 460 462 484 563 579 589 609 624 625 686 690 693 694 709 715 760 805 814 815 830 832 835 849 853 856 915 950 952 972 993 994 1009 1010 1012 1012 1013 1022 1041 1042 1052 1095 1095 1136 1137 1141 1172 1173 1173 1183 1184 1185 1215 1230 1271 1306 1323 1332 1333 1357 1359 1379 1400 1418 1436 1456 1470 1473 1474 1478 1497 1501 1512 1514 1516 1621 1622 1637 1641 1643 1656 1686 1771 3041 3055 3056 3098 3118 3146 3147 3158 3172 3180 3181 3182 3191 3191 3201 3201 3212 3214 3215 3218
TS2-e	-364 11 15 18 22 26 30 33 38 41 46 56 65 66 68 75 81 86 88 95 102 110 123 127

132 136 143 154 155 162 164 177 184 196 226 242 249 261 271 278 306 311 345 377 383 401 412 414 421 426 439 451 473 495 555 560 562 575 612 625 626 635 689 697 698 712 719 737 759 809 814 821 824 835 840 855 856 859 923 944 952 953 966 993 995 1008 1011 1013 1013 1016 1030 1041 1043 1051 1067 1073 1092 1100 1118 1125 1136 1151 1153 1171 1171 1174 1174 1176 1183 1187 1223 1243 1290 1302 1305 1324 1334 1355 1361 1364 1373 1399 1412 1413 1430 1436 1453 1454 1471 1473 1474 1478 1481 1492 1497 1502 1506 1511 1517 1517 1519 1535 1606 1624 1640 1644 1646 1687 1691 1706 1767 3041 3055 3056 3059 3059 3092 3116 3137 3141 3141 3144 3164 3165 3178 3179 3183 3187 3191 3192 3197 3198 3199 3206 3209 3211 3214

Table S2-4. Frequencies of some stationary points for the reduction process, involved in the discussion on Cu(OAc)₂ as catalyst, computed at IDSCRF (PCM)-B3LYP/DZVP level in formamide at 343K.

Species	Frequencies (cm ⁻¹)													
pre-CAT-OAc	10	19	20	23	27	28	36	54	56	63	65	77		
	105	107	117	147	173	179	187	190	201	218	230	273		
	285	331	335	369	454	459	548	558	610	610	612	616		
	667	676	684	687	950	951	951	956	1020	1020	1046	1047	1063	
	1063	1067	1067	1387	1388	1388	1390	1443	1447	1448	1449	1469	1471	
	1475	1475	1493	1494	1510	1513	1518	1519	1553	1597	3060	3060	3062	
	3062	3147	3147	3151	3151	3181	3182	3187	3187					
H₂O...H₂O	66	215	233	248	384	684	1632	1686	3550	3627	3717	3729		
LE-INT1	15	16	23	27	28	31	32	34	35	38	45	50		
	54	61	65	70	74	79	84	104	108	111	117	124		
	133	139	145	159	164	178	182	193	202	208	213	242		
	251	265	286	295	326	340	359	359	390	394	404	452		
	457	489	519	527	543	609	610	611	613	658	662	669		
	673	680	682	871	889	934	946	948	950	1020	1021	1025		
	1034	1044	1062	1062	1066	1067	1079	1121	1128	1134	1178	1273	1363	
	1384	1388	1388	1413	1415	1441	1446	1451	1453	1456	1472	1473	1476	
	1477	1477	1489	1491	1491	1505	1507	1510	1511	1525	1530	1545	1582	1618
	1642	1687	1690	2771	3044	3049	3056	3059	3059	3060	3087	3121	3123	3139
	3145	3146	3146	3162	3174	3178	3179	3182	3193	3308	3588	3663		
LE-TS1	-528	11	13	14	26	27	29	31	31	34	39	43		
	48	57	69	73	78	82	92	97	100	108	113	115		
	130	140	143	147	159	164	175	190	196	198	240	250		
	260	276	293	308	330	353	356	396	403	420	453	459		
	521	538	543	592	609	611	613	616	653	662	668	677		
	678	696	777	797	870	940	945	948	950	1021	1022	1023		
	1043	1046	1062	1065	1066	1067	1079	1119	1128	1178	1230	1273	1384	
	1385	1387	1388	1416	1432	1441	1446	1452	1454	1456	1460	1473	1474	

	1474 1476 1478 1491 1492 1495 1501 1503 1510 1511 1528 1534 1545 1578 1630 1689 1693 1732 1870 3043 3048 3058 3059 3059 3060 3079 3119 3121 3144 3145 3145 3146 3162 3178 3178 3181 3182 3192 3595 3654
LE-INT2	8 10 14 17 20 22 27 28 34 41 44 50 53 66 71 73 77 89 95 99 102 109 110 116 124 130 131 148 159 162 178 180 191 196 224 250 259 273 292 298 330 351 355 376 399 403 446 454 459 497 536 544 566 603 610 612 613 619 667 668 678 680 870 872 881 914 947 949 951 1021 1021 1022 1029 1043 1062 1066 1067 1067 1072 1079 1119 1128 1177 1273 1318 1385 1387 1388 1403 1416 1441 1446 1452 1456 1457 1471 1473 1474 1477 1478 1485 1486 1491 1492 1504 1505 1510 1511 1531 1532 1545 1578 1692 1709 1722 2867 3043 3048 3059 3059 3060 3063 3075 3119 3121 3143 3145 3145 3146 3161 3178 3178 3182 3190 3192 3338 3555 3682
LE-TS2	-125 9 11 16 22 25 30 34 35 39 40 43 47 52 61 72 80 83 88 91 94 101 103 108 113 128 135 136 154 159 169 180 197 200 206 227 251 271 279 298 323 330 370 409 420 430 438 457 458 464 517 540 600 603 610 612 616 630 667 675 679 681 847 858 880 915 917 946 948 1021 1030 1030 1031 1043 1063 1063 1067 1067 1067 1095 1111 1120 1171 1253 1298 1314 1361 1384 1387 1403 1416 1436 1442 1455 1457 1472 1472 1475 1476 1484 1485 1487 1492 1493 1496 1506 1506 1507 1525 1532 1571 1575 1637 1678 1727 1938 2895 3043 3049 3059 3059 3062 3063 3117 3123 3143 3144 3144 3145 3177 3178 3181 3189 3189 3192 3228 3570 3674
LE-INT3	16 17 21 28 30 31 31 36 39 42 45 45 50 55 66 76 79 83 87 91 96 100 107 109 120 126 130 138 139 154 169 172 178 199 222 233 246 264 272 297 320 321 337 379 414 441 448 458 465 494 518 530 548 598 601 611 614 616 651 653 663 670 680 806 886 888 890 928 944 949 1020 1022 1030 1041 1043 1062 1066 1067 1067 1075 1120 1125 1175 1223 1265 1312 1363 1382 1387 1403 1418 1426 1436 1441 1458 1469 1471 1476 1476 1478 1484 1484 1487 1494 1499 1506 1509 1513 1533 1534 1577 1623 1685 1726 1740 2877 3035 3043 3058 3058 3063 3066 3103 3115 3143 3144 3144 3147 3164 3177 3178 3185 3188 3189 3197 3397 3589 3677
LE-INT4a	15 28 35 41 46 49 77 85 101 117 138 142 147 153 167 189 220 262 269 312 389 423 449 476 535 602 613 633 671 676 893 921 946 1007 1023 1044 1066 1067 1071 1118 1125 1172 1265 1353 1384 1407 1419 1432 1459 1465 1470 1473 1485 1490 1494 1498 1507 1510 1526 1555 1579 1670 2583 3040 3045 3059 3064 3110 3116 3142 3148 3177 3185 3194 3195
LE-INT4b	24 25 29 39 59 78 98 109 138 159 179 190 238 251 311 345 405 426 452 490 513 580 607 610

	642 684 838 920 951 1022 1034 1057 1066 1067 1139 1362 1388 1412 1454 1473 1475 1486 1506 1518 1529 1641 1679 2384 2807 3060 3064 3147 3148 3181 3194 3610 3659
CAT-OAc	27 34 44 48 62 92 101 164 179 233 333 481 521 544 611 620 653 679 906 927 1031 1036 1061 1066 1235 1350 1382 1412 1437 1476 1480 1486 1491 1638 1702 3054 3065 3133 3152 3170 3200 3315
N...H₂O	25 41 77 86 102 118 153 222 230 318 398 436 516 566 592 757 780 1033 1085 1130 1144 1177 1286 1301 1445 1449 1484 1505 1511 1516 1547 1665 1743 3037 3042 3106 3116 3195 3195 3467 3660 3764

Table S3-1. The total energies ($E_{\text{tot/a.u.}}=E_{\text{elec/a.u.}}+ZPE/a.u.$), zero-point energies (ZPE/a.u.) and Gibbs free energies (G/a.u.) for the entire catalytic cycle, involved in the discussion on TBHP (**OX-a**) as oxidant, computed at IDSCRF(PCM)-B3LYP/DZVP level in formamide at 343K.

Species	$E_{\text{tot/a.u.}}$	ZPE/a.u.	G/a.u.
CAT	-2560.748721	0.158235	-2560.79165
COM1-a	-2869.476457	0.297453	-2869.53858
TS1-a1	-2869.460096	0.294980	-2869.51806
INT1-a1	-2636.544359	0.170155	-2636.59176
INT2-a1	-2885.012453	0.275399	-2885.07329
TS2-a1	-481.366744	0.221802	-481.40547
TS3-a1	-3132.806023	0.361436	-3132.87983
INT3	-2884.366808	0.264546	-2884.42445
TS4	-2884.357795	0.264156	-2884.41308
INT4	-2884.364675	0.264441	-2884.42129
TS5	-2884.328074	0.259281	-2884.38290
INT5	-2884.436609	0.264551	-2884.49612
TS6	-2884.437018	0.265345	-2884.49446
INT6	-2884.438610	0.266256	-2884.49835
CAT-H₂O	-2637.180204	0.180883	-2637.23000
TS7	-2945.904163	0.320234	-2945.97087
COM2-a	-2945.905480	0.320536	-2945.97439
DMF-H₂O	-324.882970	0.126354	-324.91401
1a	-460.267084	0.155746	-460.30062
3a	-707.523201	0.239350	-707.56856
DMF	-248.453761	0.102658	-248.4765
TBHP	-308.720775	0.137849	-308.74759
CuCl	-2100.443557	0.000755	-2100.45301
C3H9CO•	-232.919324	0.122418	-232.94278
(CH₃)₂N(O)C•	-247.806897	0.090161	-247.83051
BuOH	-233.576649	0.135426	-233.59929

Table S3-2. The total energies ($E_{\text{tot/a.u.}}=E_{\text{elec/a.u.}}+ZPE/\text{a.u.}$), zero-point energies (ZPE/a.u.) and Gibbs free energies (G/a.u.) for the entire catalytic cycle, involved in the discussion on m-CPBA (**OX-b**) as oxidant, computed at IDSCRF(PCM)-B3LYP/DZVP level in formamide at 343K.

Species	$E_{\text{tot/a.u.}}$	ZPE/a.u.	G/a.u.
COM1-b1	-3516.222326	0.265460	-3516.29181
TS1-b1	-3516.209066	0.263236	-3516.27432
INT1-b1	-3440.486740	0.253103	-3440.54691
TS2-b1	-3688.282133	0.339039	-3688.35752
INT2-b1	-3439.829199	0.241965	-3439.88687
INT3-b1	-3688.290560	0.345766	-3688.36483
TS3-b1	-3688.283018	0.345318	-3688.35407
INT4-b1	-3688.284053	0.345768	-3688.35579
TS4-b1	-3688.248417	0.340290	-3688.32037
INT5-b1	-3688.355556	0.346699	-3688.43224
CAT-ROH	-3441.102133	0.263901	-3441.16545
COM1-b2	-3516.29904	0.265782	-3516.29904
TS1-b2	-3516.216932	0.264302	-3516.27903
INT1-b2	-3516.247065	0.266384	-3516.30866
INT2-b2	-3764.696888	0.369620	-3764.77591
TS2-b2	-3764.682491	0.365320	-3764.757
TS2-b2'	-3764.705144	0.366938	-3764.78391
m-CBA	-880.344689	0.104617	-880.37141
m-CPBA	-955.478271	0.107118	-955.50838

Table S3-3. The total energies ($E_{\text{tot/a.u.}}=E_{\text{elec/a.u.}}+ZPE/\text{a.u.}$), zero-point energies (ZPE/a.u.) and Gibbs free energies (G/a.u.) for the entire catalytic cycle, involved in the discussion on TBPB (**OX-d**) and BP (**OX-e**) as oxidant, computed at IDSCRF(PCM)-B3LYP/DZVP level in formamide at 343K.

Species	$E_{\text{tot/a.u.}}$	ZPE/a.u.	G/a.u.
TBPB	-653.065243	0.229537	-653.1058
COM1-d	-3213.818587	0.388317	-3213.89391
TS1-d	-3213.800412	0.387104	-3213.86976
INT1-d	-3213.825792	0.388399	-3213.89385
TS2-d	-3462.281901	0.487019	-3462.36459
INT2-d	-2980.915420	0.262812	-2980.97355
BP	-840.245782	0.208094	-840.28724
COM1-e	-3400.995947	0.366737	-3401.07415
TS1-e	-3400.979148	0.364677	-3401.05246
INT1-e	-3401.022427	0.366670	-3401.09566
TS2-e	-3649.471928	0.464866	-3649.55894
INT2-e	-2980.915420	0.262812	-2980.97355

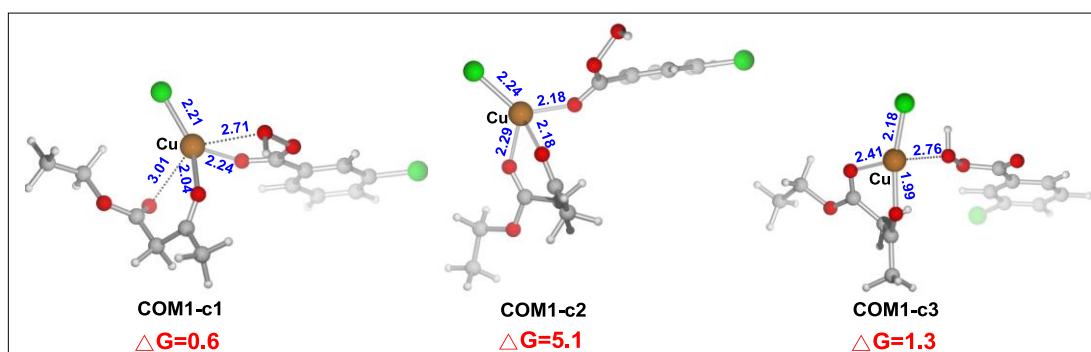
Table S3-4. The total energies ($E_{\text{tot/a.u.}}=E_{\text{elec/a.u.}}+ZPE/\text{a.u.}$), zero-point energies ($ZPE/\text{a.u.}$) and Gibbs free energies ($G/\text{a.u.}$) for the reduction process, involved in the discussion on $\text{Cu}(\text{OAc})_2$ as catalyst, computed at IDSCRF(PCM)-B3LYP/DZVP level in formamide at 343K.

Species	$E_{\text{tot/a.u.}}$	$ZPE/\text{a.u.}$	$G/\text{a.u.}$
pre-CAT-OAc	-4194.4863	0.102112	-4194.5514
$\text{H}_2\text{O}\dots\text{H}_2\text{O}$	-152.85524	0.045041	-152.87081
LE-INT1	-4595.8091	0.358786	-4595.89574
LE-TS1	-4595.8059	0.354065	-4595.89224
LE-INT2	-4595.8152	0.359110	-4595.90541
LE-TS2	-4595.7663	0.355331	-4595.85415
LE-INT3	-4595.7889	0.357411	-4595.87667
LE-INT4a	-2345.6747	0.205065	-2345.72728
LE-INT4b	-2250.0871	0.150249	-2250.13237
CAT-OAc	-2097.8395	0.113066	-2097.87784
$\text{N}\dots\text{H}_2\text{O}$	-400.135521	0.129899	-400.16913

TS(double radical): $\left[\begin{array}{c} \text{R}_2 \\ | \\ \text{O}_b \\ \vdots \\ \text{O}_a \\ | \\ \text{R}_1 \end{array} \right]$

Oxidant 	TS(double radical)		radical a+ radical b		Expt.yield(%)
	ΔE	ΔG	ΔE	ΔG	
 (TBHP)	—	—	33.5	34.4	99
 (CPBA)	—	—	32.8	32.8	20
 (DTBP)	—	—	24.5	19.1	n.d
 (TBPB)	25.4	25.3	23.8	18.8	n.r.
 (BP)	23.8	19.1	18.6	13.3	n.d.

Table S4. The relative energies (ΔE , kcal/mol) and Gibbs free energies (ΔG , kcal/mol) for different oxidants to form the correspondent radicals.



Scheme S1. Comparative structures and Gibbs free-energies (ΔG , kcal/mol) at B3LYP/DZVP level of theory of the complex COM1-b1, COM1-b2 and COM1-b3.

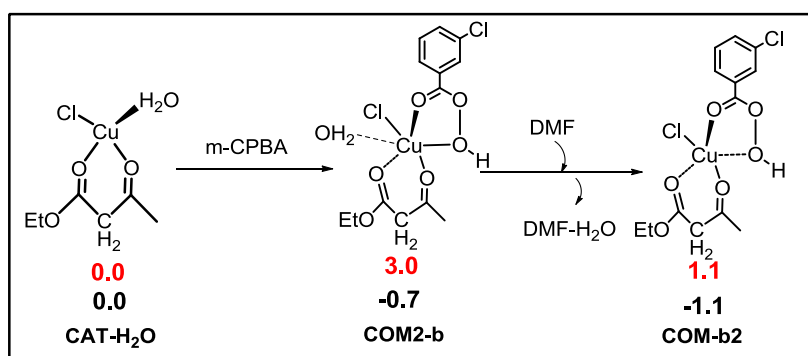


Figure S1. The relative energies (ΔE , kcal/mol) and Gibbs free energies (ΔG , kcal/mol) for the recycling of catalyst step of 1b with the schematic representation of stationary points along the reaction coordinates.

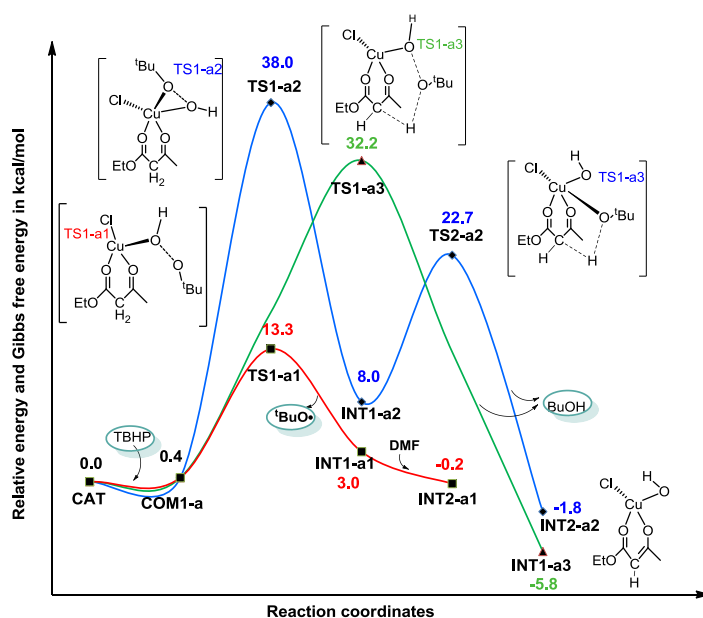


Figure S2. Gibbs free-energy profiles (ΔG , kcal/mol) for the oxidation step of 1a with the schematic representation of stationary points along the reaction coordinates.

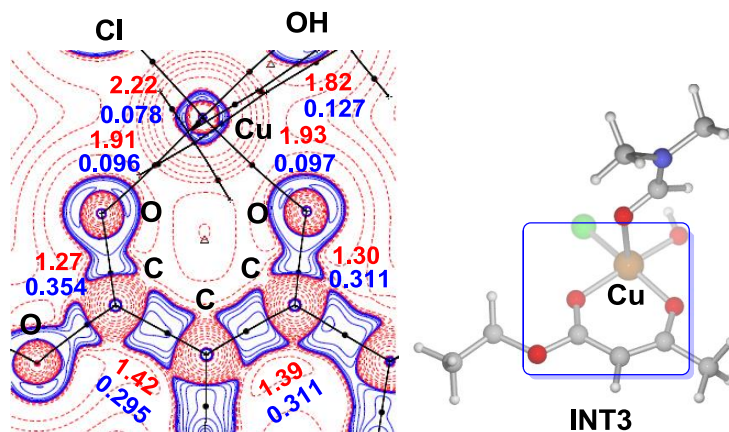


Figure S3. ORTEP plot of INT3, in which the weak interatomic interactions are represented by black dashed lines. Depiction of the “onion layer” 2-D isodensity surfaces was provided from the Laplacian of electron densities $\nabla^2\rho$ in different planes selected, with the bond lengths (Å), bond paths, electron densities (ρ_b in au), and bond critical points shown in red text, solid black lines, blue text, and small black dots, respectively.

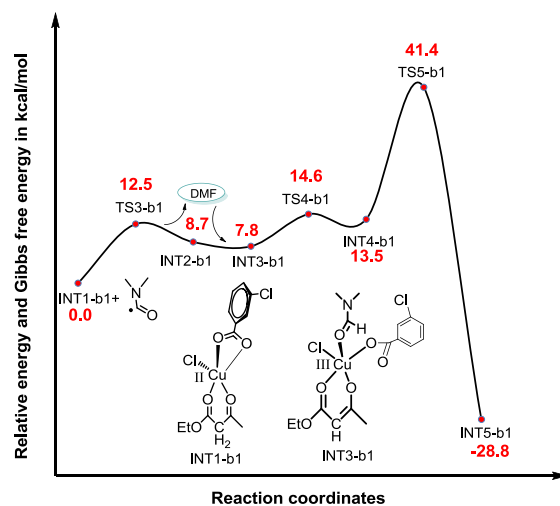


Figure S4. Gibbs free-energy profiles (ΔG , kcal/mol) for INT1-b1 \rightarrow INT5-b1 steps, involved m-CPBA as oxidant.

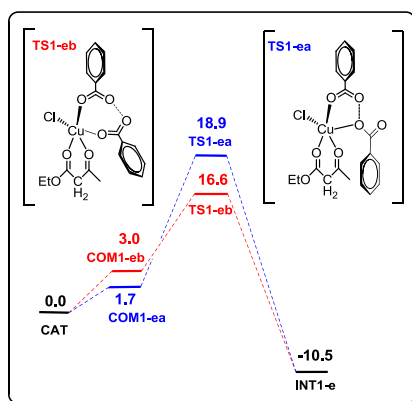


Figure S5. Gibbs free-energy profiles (ΔG , kcal/mol) for the oxidation step, involved BP as oxidant, with the schematic representation of stationary points along the reaction coordinates.

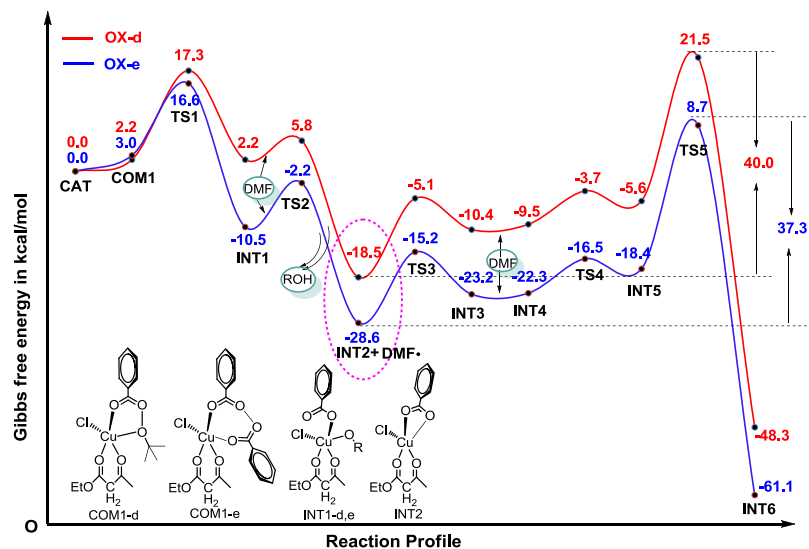


Figure S6. Gibbs free-energy profiles (ΔG , kcal/mol) for the entire catalytic cycle, involved in the discussion on TBPB (**OX-d**) and BP (**OX-e**) as oxidant, computed at B3LYP+IDSCRF/DZVP level in acetonitrile at 343K.

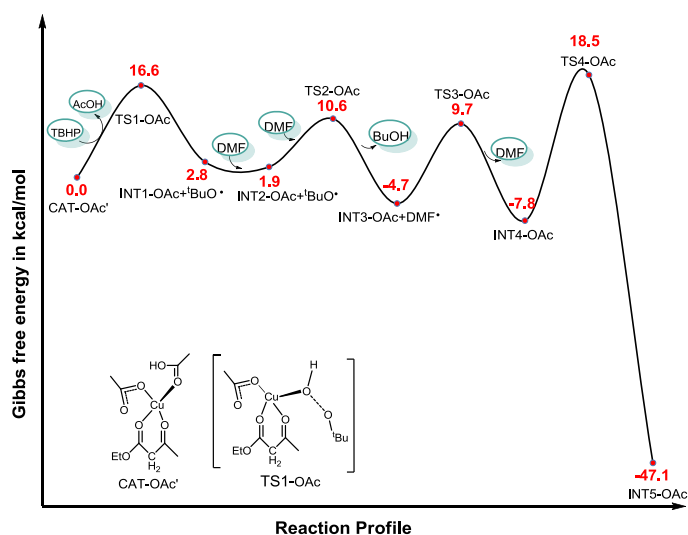


Figure S7. Gibbs free-energy profiles (ΔG , kcal/mol) for the entire catalytic cycle, involved in the discussion on CuOAc as catalyst, computed at B3LYP+IDSCRF/DZVP level in acetonitrile at 343K.

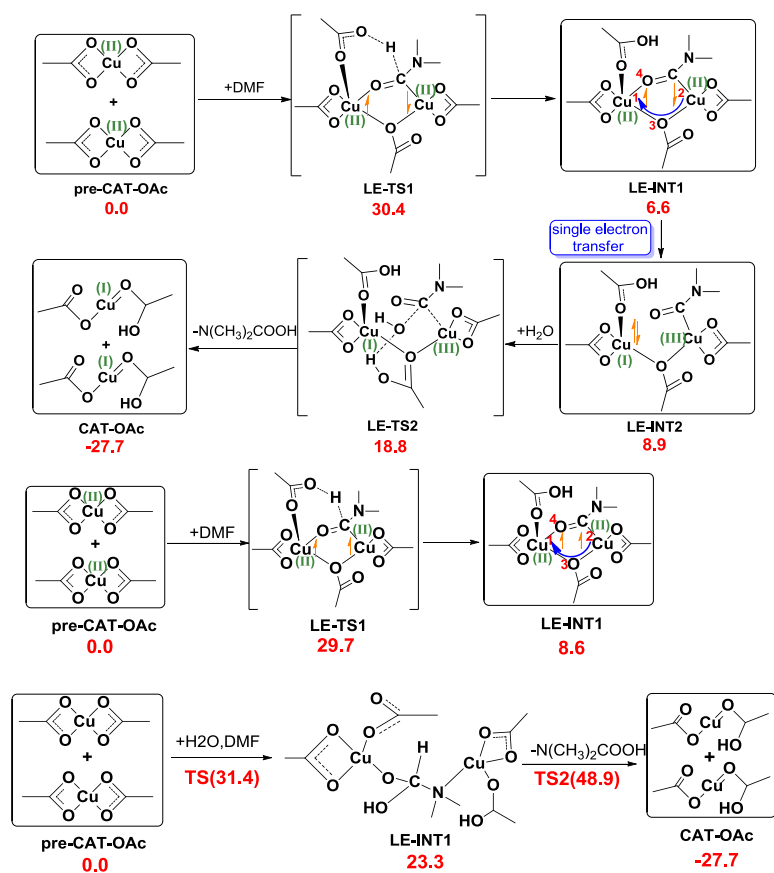


Figure S8. Gibbs free-energy profiles (ΔG , kcal/mol) for the other probable reduction steps of CuCl_2 and $\text{Cu}(\text{OAc})_2$.

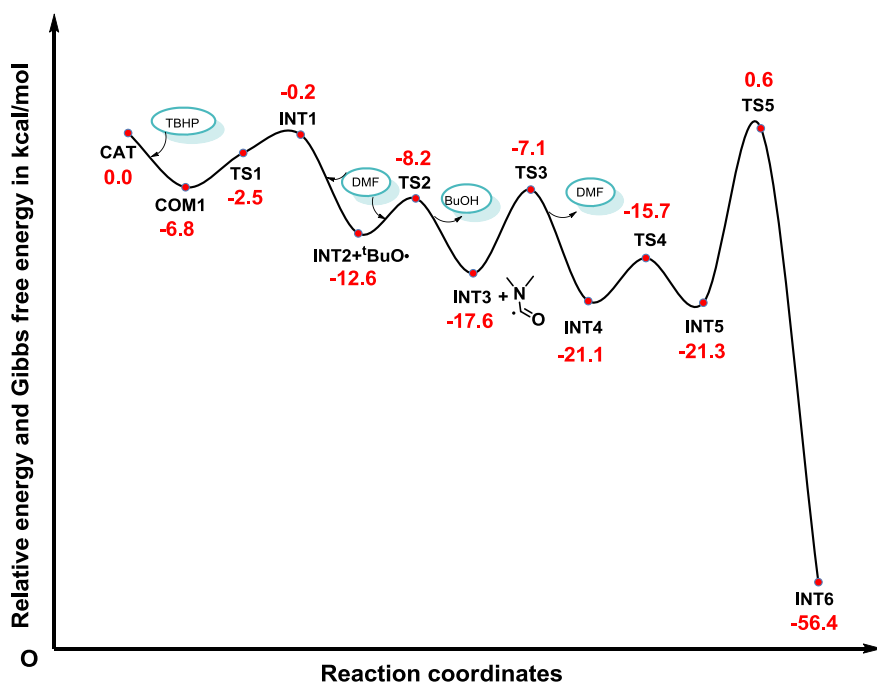


Figure S9. Gibbs free-energy profiles (ΔG , kcal/mol) for the entire catalytic cycle, involved in the discussion on TBHP as oxidant, computed at M06L+IDSCRF/DZVP level in acetonitrile at 343K.