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Supporting information: Atomistic Catalytic Reaction Networks: Case study on electrochemical reduction of CO, NO & combinations

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Computational details

The atomic structure where created using the Atomic Simulation Environment (ASE).[1] We setup a 3x3x4 fcc111 copper slab with a lattice constant of a=3.67564 .

A challenge to solve, is to translate our SMILES into correctly oriented atomic adsorbates on the Cu(111) surface. To do this the following procedure is carried out: 1) The generic atom bond 'M' is exchanged with the copper atom 'Cu' (another could be used). 2) The adsorbate including the copper atoms are made into an atomic 3D object by using mol3D from molSimplify.[2] 3) The center of mass is calculated of the atomic 3D object using ASE with and without the copper atoms. 4) A vector is now drawn by using these two center of masses, and this vector now represent the average orientation of the bonds that should be pointed to the surface. 5) The atomic 3D object is now rotated/oriented toward the surface using the normal vector of the surface and the vector from the two center of masses.

Another challenge for these following adsorption energy simulation is that several of the intermediates are very unstable and the intermediate structure breaks down during relaxation. To avoid this, we fix all four layers of the copper slab and apply a strong hookean springs to keep the intermediates intact during relaxation. This enable us to relax and obtain the bond strength of intermdiates, while avoiding a intermediate reordering during relaxation.

The DFT calculations were carried out using the GPAW calculator[3,4] in plane wave mode with the RPBE exchange-correlation functional.[5] The DFT energy for the clean slabs and adsorbates were calculated with a cut-off energy of 500 eV, a force criterion of at least 0.05 eV/Å and a $4 \times 3 \times 1$ k-point sampling grid.

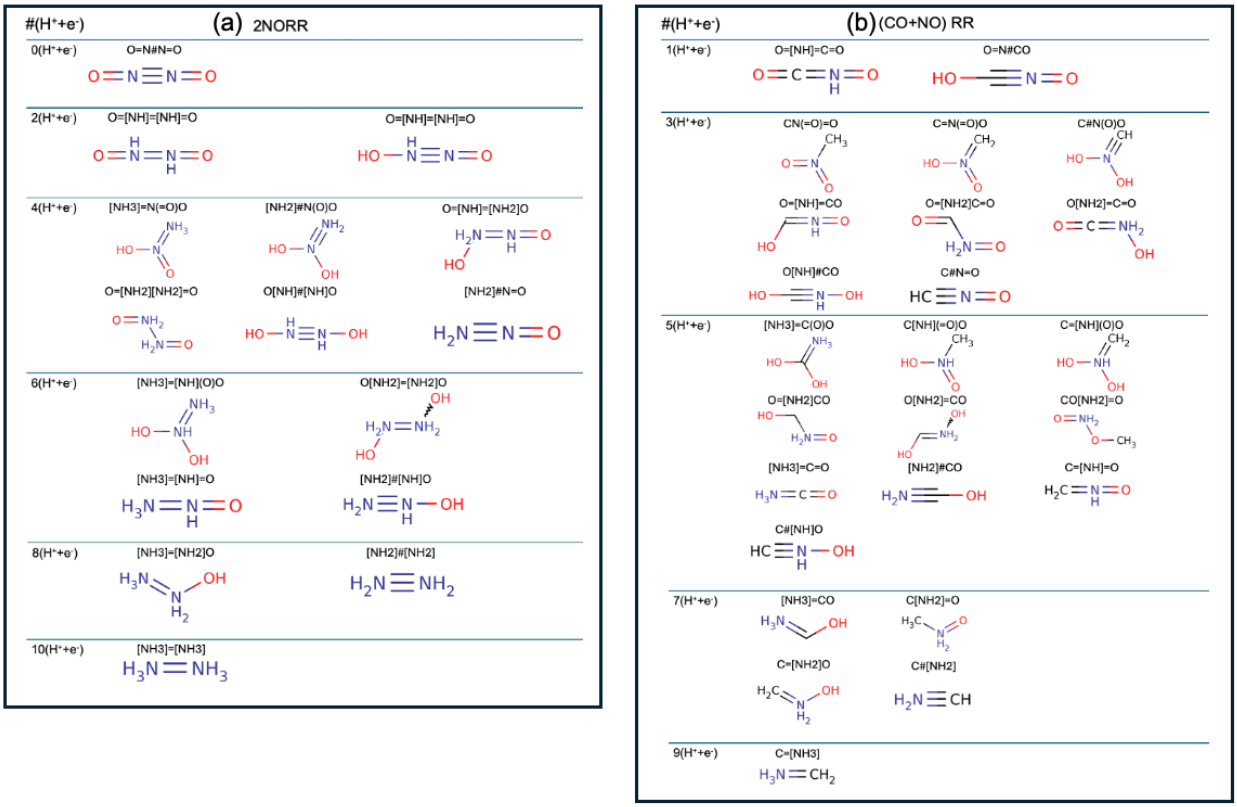

Figure S1: The automated reaction network generator list of products from reactants using nitrogen with valency 5. Here, products are depicted for (a) 2NO, and (b) CO+NO reduction reaction, all excluding ring and oxygen-oxygen bonds, and with using nitrogen valency 5 (i.e. having 5 bonds) . This enables experimentalists to prepare quantification protocols for each product, and computational tools can be used to simulate the minimum energy reaction path.

Energies calculated in Figure 3 is defined as:

$$\text{Energy} = E_{*ads} - E_{*} - 2E_{CO(g)} - n\tfrac{1}{2}E_{H_2(g)} \tag{1}$$

Where E_{*ads} is the calculated adsorption structure at some reaction coordinate, E_{*} is the copper surface, $E_{CO(g)}$ is the energy of CO in gas phase and $n\frac{1}{2}E_{H_2(g)}$ counts the hydrogen transfers (e.g. n is the reaction coordinate)

Additional data

Table S1: Product list from reducing CO & 2NO's, when disregarding R-O-O-R bonds and ring structure giving a total of 206 $CN_2O_xH_y$ products listed at 0 to 12 (H^++e^-) transfers

(H^++e^-) transfers & products
0(H^++e^-): O=C(N=O)N=O, O=C=NON=O
2(H^++e^-): O=NOC(=O)N, O=NOC(O)=N, N=NOC(=O)O, O=NNC(=O)O, ON=NC(=O)O, O=NN=C(O)O, N#CON(O)O, O=C=NN(O)O, O=C(ON)N=O, O=C(NO)N=O, OC(N=O)=NO, OC(N=O)N=O, ON(C=O)N=O, O=C=NONO, O=CNON=O, OC=NON=O', O=NCON=O, ON=CON=O, O=NNOC=O, ON=NOC=O, O=C=NN=O, N#CON=O
4(H^++e^-): OC(N=N)(O)O, NC(N=O)(O)O, ONOC(=O)N, ONOC(O)=N, O=NOC(O)N, NNOC(=O)O, N=NOC(O)O, ONNC(=O)O, ONN=C(O)O, O=NNC(O)O, ON=NC(O)O, NONC(=O)O, NON=C(O)O, O=CON(O)N, N=CON(O)O, O=CNN(O)O, OC=NN(O)O, O=NON(O)C, C=NON(O)O, O=NCN(O)O, ON=CN(O)O, OC(=O)N(O)N, NC(=O)N(O)O, N=C(O)N(O)O, O=C(ON)ON, O=C(ON)NO, OC(ON)=NO, OC(ON)N=O, O=C(NO)NO, OC(NO)=NO, OC(NO)N=O, ON(OC)N=O, ON(ON)C=O, ON(CO)N=O, ON(C=O)NO, O=CNONO, OC=NONO, OCNON=O, O=NCONO, ON=CONO, ONCON=O, O=NNOCO, ON=NOCO, ONNOC=O, CONON=O, NOCON=O, NONOC=O, OC(=O)N=N, NC(=O)N=O, N=C(O)N=O, ON(O)C#N, ON=C=NO, O=NC=NO, O=NCN=O, NON=C=O, O=CN=NO, OC=NN=O, O=C=NNO, O=CNN=O, C=NON=O, N=NOC=O, N=CON=O, N#CONO, O=NC#N
6(H^++e^-): NC(ON)(O)O, OC(NN)(O)O, NC(NO)(O)O, ONOC(O)N, NNOC(O)O, ONNC(O)O, NONC(O)O, OCON(O)N, NCON(O)O, OCNN(O)O, ONON(O)C, CNON(O)O, ONCN(O)O, CONN(O)O, NOCN(O)O, OC(O)N(O)N, NC(O)N(O)O, CN(O)N(O)O, OC(ON)ON, OC(ON)NO, OC(NO)NO, ON(OC)ON, ON(OC)NO, ON(ON)CO, ON(CO)NO, OCNONO, ONCONO, ONNOCO, CONONO, NOCONO, NONOCO, NC(=O)ON, N=C(O)ON, OC(=O)NN, OC(O)=NN, OC(O)N=N, NC(=O)NO, N=C(O)NO, NC(O)=NO, NC(O)N=O, ON(O)N=C, ON(O)C=N, CN(O)N=O, NN(O)C=O, NOC=NO, NOCN=O, ONC=NO, ONCN=O, CON=NO, CONN=O, NON=CO, NONC=O, OCN=NO, OC=NNO, OCNN=O, O=CNNO, CNON=O, C=NONO, NNOC=O, N=NOCO, NCON=O, N=CONO, O=NC=N, ON=C=N, ONC#N, C=NN=O, N=NC=O, NN=C=O, NOC#N
8(H^++e^-): NC(N)(O)O, NC(O)ON, OC(O)NN, NC(O)NO, NN(O)OC, ON(O)NC, CN(O)ON, ON(O)CN, CN(O)NO, NN(O)CO, NOCON, NOCNO, ONCNO, CONON, CONNO, NONCO, OCNNO, CNONO, NNOCO, NCONO, **NC(=O)N**, NC(O)=N, O=NCN, ON=CN, ONC=N, C=NNO, CN=NO, CNN=O, N=NCO, NN=CO, NNC=O, NON=C, CON=N, NOC=N, N=C=N, NC#N
10(H^++e^-): NC(O)N, CN(O)N, ONCN, CNNO, NNCO, NONC, CONN, NOCN, NC=N, CN=N, C=NN
12(H^++e^-): NCN, CNN

Table S2: Product list from reducing 4 CO's, thus all $C_4O_xH_y$ products listed at 2 to 14 (H^++e^-) transfers

(H^++e^-) transfers & products
2(H^++e^-): OC(=O)C#CC(=O)O, OC(=O)OC(=O)C#C, O=COC#CC(=O)O, O=C=C=COC(=O)O, O=CC#COC(=O)O, C#COC(=O)OC=O, O=C=CC(=O)OC=O, OC#CC(=O)OC=O, O=C=C=C(O)OC=O, OC(=O)C(=O)OC#C, OC(=O)C(=O)C=C=O, OC(=O)C(=O)C#CO, OC(=O)C(O)=C=C=O, O=C=C(O)C(=O)C=O, O=CC(=O)C(=O)C=O, O=C=C(O)C(O)=C=O, O=C(C=O)OC=C=O, O=C(C=O)OC#CO, OC(=C=O)OC=C=O, OC(=C=O)OC#CO, O=COC(C=O)=C=O, OC(=O)C(C=O)=C=O, O=COC#COC=O,
4(H^++e^-): C#CC(=O)C(O)(O)O, OC(C=C=C=O)(O)O, OC(C#CC=O)(O)O, O=COC(C#C)(O)O, C#COC(C=O)(O)O, O=C=CC(C=O)(O)O, OC#CC(C=O)(O)O, OC(=O)C(C#C)(O)O, OC(=O)C=C=C(O)O, OC(O)=C=C=C(O)O, OC(=O)C=CC(=O)O, OC(O)C#CC(=O)O, OC(=O)OC(=O)C=C, OC(O)OC(=O)C#C, OC(=O)OC(O)=C=C, OC(=O)OC(O)C#C, OC(=O)OC(=C)C=O, OC(=O)OC(C)=C=O, CC(=O)OC(=O)C=O, C=C(O)OC(=O)C=O, CC(=O)OC(O)=C=O, C=C(O)OC(O)=C=O, OC(=O)CC(=O)C=O, OC(O)=CC(=O)C=O, OC(=O)C=C(O)C=O, OC(O)=C=C(O)C=O, OC(=O)CC(O)=C=O, OC(O)=CC(O)=C=O, C#COCOC(=O)O, O=COC=CC(=O)O, OCOC#CC(=O)O, O=COC=C=C(O)O, O=COC#CC(O)O, O=C=CCOC(=O)O, O=CC=COC(=O)O, OC=C=COC(=O)O, OC#CCOC(=O)O, OCC#COC(=O)O, O=C=C=COC(O)O, O=CC#COC(O)O, O=C=COCC(=O)O, OC#COCC(=O)O, O=C=COC=C(O)O, OC#COC=C(O)O, COC#COC(=O)O, O=COC(=C)OC=O, C=COC(=O)OC=O, C#COC(=O)OCO, C#COC(O)OC=O, O=CCC(=O)OC=O, OC=CC(=O)OC=O, O=C=CC(=O)OCO, OC#CC(=O)OCO, O=CC=C(O)OC=O, OC=C=C(O)OC=O, O=C=C=C(O)OCO, O=C=CC(O)OC=O, OC#CC(O)OC=O, OC(=O)C(=C)OC=O, OC(O)=C(O)OC#C, OC(=O)C(=O)OC=C, OC(O)C(=O)OC#C, OC(=O)C(O)OC#C, OC(O)=C(O)C=C=O, OC(O)=C(O)C#CO, OC(O)C(=O)C=C=O, OC(=O)C(=O)CC=O, OC(=O)C(=O)C=CO, OC(O)C(=O)C#CO, OC(O)C(O)=C=C=O, OC(=O)C(O)=CC=O, OC(=O)C(O)=C=CO, OC(=O)C(O)C=C=O, OC(=O)C(O)C#CO, CC(=O)C(=O)OC=O, C=C(O)C(=O)OC=O, OC(=O)C(=C)C(=O)O, CC(=O)C(=O)C(=O)O, C=C(O)C(=O)C(=O)O, OC(C=O)(C=O)C=O, O=C=C(O)C(=O)CO, O=CC(O)C(=O)C=O, O=CC(=O)C(=O)CO, OC=C(O)C(=O)C=O, O=C=C(O)C(O)=CO, O=CC(O)C(O)=C=O, O=CC(O)=C(O)C=O, COC(=O)C(=O)C=O, COC(=O)C(O)=C=O, O=C(OC)OC=C=O, O=C(OC)OC#CO, O=C(C=O)OC=CO, O=C(CO)OC=C=O, O=C(CO)OC#CO, O=C(C=O)OCC=O, OC(=C=O)OC=CO, OC(=CO)OC=C=O, OC(=CO)OC#CO, OC(=C=O)OCC=O, OC(C=O)OC=C=O, OC(C=O)OC#CO, O=C(C=O)COC=O, OC(C=O)=COC=O, OC(=C=O)COC=O, O=COC(OC)=C=O, O=COC(CO)=C=O, O=COC(C=O)=CO, OCOC(C=O)=C=O, O=COC(C=O)C=O, OC(=O)C(OC)=C=O, OC(O)=C(C=O)C=O, OC(=O)C(CO)=C=O, OC(=O)C(C=O)=CO, OC(O)C(C=O)=C=O, OC(=O)C(C=O)C=O, O=COC=COC=O, O=COC#COCO, O=C=COCOC=O, OC#COCOC=O, OC(=O)C=C=C=O, OC(=O)C#CC=O, OC(O)=C=C=C=O, O=COC(=O)C#C, C#COC(=O)C=O, C#COC(O)=C=O, O=C=CC(=O)C=O, OC#CC(=O)C=O, O=C=C=C(O)C=O, O=C=CC(O)=C=O, OC#CC(O)=C=O, OC(=O)C(=O)C#C, O=CC(C=O)=C=O, O=C=COC=C=O, O=C=COC#CO, OC#COC#CO, O=C=C=COC=O, O=CC#COC=O, O=C=C=C=C=O

Continued on next page

Table S2: Product list from reducing 4 CO's, thus all $C_4O_xH_y$ products listed at 2 to 14 (H^++e^-) transfers (Continued)

(H^++e^-) transfers & products
6(H^++e^-): O=C=C(C)C(O)(O)O, O=CC(=C)C(O)(O)O, O=C=C(O)C(C)(O)O, O=CC(=O)C(C)(O)O, C=C=C(O)C(O)(O)O, C=CC(=O)C(O)(O)O, C#CC(O)C(O)(O)O, OC(C#COC)(O)O, OC(OC=C=C)(O)O, OC(OC#CC)(O)O, OC(OCC#C)(O)O, CC(OC=C=O)(O)O, CC(OC#CO)(O)O, OC(C=C=CO)(O)O, OC(C=CC=O)(O)O, OC(C#CCO)(O)O, OC(CC=C=O)(O)O, OC(CC#CO)(O)O, OC(COC#C)(O)O, C#COC(OC)(O)O, O=C=CC(OC)(O)O, OC#CC(OC)(O)O, O=COC(C=C)(O)O, OCOC(C#C)(O)O, O=COC(C=O)(O)C, C=COC(C=O)(O)O, C#COC(CO)(O)O, O=C=CC(CO)(O)O, O=CCC(C=O)(O)O, OC=CC(C=O)(O)O, OC#CC(CO)(O)O, OC(=O)C(C=C)(O)O, OC(O)C(C#C)(O)O, OC(=O)C(C=O)(O)C, CC(=O)C(C=O)(O)O, C=C(O)C(C=O)(O)O, OC(=O)CC=C(O)O, OC(O)=CC=C(O)O, OC(O)C=C=C(O)O, OC(=O)CCC(=O)O, OC(O)C=CC(=O)O, OC(O)C#CC(O)O, OC(=O)COC(=O)C, OC(O)=COC(=O)C, OC(=O)COC(O)=C, OC(O)=COC(O)=C, CC(=O)COC(=O)O, C=C(O)COC(=O)O, CC(O)=COC(=O)O, OC(=O)OC(=C)OC, CC(=O)OC(=O)OC, C=C(O)OC(=O)OC, OC(=O)CC(=O)OC, OC(O)=CC(=O)OC, OC(=O)C=C(O)OC, OC(O)=C=C(O)OC, OC(=O)OC(=O)CC, OC(O)OC(=O)C=C, OC(=O)OC(O)=CC, OC(O)OC(O)=C=C, OC(=O)OC(O)C=C, OC(O)OC(O)C#C, OC(=O)OC(=C)CO, OC(O)OC(=C)C=O, OC(=O)OC(C)=CO, OC(O)OC(C)=C=O, OC(=O)OC(C)C=O, CC(=O)OC(=O)CO, C=C(O)OC(=O)CO, CC(O)OC(=O)C=O, CC(=O)OC(O)=CO, C=C(O)OC(O)=CO, CC(O)OC(O)=C=O, CC(=O)OC(O)C=O, C=C(O)OC(O)C=O, OC(=O)CC(=O)CO, OC(O)=CC(=O)CO, OC(O)CC(=O)C=O, OC(=O)C=C(O)CO, OC(O)=C=C(O)CO, OC(O)C=C(O)C=O, OC(=O)CC(O)=CO, OC(O)=CC(O)=CO, OC(O)CC(O)=C=O, OC(=O)CC(O)C=O, OC(O)=CC(O)C=O, O=COCOC(=O)C, O=COCOC(O)=C, C=COCOC(=O)O, C#COCOC(O)O, O=COCCC(=O)O, OCOC=CC(=O)O, O=COCC=C(O)O, OCOC=C=C(O)O, O=COC=CC(O)O, OCOC#CC(O)O, O=CCCOC(=O)O, OC=CCOC(=O)O, OCC=COC(=O)O, O=C=CCOC(O)O, O=CC=COC(O)O, OC=C=COC(O)O, OC#CCOC(O)O, OCC#COC(O)O, O=CCOCC(=O)O, OC=COCC(=O)O, O=CCOC=C(O)O, OC=COC=C(O)O, O=C=COCC(O)O, OC#COCC(O)O, COC=COC(=O)O, COC#COC(O)O, OCOC(=C)OC=O, O=COC(C)OC=O, CCOC(=O)OC=O, C=COC(=O)OCO, C=COC(O)OC=O, C#COC(O)OCO, OCCC(=O)OC=O, O=CCC(=O)OCO, OC=CC(=O)OCO, OCC=C(O)OC=O, O=CC=C(O)OCO, OC=C=C(O)OCO, O=CCC(O)OC=O, OC=CC(O)OC=O, O=C=CC(O)OCO, OC#CC(O)OCO, O=COC(=O)COC, O=COC(O)=COC, OC(O)=C(C)OC=O, OC(O)C(=C)OC=O, OC(=O)C(=C)OCO, OC(=O)C(C)OC=O, OC(O)=C(O)OC=C, OC(O)C(=O)OC=C, OC(=O)C(=O)OCC, OC(=O)C(O)OC=C, OC(O)C(O)OC#C, OC(O)=C(O)CC=O, OC(O)=C(O)C=CO, OC(O)C(=O)CC=O, OC(O)C(=O)C=CO, OC(=O)C(=O)CCO, OC(O)C(O)=CC=O, OC(O)C(O)=C=CO, OC(=O)C(O)=CCO, OC(O)C(O)C=C=O, OC(=O)C(O)CC=O, OC(=O)C(O)C=CO, OC(O)C(O)C#CO, CC(O)=C(O)OC=O, CC(O)C(=O)OC=O, CC(=O)C(=O)OCO, C=C(O)C(=O)OCO, CC(=O)C(O)OC=O, C=C(O)C(O)OC=O, OC(=O)C(=O)COC, OC(=O)C(O)=COC, OC(=O)C(C)=C(O)O, OC(O)C(=C)C(=O)O, OC(=O)C(C)C(=O)O, CC(=O)C(O)=C(O)O, C=C(O)C(O)=C(O)O, CC(O)=C(O)C(=O)O, CC(O)C(=O)C(=O)O, CC(=O)C(=O)C(O)O, C=C(O)C(=O)C(O)O, CC(=O)C(O)C(=O)O, C=C(O)C(O)C(=O)O, OC(OC)(C=O)C=O, OC(CO)(C=O)C=O, O=CC(O)C(=O)CO, OC=C(O)C(=O)CO, OCC(O)C(=O)C=O, OCC(=O)C(=O)CO, O=CC(O)C(O)=CO, OC=C(O)C(O)=CO, OCC(O)C(O)=C=O, O=CC(O)=C(O)CO, O=CC(O)C(O)C=O, COC(=O)C(=O)OC, COC(O)C(=O)C=O, COC(=O)C(=O)CO, COC(O)C(O)=C=O, COC(=O)C(O)=CO, COC(O)=C(O)C=O, COC(=O)C(O)C=O, O=C(OC)OC=CO, O=C(OC)OCC=O, OC(OC)OC=C=O, OC(OC)OC#CO, O=C(C=O)OCOC, OC(=C=O)OCOC, O=C(CO)OC=CO, O=C(C=O)OCCO, O=C(CO)OCC=O, OC(=CO)OC=CO, OC(=C=O)OCCO, OC(=CO)OCC=O, OC(C=O)OC=CO, OC(CO)OC=C=O, OC(CO)OC#CO, OC(C=O)OCC=O, O=C(OC)COC=O, OC(OC)=COC=O, O=C(C=O)COCO, O=C(CO)COC=O, OC(C=O)=COCO, OC(CO)=COC=O, OC(=C=O)COCO, OC(=CO)COC=O, OC(C=O)COC=O, O=COC(OC)=CO, OCOC(OC)=C=O, O=COC(OC)C=O, O=COC(CO)=CO, OCOC(CO)=C=O, OCOC(C=O)=CO, O=COC(CO)C=O, OCOC(C=O)C=O, OC(O)=C(OC)C=O, OC(=O)C(OC)=CO, OC(O)C(OC)=C=O, OC(=O)C(OC)C=O, OC(O)=C(CO)C=O, OC(=O)C(CO)=CO, OC(O)C(CO)=C=O, OC(O)C(C=O)=CO, OC(=O)C(CO)C=O, OC(O)C(C=O)C=O, O=COC=COCO, O=COCCOC=O, OCOC#COCO, O=C=COCOCO, O=CCOCOC=O, OC=COCOC=O, OC#COCOCO, OC(C#C)(O)C=O, OC(=O)C#COC, OC(=O)OC=C=C, OC(=O)OC#CC, OC(=O)OCC#C, CC(=O)OC=C=O, CC(=O)OC#CO, C=C(O)OC=C=O, C=C(O)OC#CO, OC(=O)C=C=CO, OC(=O)C=CC=O, OC(=O)C#CCO, OC(=O)CC=C=O, OC(=O)CC#CO, OC(O)=C=C=CO, OC(O)=C=CC=O, OC(O)=CC=C=O, OC(O)=CC#CO, OC(O)C=C=C=O, OC(O)C#CC=O, OC(=O)COC#C, OC(O)=COC#C, C#COC(=O)OC, O=C=CC(=O)OC, OC#CC(=O)OC, O=C=C=C(O)OC, O=COC(=O)C=C, OCOC(=O)C#C, O=COC(O)=C=C, O=COC(O)C#C, O=COC(=C)C=O, O=COC(C)=C=O, C=COC(=O)C=O, C#COC(=O)CO, C=COC(O)=C=O, C#COC(O)=CO, C#COC(O)C=O, O=C=CC(=O)CO, O=CCC(=O)C=O, OC=CC(=O)C=O, OC#CC(=O)CO, O=C=C=C(O)CO, O=CC=C(O)C=O, OC=C=C(O)C=O, O=C=CC(O)=CO, O=CCC(O)=C=O, OC=CC(O)=C=O, OC#CC(O)=CO, O=C=CC(O)C=O, OC#CC(O)C=O, OC(O)=C(O)C#C, OC(=O)C(=O)C=C, OC(O)C(=O)C#C, OC(=O)C(O)=C=C, OC(=O)C(O)C#C, OC(=O)C(=C)C=O, OC(=O)C(C)=C=O, CC(=O)C(=O)C=O, C=C(O)C(=O)C=O, CC(=O)C(O)=C=O, C=C(O)C(O)=C=O, COC(C=O)=C=O, OCC(C=O)=C=O, O=CC(C=O)=CO, O=CC(C=O)C=O, OC=COC=C=O, O=CCOC=C=O, OC=COC#CO, O=CCOC#CO, COC#COC=O, OC=C=COC=O, O=C=C=COCO, O=CC=COC=O, OCC#COC=O, O=CC#COCO, O=C=CCOC=O, OC#CCOC=O, C#COCOC=O, O=C(C#C)C=O, OC(C#C)=C=O, O=C=C=C=CO, O=CC=C=C=O, O=CC#CC=O, O=C=CC=C=O, O=C=CC#CO, OC#CC#CO, O=C=COC#C, OC#COC#C,

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Table S2: Product list from reducing 4 CO's, thus all $C_4O_xH_y$ products listed at 2 to 14 (H^++e^-) transfers (Continued)

(H^++e^-) transfers & products
8(H^++e^-): OC(=O)OC(C)(O)C, CC(=O)OC(C)(O)O, C=C(O)OC(C)(O)O, OC(=O)CC(C)(O)O, OC(O)=CC(C)(O)O, CC(=C)OC(O)(O)O, CC(=O)CC(O)(O)O, C=C(O)CC(O)(O)O, CC(O)=CC(O)(O)O, O=CC(C)C(O)(O)O, OC=C(C)C(O)(O)O, OCC(=C)C(O)(O)O, O=CC(O)C(C)(O)O, OC=C(O)C(C)(O)O, OCC(=O)C(C)(O)O, C=CC(O)C(O)(O)O, CC=C(O)C(O)(O)O, CCC(=O)C(O)(O)O, COC(=C)C(O)(O)O, COC(=O)C(C)(O)O, OC(C=COC)(O)O, OC(OC=CC)(O)O, OC(OCC=C)(O)O, CC(OC=CO)(O)O, CC(OCC=O)(O)O, OC(C=CCO)(O)O, OC(CC=CO)(O)O, OC(CCC=O)(O)O, OC(COC=C)(O)O, CC(COC=O)(O)O, O=COC(OC)(O)C, C=COC(OC)(O)O, O=CCC(OC)(O)O, OC=CC(OC)(O)O, O=COC(CC)(O)O, OCOC(C=C)(O)O, O=COC(CO)(O)C, OCOC(C=O)(O)C, C=COC(CO)(O)O, CCOC(C=O)(O)O, O=CCC(CO)(O)O, OC=CC(CO)(O)O, OCCC(C=O)(O)O, COCC(C=O)(O)O, OC(=O)C(OC)(O)C, CC(=O)C(OC)(O)O, C=C(O)C(OC)(O)O, OC(=O)C(CC)(O)O, OC(O)C(C=C)(O)O, OC(=O)C(CO)(O)C, OC(O)C(C=O)(O)C, CC(=O)C(CO)(O)O, C=C(O)C(CO)(O)O, CC(O)C(C=O)(O)O, OC(O)CC=C(O)O, OC(O)CCC(=O)O, OC(O)C=CC(O)O, OC(O)COC(=O)C, OC(O)COC(O)=C, OC(=O)COC(O)C, OC(O)=COC(O)C, CC(O)COC(=O)O, CC(=O)COC(O)O, C=C(O)COC(O)O, CC(O)=COC(O)O, OC(O)OC(=C)OC, OC(=O)OC(C)OC, CC(O)OC(=O)OC, CC(=O)OC(O)OC, C=C(O)OC(O)OC, OC(O)CC(=O)OC, OC(O)C=C(O)OC, OC(=O)CC(O)OC, OC(O)=CC(O)OC, OC(O)OC(=O)CC, OC(O)OC(O)=CC, OC(=O)OC(O)CC, OC(O)OC(O)C=C, OC(O)OC(=C)CO, OC(O)OC(C)=CO, OC(=O)OC(C)CO, OC(O)OC(C)C=O, CC(O)OC(=O)CO, CC(O)OC(O)=CO, CC(=O)OC(O)CO, C=C(O)OC(O)CO, CC(O)OC(O)C=O, OC(O)CC(=O)CO, OC(O)C=C(O)CO, OC(O)CC(O)=CO, OC(=O)CC(O)CO, OC(O)=CC(O)CO, OC(O)CC(O)C=O, OCOCOC(=O)C, OCOCOC(O)=C, O=COCOC(O)C, CCOCOC(=O)O, C=COCOC(O)O, OCOCCC(=O)O, OCOCC=C(O)O, O=COCCC(O)O, OCOC=CC(O)O, OCCCOC(=O)O, O=CCCOC(O)O, OC=CCOC(O)O, OCC=COC(O)O, OCCOCC(=O)O, OCCOC=C(O)O, O=CCOCC(O)O, OC=COCC(O)O, COCCOC(=O)O, COC=COC(O)O, COCOCC(=O)O, COCOC=C(O)O, OCOC(=C)OCO, OCOC(C)OC=O, CCOC(=O)OCO, CCOC(O)OC=O, C=COC(O)OCO, OCCC(=O)OCO, OCC=C(O)OCO, OCCC(O)OC=O, O=CCC(O)OCO, OC=CC(O)OCO, OCOC(=O)COC, OCOC(O)=COC, O=COC(O)COC, OC(O)=C(C)OCO, OC(O)C(=C)OCO, OC(O)C(C)OC=O, OC(=O)C(C)OCO, OC(O)=C(O)OCC, OC(O)C(=O)OCC, OC(O)C(O)OC=C, OC(=O)C(O)OCC, OC(O)=C(O)CCO, OC(O)C(=O)CCO, OC(O)C(O)=CCO, OC(O)C(O)CC=O, OC(O)C(O)C=CO, OC(=O)C(O)CCO, CC(O)=C(O)OCO, CC(O)C(=O)OCO, CC(O)C(O)OC=O, CC(=O)C(O)OCO, C=C(O)C(O)OCO, OC(O)=C(O)COC, OC(O)C(=O)COC, OC(O)C(O)=COC, OC(=O)C(O)COC, OC(O)C(C)=C(O)O, OC(O)C(=C)C(O)O, OC(O)C(C)C(=O)O, CC(O)C(O)=C(O)O, CC(O)=C(O)C(O)O, CC(O)C(=O)C(O)O, CC(O)C(O)C(=O)O, CC(=O)C(O)C(O)O, C=C(O)C(O)C(O)O, OC(OC)(OC)C=O, OC(OC)(CO)C=O, OC(CO)(CO)C=O, OCC(O)C(=O)CO, OCC(O)C(O)=CO, OCC(O)=C(O)CO, O=CC(O)C(O)CO, COC(O)C(=O)OC, COC(O)=C(O)OC, COC(O)C(=O)CO, COC(O)C(O)=CO, COC(O)=C(O)CO, COC(O)C(O)C=O, COC(=O)C(O)CO, O=C(OC)OCOC, O=C(OC)OCCO, OC(OC)OC=CO, OC(OC)OCC=O, O=C(CO)OCOC, OC(=CO)OCOC, OC(C=O)OCOC, O=C(CO)OCCO, OC(=CO)OCCO, OC(CO)OC=CO, OC(C=O)OCCO, OC(CO)OCC=O, O=C(OC)COCO, OC(OC)=COCO, OC(OC)COC=O, O=C(CO)COCO, OC(CO)=COCO, OC(=CO)COCO, OC(C=O)COCO, OC(CO)COC=O, O=COC(OC)OC, OCOC(OC)=CO, O=COC(OC)CO, OCOC(OC)C=O, OCOC(CO)=CO, O=COC(CO)CO, OCOC(CO)C=O, OC(O)=C(OC)OC, OC(=O)C(OC)OC, OC(O)=C(OC)CO, OC(O)C(OC)=CO, OC(=O)C(OC)CO, OC(O)C(OC)C=O, OC(O)=C(CO)CO, OC(O)C(CO)=CO, OC(O)C(CO)C=O, OC(=O)C(CO)CO, OC(O)C(CO)C=O, O=COCCOCO, OCOC=COCO, O=CCOCOCO, OC=COCOCO, OCCOCOC=O, COCOCOC=O, C#COC(C)(O)O, O=C=CC(C)(O)O, OC#CC(C)(O)O, C=C=CC(O)(O)O, C#CCC(O)(O)O, CC#CC(O)(O)O, CC(=O)OC(=O)C, C=C(O)OC(=O)C, C=C(O)OC(O)=C, CC(=C)OC(=O)O, CC(=O)CC(=O)O, C=C(O)CC(=O)O, CC(O)=CC(=O)O, CC(=O)C=C(O)O, C=C(O)C=C(O)O, CC(O)=C=C(O)O, OC(C#C)(O)OC, OC(C=C)(O)C=O, OC(C#C)(O)CO, CC(C=O)(O)C=O, OC(=O)C=COC, OC(O)=C=COC, OC(O)C#COC, OC(=O)OC=CC, OC(=O)OCC=C, OC(O)OC=C=C, OC(O)OC#CC, OC(O)OCC#C, CC(=O)OC=CO, CC(=O)OCC=O, C=C(O)OC=CO, C=C(O)OCC=O, CC(O)OC=C=O, CC(O)OC#CO, OC(=O)C=CCO, OC(=O)CC=CO, OC(=O)CCC=O, OC(O)=C=CCO, OC(O)=CC=CO, OC(O)=CCC=O, OC(O)C=C=CO, OC(O)C=CC=O, OC(O)C#CCO, OC(O)CC=C=O, OC(O)CC#CO, OC(=O)COC=C, OC(O)=COC=C, OC(O)COC#C, CC(=O)COC=O, C=C(O)COC=O, CC(O)=COC=O, O=COC(=C)OC, C=COC(=O)OC, C#COC(O)OC, O=CCC(=O)OC, OC=CC(=O)OC, O=CC=C(O)OC, OC=C=C(O)OC, O=C=CC(O)OC, OC#CC(O)OC, O=COC(=O)CC, OCOC(=O)C=C, O=COC(O)=CC, OCOC(O)=C=C, O=COC(O)C=C, OCOC(O)C#C, O=COC(=C)CO, OCOC(=C)C=O, O=COC(=C)C=O, OCOC(C)=C=O, O=COC(C)C=O, C=COC(=O)CO, CCOC(=O)C=O, C=COC(O)=CO, CCOC(O)=C=O, C=COC(O)C=O, C#COC(O)CO, O=CCC(=O)CO, OC=CC(=O)CO, OCCC(=O)C=O, O=CC=C(O)CO, OC=C=C(O)CO, OCC=C(O)C=O, O=CCC(O)=CO, OC=CC(O)=CO, OCCC(O)=C=O, O=C=CC(O)CO, O=CCC(O)C=O, OC=CC(O)C=O, OC#CC(O)CO, COCC(=O)C=O, COC=C(O)C=O, COCC(O)=C=O, OC(=O)C(=C)OC, CC(=O)C(=O)OC, C=C(O)C(=O)OC, OC(O)=C(O)C=C, OC(=O)C(=O)CC, OC(O)C(=O)C=C, OC(=O)C(O)=CC, OC(O)C(O)=C=C, OC(=O)C(O)C=C, OC(O)C(O)C#C, OC(O)=C(C)C=O, OC(=O)C(=C)CO, OC(O)C(=C)C=O, OC(=O)C(C)=CO, OC(O)C(C)=C=O, OC(=O)C(C)C=O, CC(O)=C(O)C=O, CC(=O)C(=O)CO, C=C(O)C(=O)CO, CC(O)C(O)=C=O, CC(=O)C(O)C=O, C=C(O)C(O)=CO, CC(O)C(O)=C=O, C=C(O)C(O)C=O, COC(OC)=C=O, COC(CO)=C=O, COC(C=O)=CO, COC(C=O)C=O, OCC(CO)=C=O, OCC(C=O)=CO, OCC(C=O)C=O, COCOC=C=O, COCOC#CO, OC=COC=CO, OCCOC=C=O, O=CCOC=CO, OCCOC#CO, O=CCOCC=O, COC=COC=O, COC#COCO, OC=C=COCO, OCC=COC=O, O=CC=COCO, OCC#COCO, OC=CCOC=O, O=C=CCOCO, OC#CCOCO, O=CCCOC=O, C=COCOC=O, C#COCOCO, C#COC(=O)C, C#COC(O)=C, O=C=CC(=O)C, OC#CC(=O)C, O=C=CC(O)=C, OC#CC(O)=C, O=C=C=C(O)C, C=C=CC(=O)O, C#CCC(=O)O, CC#CC(=O)O, C=C=C=C(O)O, C#CC=C(O)O, O=C(C#C)OC, O=C(C=C)C=O, O=C(C#C)CO, OC(C=C)=C=O, OC(=C=C)C=O, OC(C#C)C=O, C=C(C=O)C=O, CC(C=O)=C=O, O=CC=C=CO, OC=C=C=CO, OCC=C=C=O, O=CC=CC=O, O=CC#CCO, O=C=CC=CO, O=CCC=C=O, O=CCC#CO, OC=CC#CO, COC=C=C=O, COC#CC=O, O=C=COC=C, O=CCOC#C, OC=COC#C, OC#COC=C, C=C=COC=O, C#CCOC=O, CC#COC=O, C=C=C=C=O, C#CC=C=O, C#CC#CO, C#COC#C,

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Table S2: Product list from reducing 4 CO's, thus all $C_4O_xH_y$ products listed at 2 to 14 (H^++e^-) transfers (Continued)

(H^++e^-) transfers & products
10(H^++e^-): OC(O)OC(C)(O)C, CC(O)OC(C)(O)O, OC(O)CC(C)(O)O, CC(C)OC(O)(O)O, CC(O)CC(O)(O)O, CC(O)(O)C(C)(O)O, CC(C)(O)C(O)(O)O, OCC(C)C(O)(O)O, OCC(O)C(C)(O)O, CCC(O)C(O)(O)O, COC(C)C(O)(O)O, COC(O)C(C)(O)O, CC(OCOC)(O)O, OC(CCOC)(O)O, OC(OCCC)(O)O, CC(OCCO)(O)O, OC(CCCO)(O)O, OC(COCC)(O)O, CC(COCO)(O)O, OCOC(OC)(O)C, CCOC(OC)(O)O, OCCC(OC)(O)O, OCOC(CC)(O)O, OCOC(CO)(O)C, CCOC(CO)(O)O, OCCC(CO)(O)O, COCC(OC)(O)O, COCC(CO)(O)O, OC(O)C(OC)(O)C, CC(O)C(OC)(O)O, OC(O)C(CC)(O)O, OC(O)C(CO)(O)C, CC(O)C(CO)(O)O, OC(O)CCC(O)O, OC(O)COC(O)C, CC(O)COC(O)O, OC(O)OC(C)OC, CC(O)OC(O)OC, OC(O)CC(O)OC, OC(O)OC(O)CC, OC(O)OC(C)CO, CC(O)OC(O)CO, OC(O)CC(O)CO, OCOCOC(O)C, CCOCOC(O)O, OCOCCC(O)O, OCCCOC(O)O, OCCOCC(O)O, COCCOC(O)O, COCOCC(O)O, OCOC(C)OCO, CCOC(O)OCO, OCCC(O)OCO, OCOC(O)COC, OC(O)C(C)OCO, OC(O)C(O)OCC, OC(O)C(O)CCO, CC(O)C(O)OCO, OC(O)C(O)COC, OC(O)C(C)C(O)O, CC(O)C(O)C(O)O, OC(OC)(OC)OC, OC(OC)(OC)CO, OC(OC)(CO)CO, OC(CO)(CO)CO, OCC(O)C(O)CO, COC(O)C(O)OC, COC(O)C(O)CO, OC(OC)OCOC, OC(OC)OCCO, OC(CO)OCOC, OC(CO)OCCO, OC(OC)COCO, OC(CO)COCO, OCOC(OC)OC, OCOC(OC)CO, OCOC(CO)CO, OC(O)C(OC)OC, OC(O)C(OC)CO, OC(O)C(CO)CO, OCOC-COCO, OCCOCOCO, COCOCOCO, O=COC(C)(O)C, C=COC(C)(O)O, O=CCC(C)(O)O, OC=CC(C)(O)O, C=CCC(O)(O)O, CC=CC(O)(O)O, OC(=O)C(C)(O)C, CC(=O)C(C)(O)O, C=C(O)C(C)(O)O, CC(=C)C(O)(O)O, CC(O)OC(=O)C, CC(O)OC(O)=C, CC(C)OC(=O)O, CC(=C)OC(O)O, CC(O)CC(=O)O, CC(O)C=C(O)O, CC(=O)CC(O)O, C=C(O)CC(O)O, CC(O)=CC(O)O, OC(C=C)(O)OC, CC(OC)(O)C=O, OC(CC)(O)C=O, OC(C=C)(O)CO, CC(CO)(O)C=O, CC(=O)OCOC, C=C(O)OCOC, OC(=O)CCOC, OC(O)=CCOC, OC(O)C=COC, OC(=O)OCCC, OC(O)OC=CC, OC(O)OCC=C, CC(=O)OCCO, C=C(O)OCCO, CC(O)OC=CO, CC(O)OCC=O, OC(=O)CCCO, OC(O)=CCCO, OC(O)C=CCO, OC(O)CC=CO, OC(O)CCC=O, OC(=O)COCC, OC(O)=COCC, OC(O)COC=C, CC(=O)COCO, C=C(O)COCO, CC(O)=COCO, CC(O)COC=O, OCOC(=C)OC, O=COC(C)OC, CCOC(=O)OC, C=COC(O)OC, OCCC(=O)OC, OCC=C(O)OC, O=CCC(O)OC, OC=CC(O)OC, OCOC(=O)CC, OCOC(O)=CC, O=COC(O)CC, OCOC(O)C=C, OCOC(=C)CO, OCOC(C)=CO, O=COC(C)CO, OCOC(C)C=O, CCOC(=O)CO, CCOC(O)=CO, C=COC(O)CO, CCOC(O)C=O, OCCC(=O)CO, OCC=C(O)CO, OCCC(O)=CO, O=CCC(O)CO, OC=CC(O)CO, OCCC(O)C=O, COCC(=O)OC, COC=C(O)OC, COCC(=O)CO, COC=C(O)CO, COCC(O)=CO, COCC(O)C=O, OC(O)=C(C)OC, OC(O)C(=C)OC, OC(=O)C(C)OC, CC(O)=C(O)OC, CC(O)C(=O)OC, CC(=O)C(O)OC, C=C(O)C(O)OC, OC(O)=C(O)CC, OC(O)C(=O)CC, OC(O)C(O)=CC, OC(=O)C(O)CC, OC(O)C(O)C=C, OC(O)=C(C)CO, OC(O)C(=C)CO, OC(O)C(C)=CO, OC(=O)C(C)CO, OC(O)C(C)C=O, CC(O)=C(O)CO, CC(O)C(=O)CO, CC(O)C(O)=CO, CC(=O)C(O)CO, C=C(O)C(O)CO, CC(O)C(O)C=O, COC(OC)=CO, COC(OC)C=O, COC(CO)=CO, COC(CO)C=O, OCC(CO)=CO, OCC(CO)C=O, COCOC=CO, CO-COCC=O, OCCOC=CO, OCCOCC=O, COC=COCO, COCCOC=O, OCC=COCO, OC=CCOCO, OCCCOC=O, O=CCCOCO, CCOCOC=O, C=COCOCO, CC(C#C)(O)O, O=COC(=C)C, C=COC(=O)C, C=COC(O)=C, C#COC(O)C, O=CCC(=O)C, OC=CC(=O)C, O=CCC(O)=C, OC=CC(O)=C, O=CC=C(O)C, OC=C=C(O)C, O=C=CC(O)C, OC#CC(O)C, C=CCC(=O)O, CC=CC(=O)O, C=CC=C(O)O, CC=C=C(O)O, C=C=CC(O)O, C#CCC(O)O, CC#CC(O)O, CC(=O)C(=O)C, C=C(O)C(=O)C, C=C(O)C(O)=C, CC(=C)C(=O)O, O=C(C=C)OC, OC(=C=C)OC, OC(C#C)OC, C=C(OC)C=O, CC(OC)=C=O, O=C(CC)C=O, O=C(C=C)CO, OC(CC)=C=O, OC(C=C)=CO, OC(=CC)C=O, OC(=C=C)CO, OC(C=C)C=O, OC(C#C)CO, C=C(CO)C=O, CC(CO)=C=O, CC(C=O)=CO, CC(C=O)C=O, OCC=C=CO, O=CC=CCO, OCC#CCO, O=CCC=CO, OC=CC=CO, OCCC=C=O, OCCC#CO, O=CCCC=O, COC#COC, COC=C=CO, COC=CC=O, COC#CCO, COCC=C=O, COCC#CO, O=C=COCC, O=CCOC=C, OC=COC=C, OC#COCC, OCCOC#C, C=C=COCO, C=CCOC=O, C#CCOCO, CC=COC=O, CC#COCO, COCOC#C, CC(=O)C#C, C=C(O)C#C, CC=C=C=O, C=C=C=CO, C=CC=C=O, C#CC=CO, C=CC#CO, C=C=CC=O, CC#CC=O, C#CCC=O, C=COC#C, C#CC#C
12(H^++e^-): OCOC(C)(O)C, CCOC(C)(O)O, OCCC(C)(O)O, CCCC(O)(O)O, COCC(C)(O)O, OC(O)C(C)(O)C, CC(O)C(C)(O)O, CC(C)C(O)(O)O, CC(O)OC(O)C, CC(C)OC(O)O, CC(O)CC(O)O, CC(OC)(O)OC, OC(CC)(O)OC, CC(OC)(O)CO, OC(CC)(O)CO, CC(CO)(O)CO, CC(O)OCOC, OC(O)CCOC, OC(O)OCCC, CC(O)OCCO, OC(O)CCCO, OC(O)COCC, CC(O)COCO, OCOC(C)OC, CCOC(O)OC, OCCC(O)OC, OCOC(O)CC, OCOC(C)CO, CCOC(O)CO, OCCC(O)CO, COCC(O)OC, COCC(O)CO, OC(O)C(C)OC, CC(O)C(O)OC, OC(O)C(O)CC, OC(O)C(C)CO, CC(O)C(O)CO, COC(OC)OC, COC(OC)CO, COC(CO)CO, OCC(CO)CO, COCOCOC, COCOCCO, OCCOCCO, COCCOCO, OCCCOCO, CCOCOCO, CC(C=C)(O)O, CC(C=O)(O)C, OCOC(=C)C, O=COC(C)C, CCOC(=O)C, CCOC(O)=C, C=COC(O)C, OCCC(=O)C, OCCC(O)=C, OCC=C(O)C, O=CCC(O)C, OC=CC(O)C, CCCC(=O)O, CCC=C(O)O, C=CCC(O)O, CC=CC(O)O, COCC(=O)C, COCC(O)=C, COC=C(O)C, CC(O)=C(O)C, CC(O)C(=O)C, CC(O)C(O)=C, CC(C)=C(O)O, CC(C)C(=O)O, CC(=C)C(O)O, C=C(OC)OC, O=C(CC)OC, OC(=CC)OC, OC(C=C)OC, C=C(OC)CO, CC(OC)=CO, CC(OC)C=O, O=C(CC)CO, OC(CC)=CO, OC(=CC)CO, OC(CC)C=O, OC(C=C)CO, C=C(CO)CO, CC(CO)=CO, CC(CO)C=O, OCC=CCO, OCCC=CO, O=CCCCO, COC=COC, COC=CCO, COCC=CO, COCCC=O, O=CCOCC, OC=COCC, OCCOC=C, C=CCOCO, CC=COCO, CCCOC=O, COCOC=C, CC(=O)C=C, C=C(O)C=C, CC(O)=C=C, CC(O)C#C, CC(=C)C=O, CC(C)=C=O, C=C=COC, CC#COC, C#CCOC, CC=C=CO, CCC=C=O, C=CC=CO, CCC#CO, CC=CC=O, C=C=CCO, CC#CCO, C=CCC=O, C#CCCO, C=COC=C, CCOC#C, C=C=C=C, C#CC=C

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Table S2: Product list from reducing 4 CO's, thus all $C_4O_xH_y$ products listed at 2 to 14 (H^++e^-) transfers (Continued)

(H^++e^-) transfers & products
14(H^++e^-) CC(OC)(O)C, CC(CC)(O)O, CC(CO)(O)C, OCOC(C)C, CCOC(O)C, OCCC(O)C, CCCC(O)O, COCC(O)C, CC(O)C(O)C, CC(C)C(O)O, CC(OC)OC, OC(CC)OC, CC(OC)CO, OC(CC)CO, CC(CO)CO, OCCCCO, COCCOC, COCCCO, OCCOCC, CCCOCO, COCOCC, CC(=C)OC, CC(=O)CC, C=C(O)CC, CC(O)=CC, CC(O)C=C, CC(=C)CO, CC(C)=CO, CC(C)C=O, CC=COC, C=CCOC, CCC=CO, CC=CCO, CCCC=O, C=CCCO, CCOC=C, C=C=CC, C=CC=C, C#CCC, CC#CC
16(H^++e^-): CC(C)(O)C, CC(C)OC, CC(O)CC, CC(C)CO, CCCOC, CCCCO, CCOCC, CC(=C)C, C=CCC, CC=CC
18(H^++e^-): CC(C)C, CCCC

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