Spatial-Confinement Induced Electroreduction of CO and CO_2 to Diols on Densely-Arrayed Cu Nanopyramids

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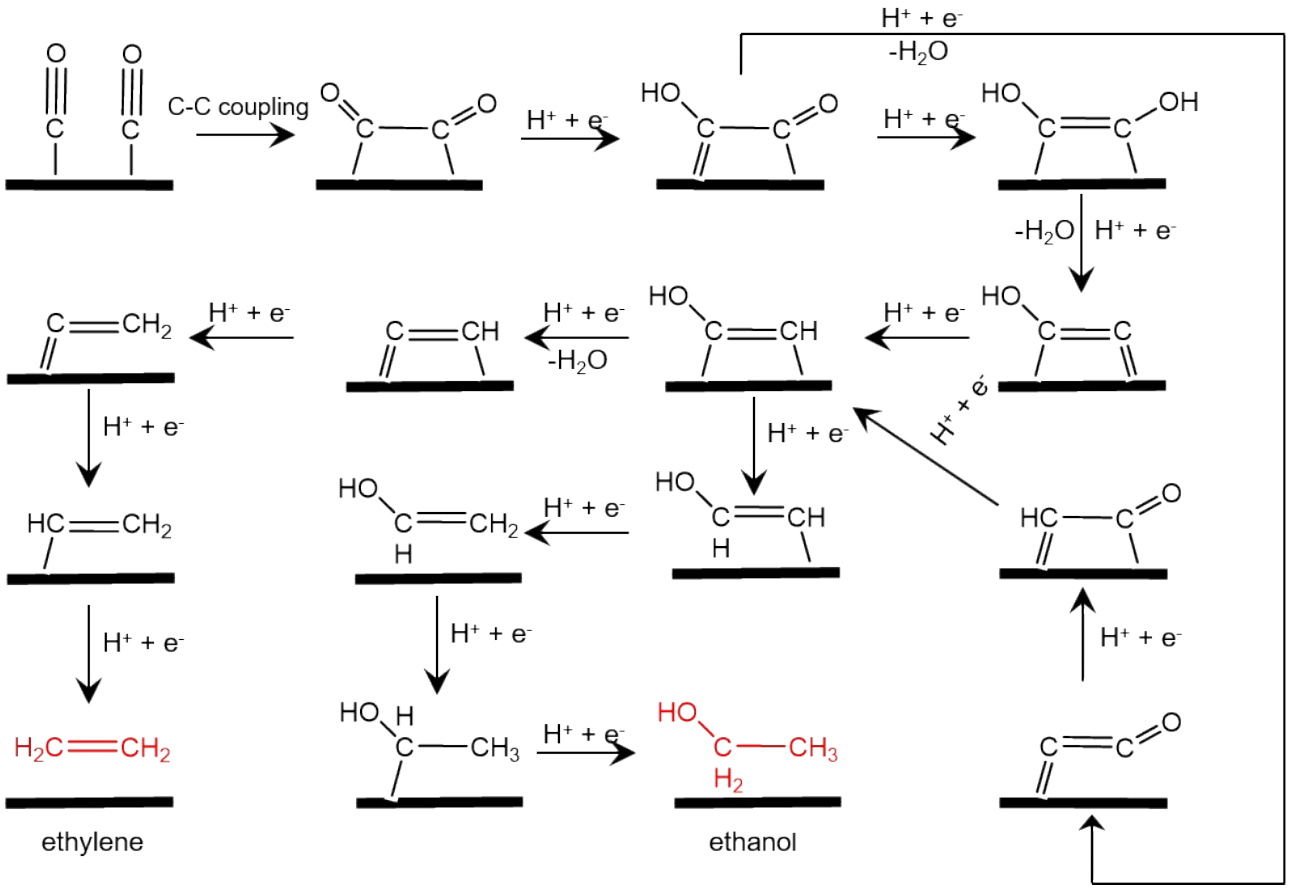
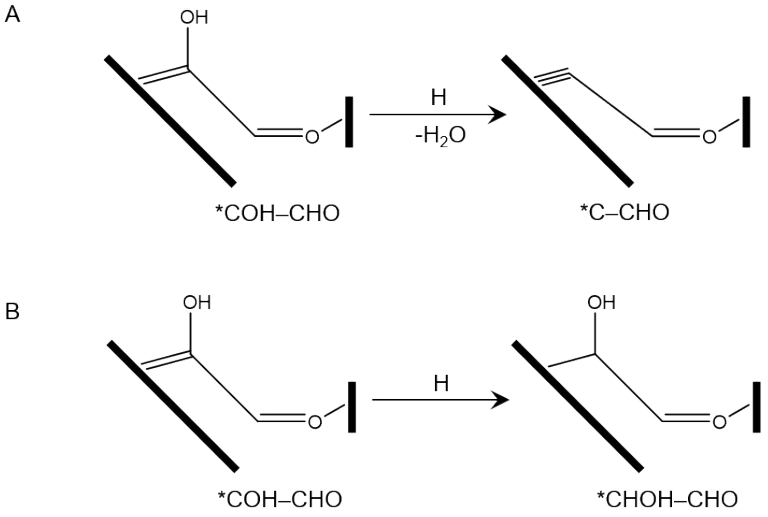


Scheme S1. Conventional *COH–COH and *C–CO pathways on Cu (100) following adsorption of two CO intermediates.[1-3]



Scheme S2. Further hydrogenation step for *COH–CHO on Cu-DAN to: (A) *C–CHO, and; (B) *CHOH–CHO.

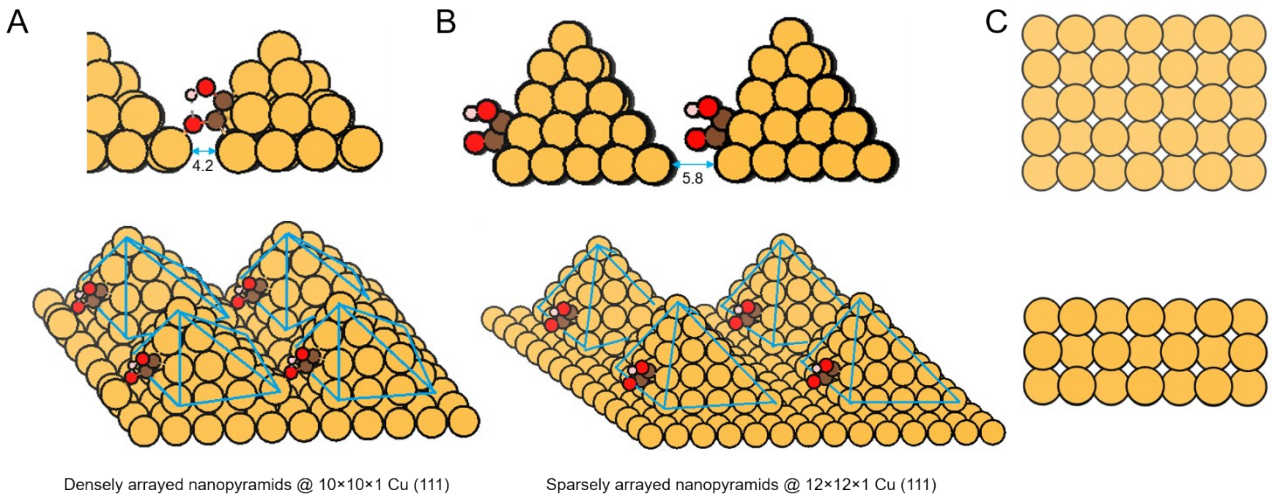


Fig. S1. Close-up (top panel) and overall (bottom panel) view of *COH–CO adsorption on: (A) densely-arrayed Cu nanopyramids, (B) sparsely-arrayed Cu nanopyramids, and top and side view of (C) planar Cu (100). The [111] diamond nanopyramid was built based on a 10×10×1 Cu surface with 4.2 Å distance between two nanopyramids to represent the dense-array, and on a 12×12×1 Cu surface to represent the sparse-array with 5.8 Å distance. Distance in figure is Å. Color code: Cu, orange; C, brown; O, red; H, pink. Solid-blue lines serve as a visual guide for the pyramid.

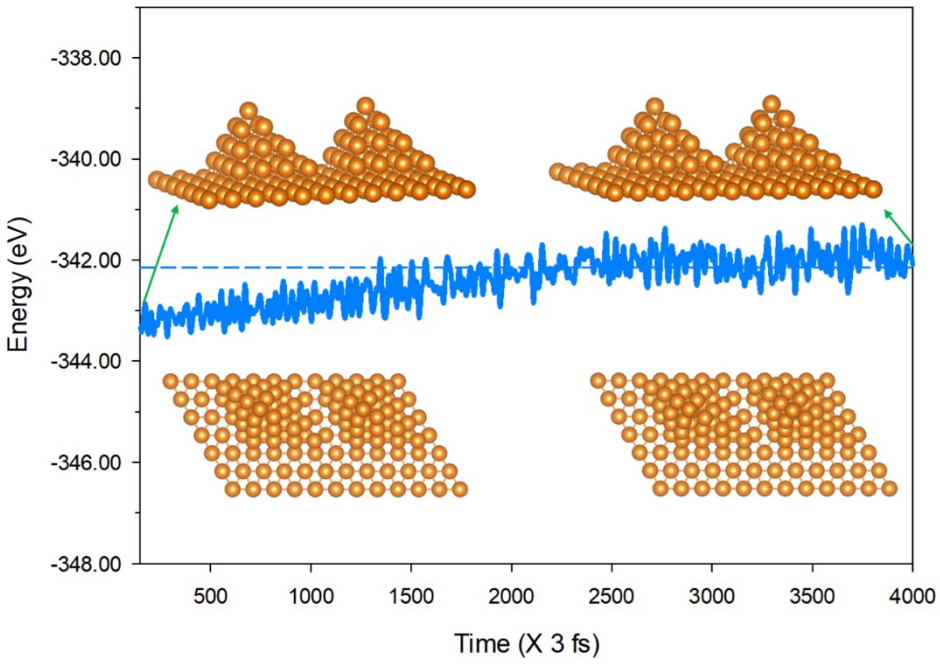


Fig. S2. *Ab initio* molecular dynamics (AIMD) simulated energy evolution for Cu-DAN at 300 K. Insets show the top and side views of the snapshots of atomic configurations at 0 and 12 ps. The blue dashed-line denotes equilibrium position.

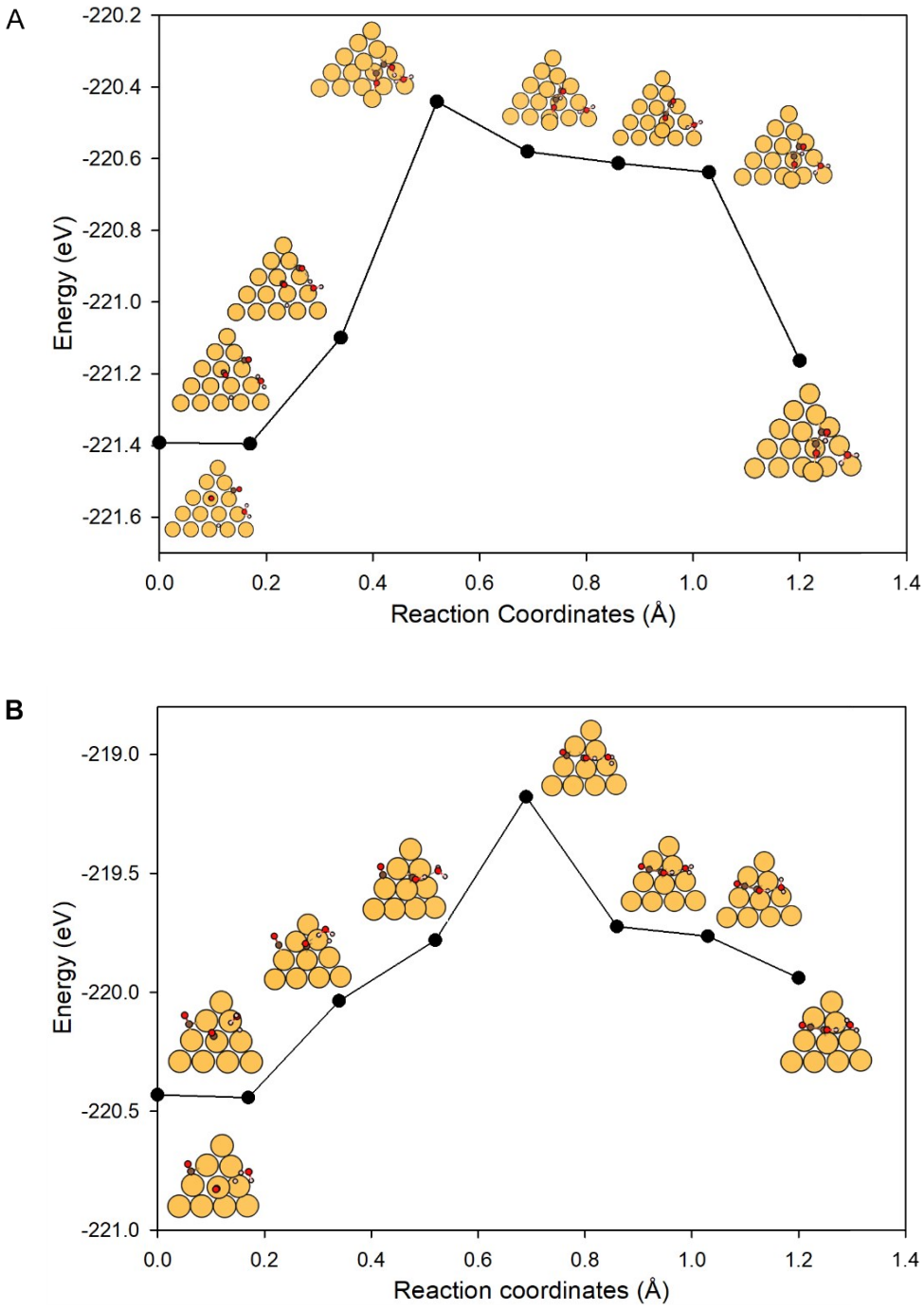


Fig. S3. Minimum energy path (MEP) involved in *CO + *CO + H^+ + e^- → *COH–CO via H-shuttling on (A) Cu-DAN, and (B) Cu-SAN. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier in (A) is $\Delta G^{\neq}(U^0)$ = 1.07 eV and in (B), $\Delta G^{\neq}(U^0)$ = 1.50 eV.

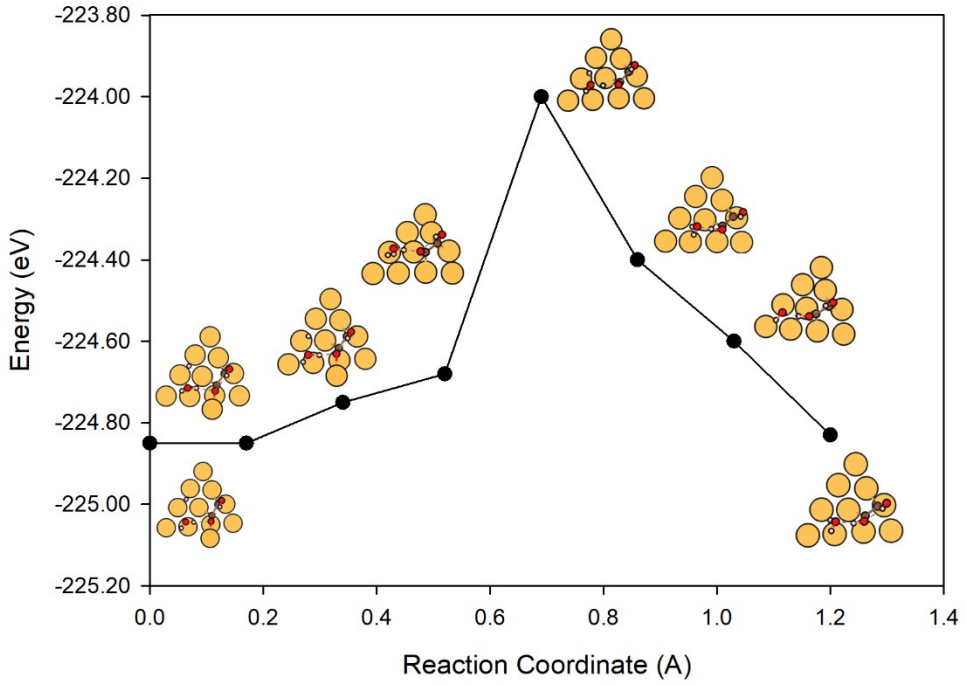


Fig. S4. MEP involved in *COH–CO + H^+ + e^- → *COH–COH on Cu-DAN via H-shuttling. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier is $\Delta G^{\neq}(U^0)$ = 0.76 eV.

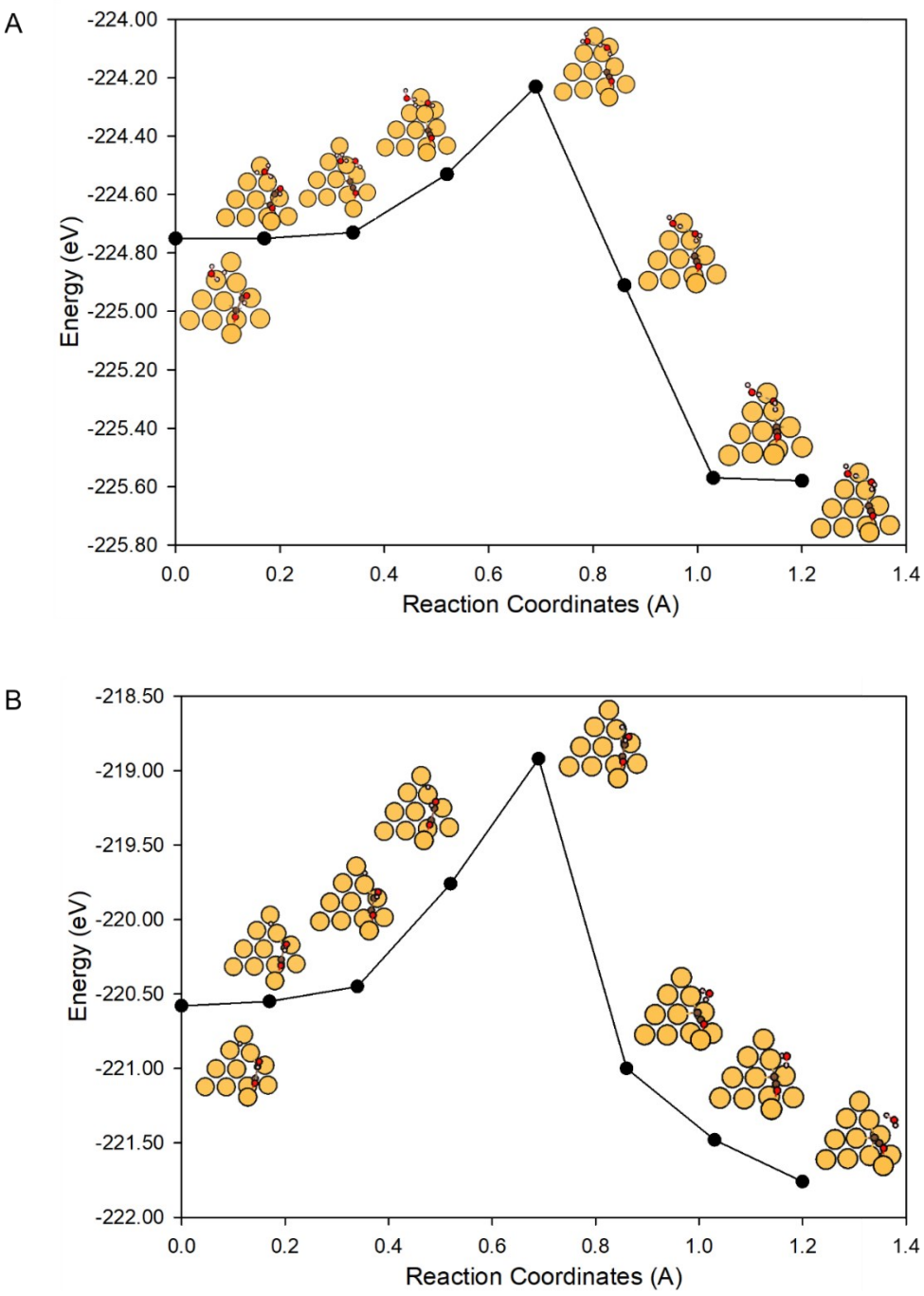


Fig. S5. MEP involved in *COH–CO + H^+ + e^- → *C–CO + H_2O on Cu-DAN via (A) H-shuttling and (B) surface *H transfer. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value in (A) is $\Delta G^{\neq}(U^0)$ = 0.72 eV and in (B), $\Delta G^{\neq}(U^0)$ = 1.66 eV

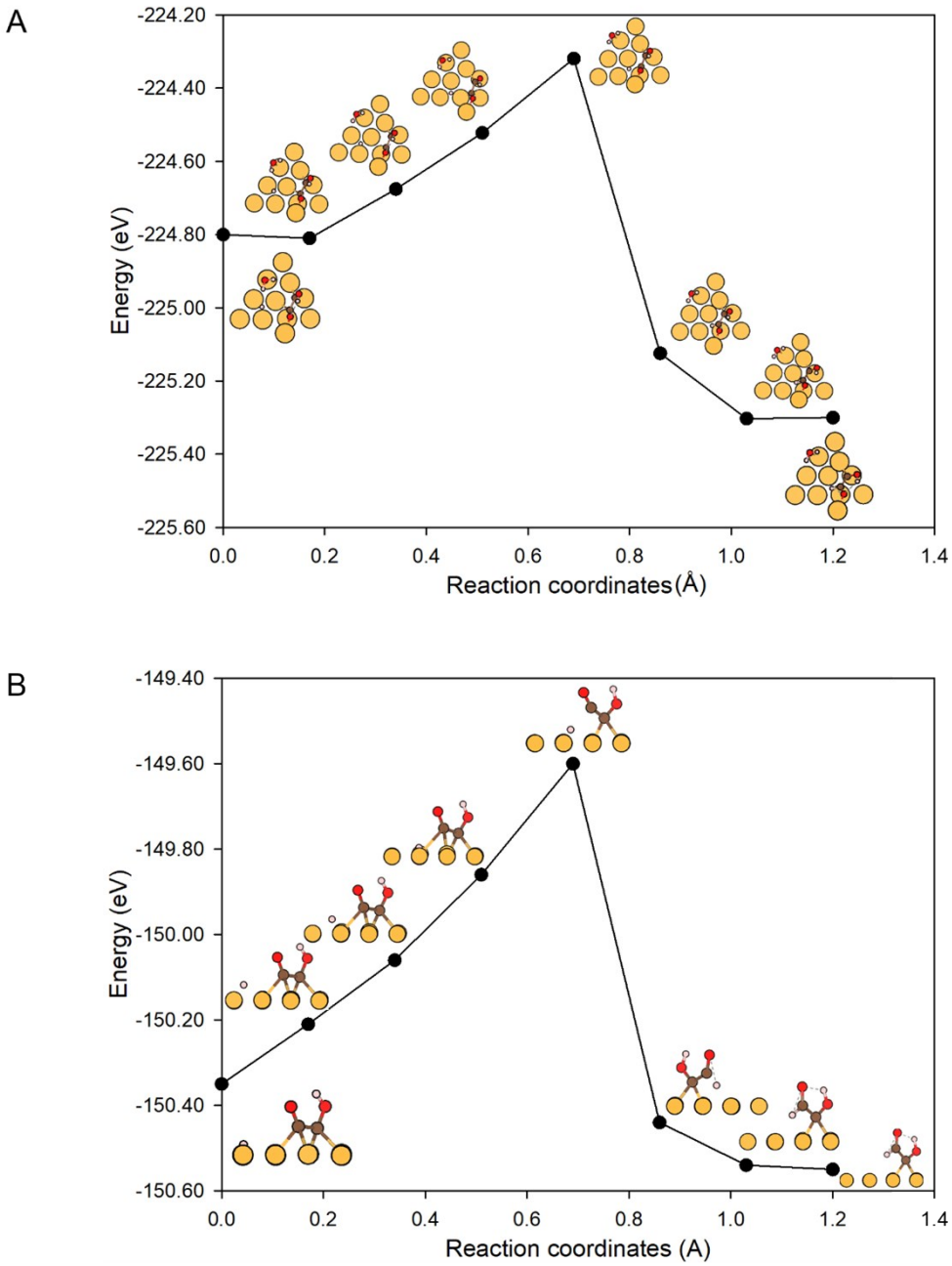


Fig. S6. MEP involved in *COH–CO + H^+ + e^- → *COH–CHO via surface *H transfer on (A) Cu-DAN and (B) planar Cu (100). Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier in (A) is $\Delta G^{\neq}(U^0)$ = 0.41 eV, in (B) $\Delta G^{\neq}(U^0)$ = 0.69 eV.

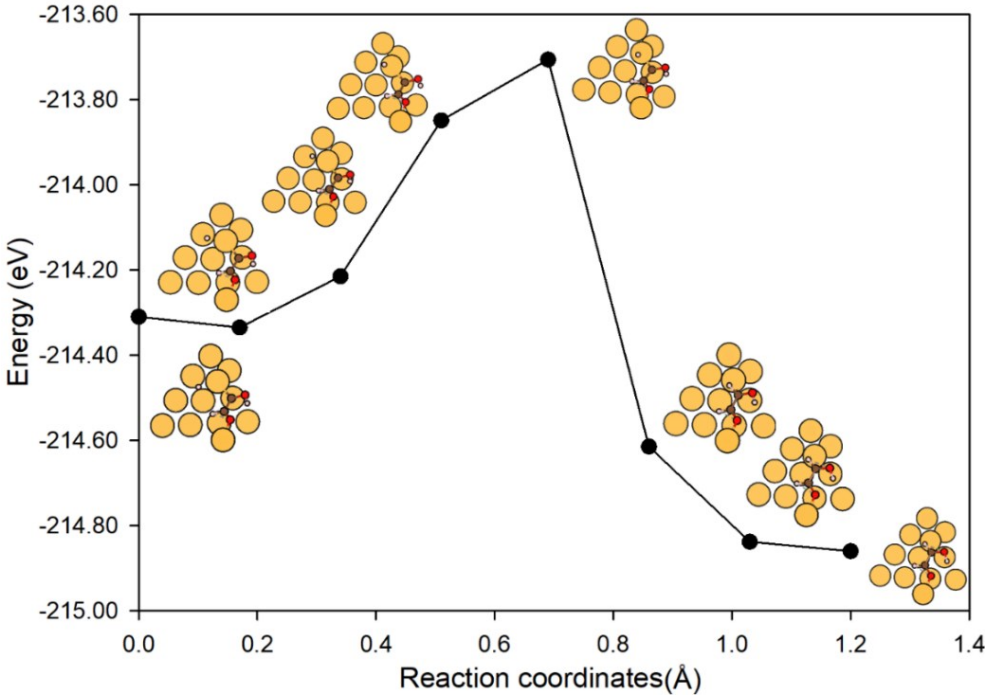


Fig. S7. MEP involved in *COH–CHO + H^+ + e^- → *CHOH–CHO via surface *H transfer on Cu-DAN. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value is $\Delta G^{\neq}(U^0)$ = 0.52 eV.

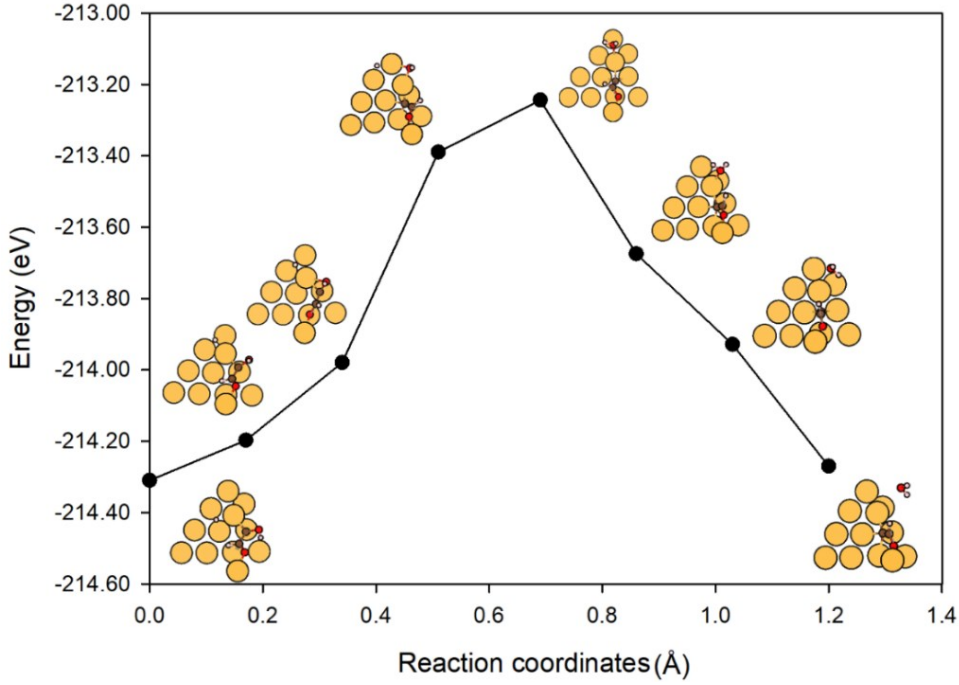


Fig. S8. MEP involved in *COH–CHO + H^+ + e^- → *C–CHO + H_2O on Cu-DAN via surface *H transfer. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value is $\Delta G^{\neq}(U^0)$ = 1.02 eV.

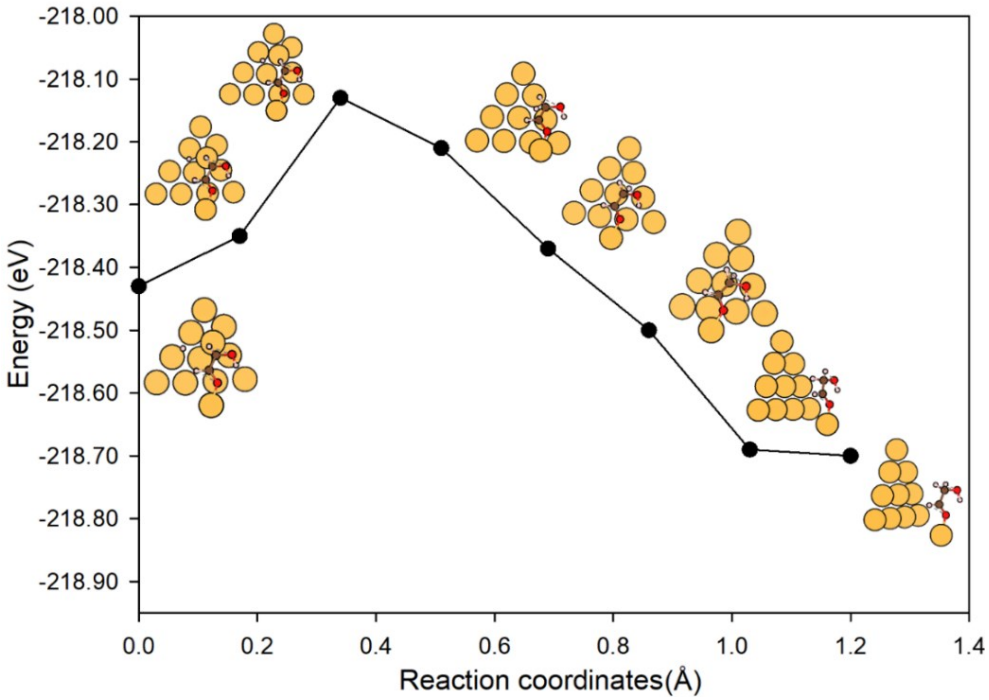


Fig. S9. MEP involved in *CHOH–CHO + H^+ + e^- → *CH_2OH–CHO on Cu-DAN via surface *H transfer. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value is $\Delta G^{\neq}(U^0)$ = 0.25 eV.

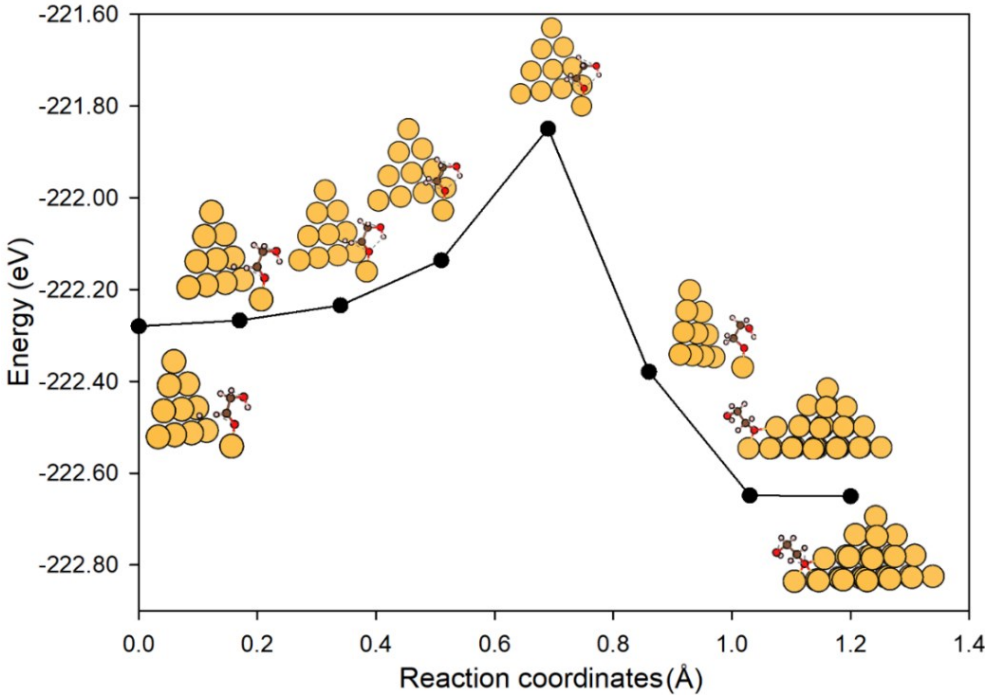


Fig. S10. MEP involved in $*CH_2OH–CHO + H^+ + e^- \rightarrow *CH_2OH–CH_2O$ on Cu-DAN via surface *H transfer. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value is $\Delta G^{\neq}(U^0) = 0.39$ eV.

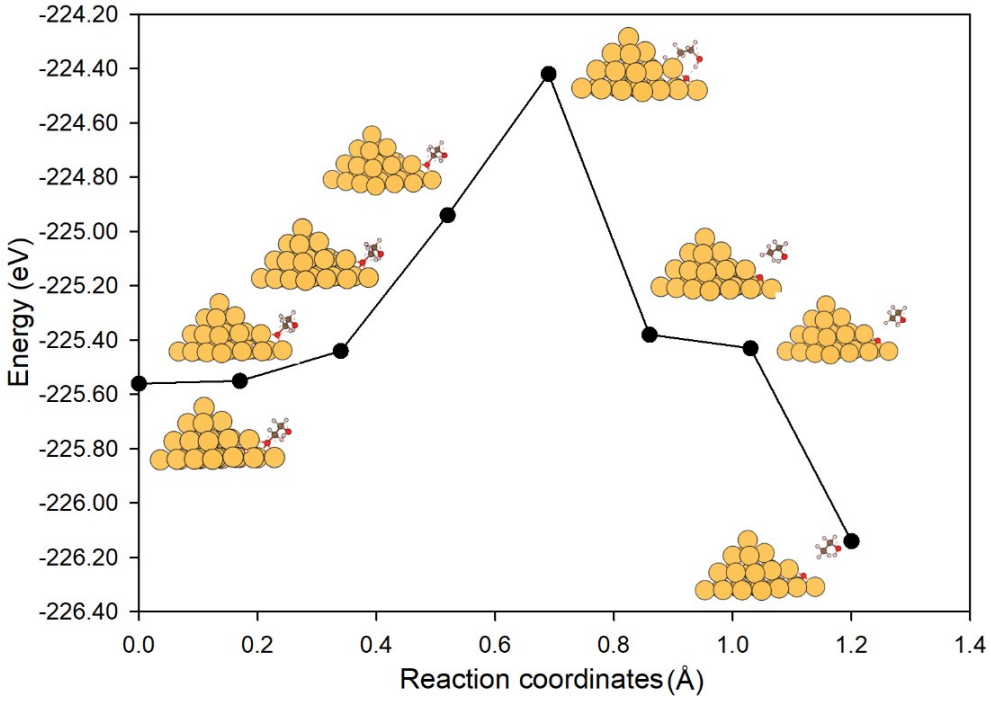


Fig. S11. MEP involved in $*CH_2OH–CH_2O + H^+ + e^- \rightarrow CH_2OH–CH_3 + *O$ on Cu-DAN via surface *H transfer. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value is $\Delta G^{\neq}(U^0)$ = 0.98 eV.

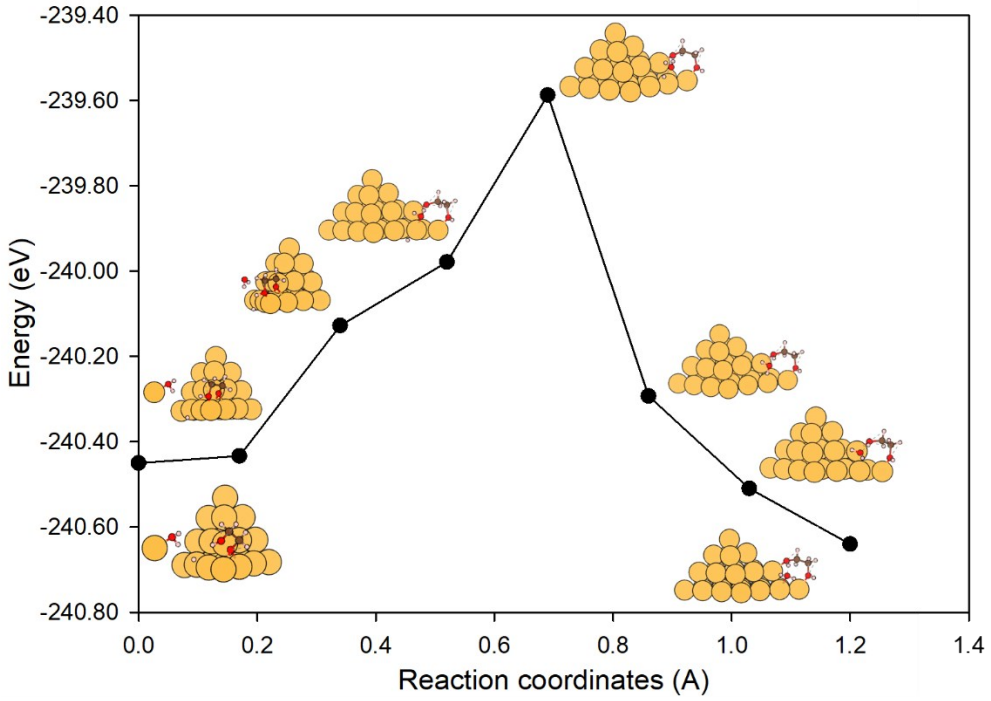


Fig. S12. MEP involved in $*CH_2OH–CH_2O + H^+ + e^- \rightarrow *CH_2OH–CH_2OH$ on Cu-DAN via H-shuttling. Color code: Cu, orange; C, brown; O, red; H, pink. Energy barrier value is $\Delta G^{\neq}(U^0)$ = 0.73 eV.

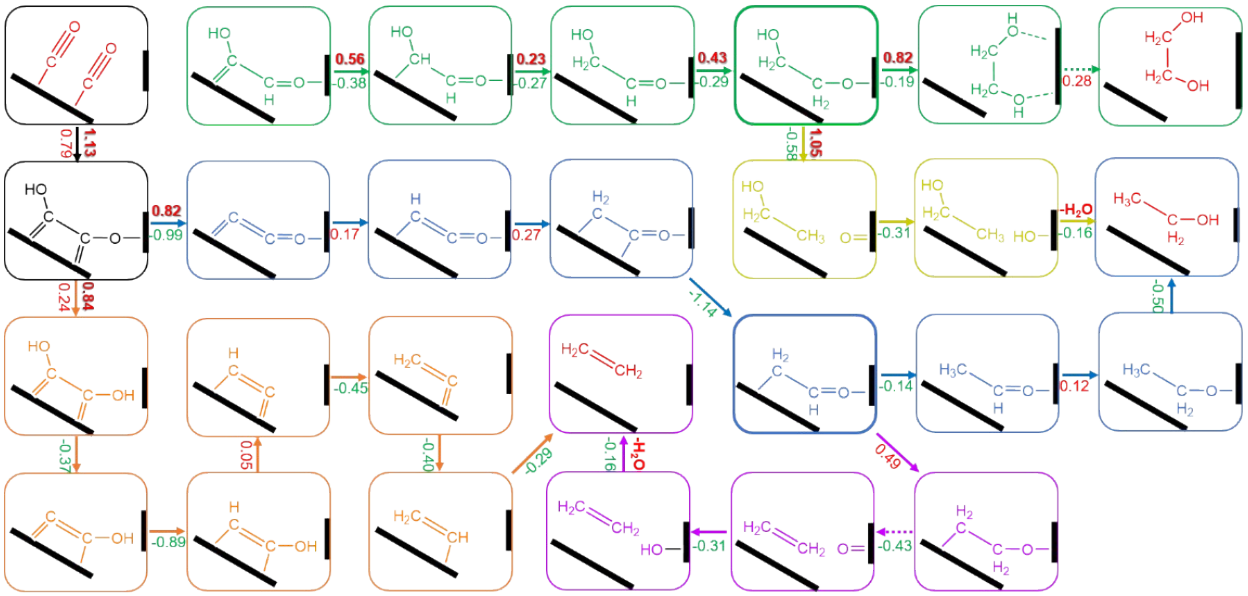


Fig. S13 Chemical structure of reaction intermediates in different pathways on Cu-DAN. Pathways toward C_2 products (ethylene, ethanol and ethylene glycol) beyond 2 *CO are shown as colored-branches: orange, *COH–COH pathway toward C_2H_4; blue, *C–CO pathway toward C_2H_5OH; purple, *C–CO pathway bifurcating to C_2H_4; green, *COH–CHO pathway toward $C_2H_6O_2$, and; brown, *COH–CHO pathway bifurcating to C_2H_5OH. Reaction barrier $\Delta G^{\neq}$ values at 0 V vs RHE appear in bolded- and shaded-font. Free energy change ΔG values appear in standard-font. Green and red values denote, respectively, exergonic and endergonic process. The solid-arrow denotes proton-coupled electron transfer ($H^+ + e^-$), and dotted-arrow denotes desorption. The unit of energy is eV.

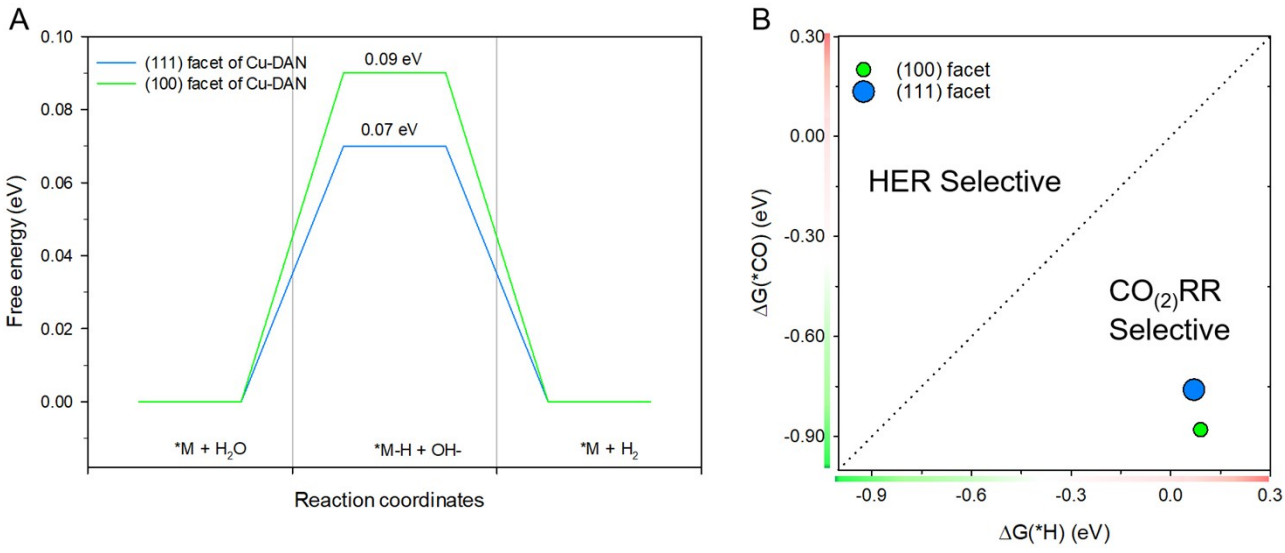


Fig. S14. (A) Free energy diagram for HER on Cu-DAN. (B) Comparison between hydrogen adsorption free energy $\Delta G(*H)$ and carbon monoxide adsorption free energy $\Delta G(*CO)$ on (111) and (100) facets of Cu-DAN.

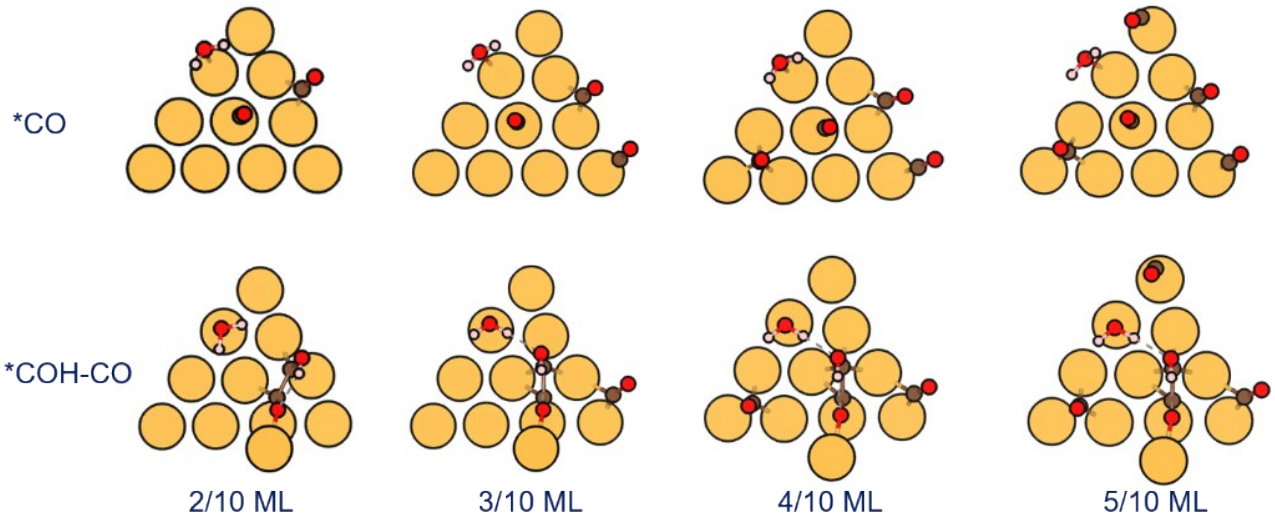


Fig. S15. Atomic structures of *CO and *COH–CO under *CO coverage of 2/10, 3/10, 4/10 and 5/10 ML. Color code: Cu, orange; C, brown; O, red; H, pink.

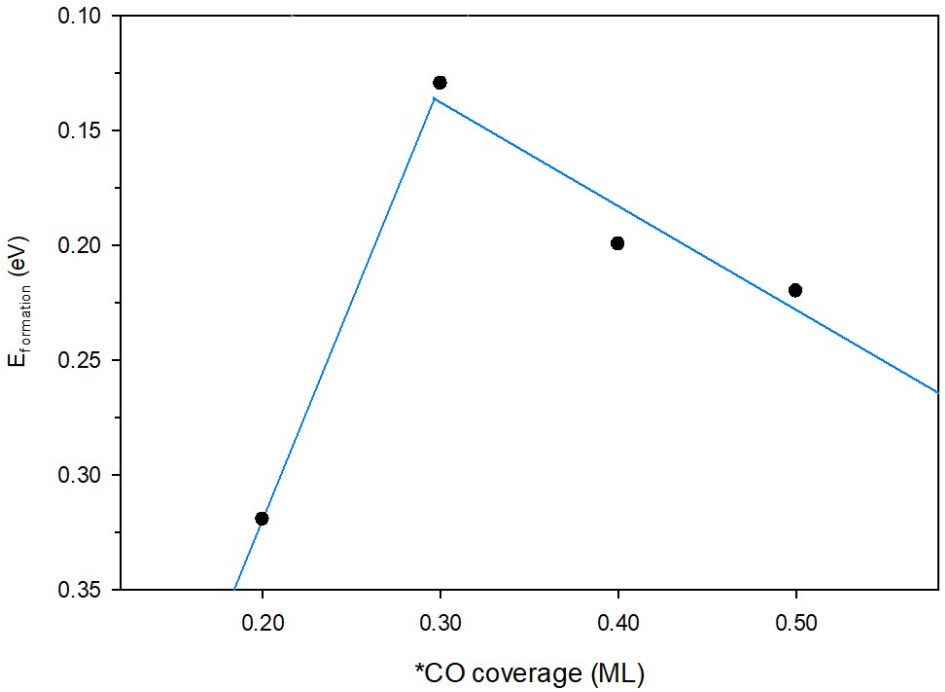


Fig. S16. Volcano-type relationship between *CO coverage and formation energy of *COH–CO.

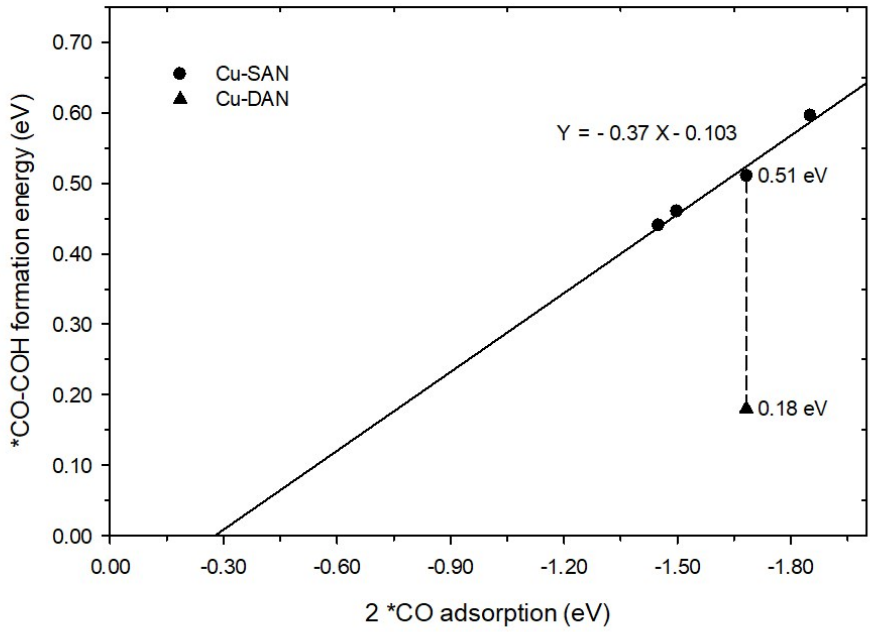


Fig. S17. Linear scaling relations between 2*CO adsorption and *COH–CO formation free energies on Cu-SAN and Cu-DAN.

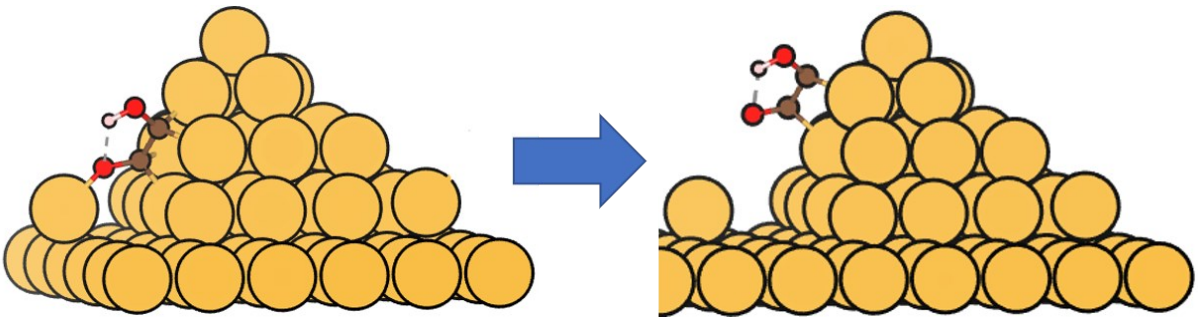


Fig. S18. Computation of Cu–O bond strength. To compute the strength of the bond between βO and Cu of the adjacent nanopyramid, we moved the *COH–CO along the nanopyramid surface until the Cu-O bond was completely broken. The energy difference between the translated structure with original is 2.63 eV (253.76 kJ mol^{-1}), and reflects the Cu–O bond strength. All atoms were fixed to compute the single-point energy of the structure.

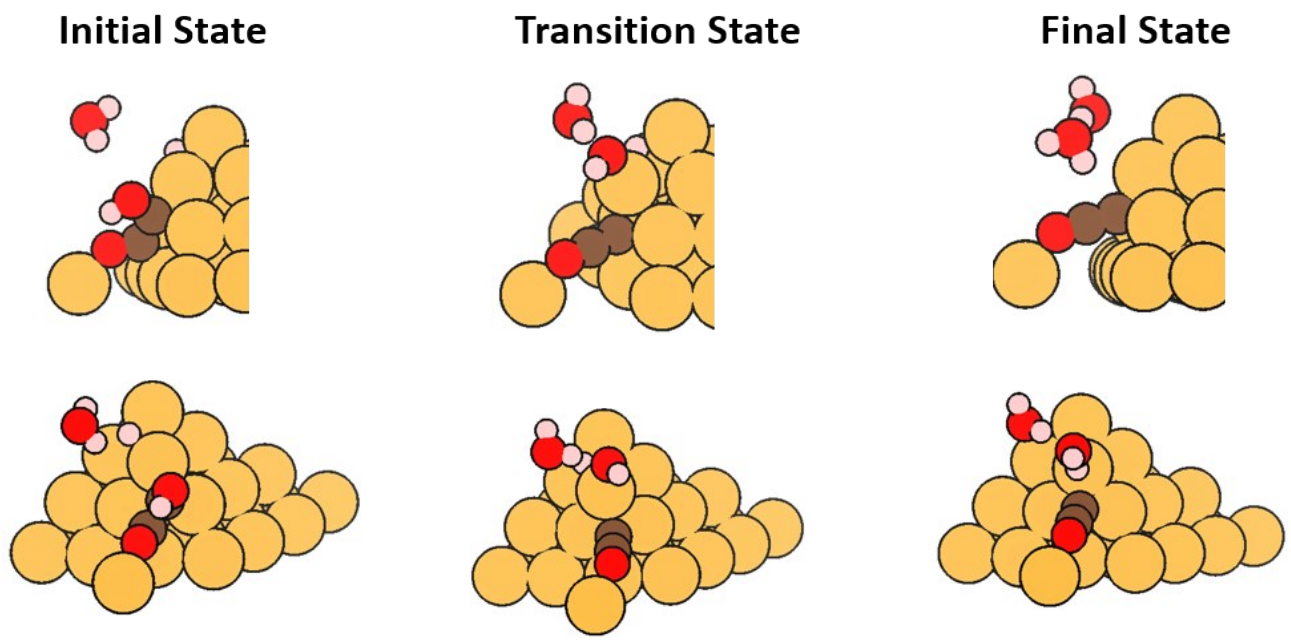


Fig. S19. Side and front view of optimized structures of, respectively, the initial, transition and final states involved in *COH–CO reduction to *C–CO on Cu-DAN. Color code: Cu, orange; C, brown; O, red; H, pink.

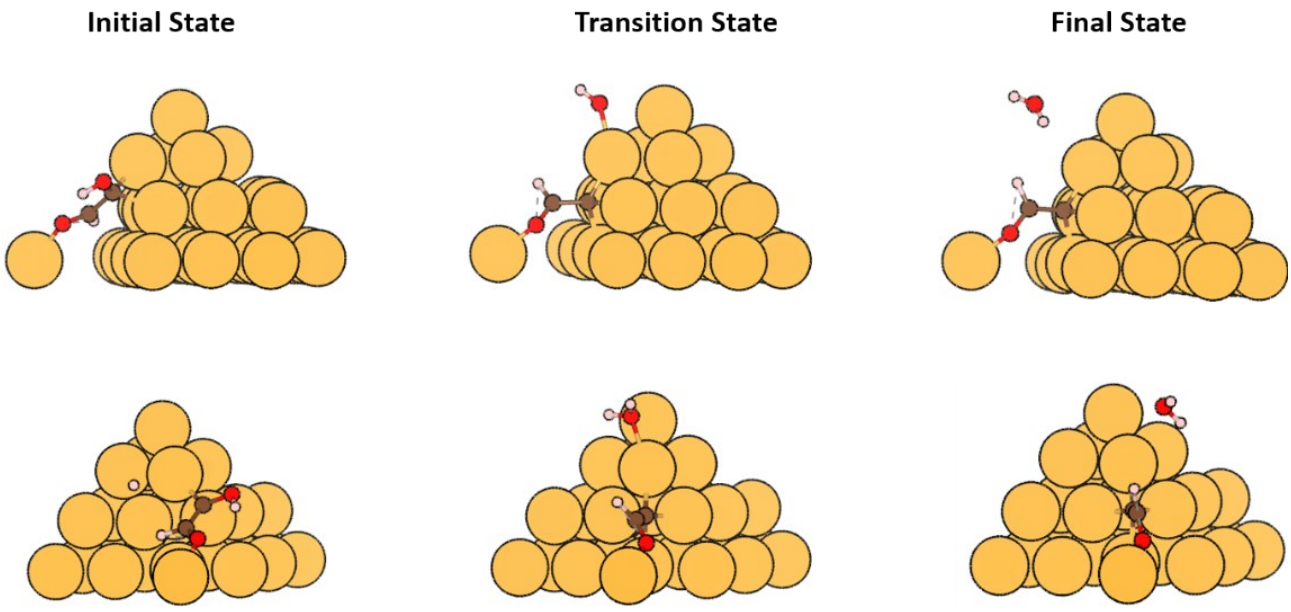


Fig. S20. Side and front view of optimized structures of, respectively, the initial, transition and final states involved in *COH–CHO reduction to *C–CHO on Cu-DAN (*COH–CHO + H^+ + e^- → *C–CHO + H_2O). Color code: Cu, orange; C, brown; O, red; H, pink.

Supplementary Note 1

Stability of Cu-DAN

Stability is a prerequisite for electrocatalytic materials. This is closely related to the experimental feasibility and catalytic activity for long-term use.

The dissolution potential (U_{diss}) of the surface atoms on nanopyramid, which assess the dissolution-resistance of one surface atom from the nanopyramid into water under an applied potential,[8] is calculated as:

$$U_{diss} = U^0_{diss(Cu)} - E_f / ne$$

where $U^0_{diss(Cu)}$ and n denote standard reduction potential of Cu and the number of electrons transferred during dissolution. The values are 0.34 V and 2, respectively.

E_f, the formation energy of one surface Cu atom, is defined as:

$$E_f = E_{nanopyramid} - E_{less} - E_{Cu}$$

where $E_{nanopyramid}$ is the total energy, E_{less} is the energy of nanopyramid without one surface Cu atom and E_{Cu} is the energy of isolated Cu atom.

The calculated positive U_{diss} of 1.72 V shows that the surface Cu atoms will be stable under electrochemical environments.

In addition, we carried out *ab initio* molecular dynamics (AIMD) simulations to explore the thermodynamic stability of the surface atoms of the Cu-DAN at 300K, as shown in Figure S2. We found that the thermal oscillations of surface Cu atoms occur near the equilibrium position following relaxation for 6 ps, and that the structure showed no significant structural distortion. This finding confirms thermodynamic stability of Cu-DAN.

Supplementary Note 2

Hydrogen evolution reaction (HER) on Cu-DAN

We used DFT computations to identity that the most stable *H adsorption sites, with minimum adsorption energy on Cu nanopyramids, is the 4-fold hollow site for (100) facets, and HCP hollow site for (111) facets, respectively. The performance of these active sites for the Volmer step of HER in alkaline condition (*M + H_2O + e^- →*M-H + OH^-) was investigated using free energy as an indicator. The free energy change of the Volmer step can be computed from:

$$\Delta G_{volmer} = (G_{*M-H} + G_{OH^-}) - (G_{*M} + G_{H2O} + G_{e^-})$$

where G_{*M} is the free energy of the original pyramidal structure, G_{*M-H} is the free energy of the pyramidal structure with adsorbed *H, G_{H2O} and G_{H2} is the free energy of a H_2O molecule and a H_2 molecule. G_{OH^-} is the free energy of a hydroxide ion (OH^-) obtained as, $G_{OH^-} = G_{H2O} - G_{H2}/2$.

The computational results are given in Figure S14A, and a comparison with *CO adsorption energy on the same sites is given in Figure S14B that indicates suppression of competing HER on Cu-DAN.

Supplementary Note 3

Effect of *CO coverage on the formation of *COH-CO

The coverage of *CO is expressed in monolayer (ML) units. These are defined as the number of adsorbed *CO molecules (*n, n* = 2, 3, 4 and 5 in this simulation) divided by the total number of atoms on one facet of Cu-DAN (10). The formation energy of intermediate *COH-CO under such *CO coverage then is computed as:

$$E_{formation} = E_{total} - (E_{slab+n*CO} + E_{H2}/2)$$

where E_{total} is the energy of the total system, $E_{slab+n*CO}$ is the energy of Cu-CAN with adsorption of n *CO molecules. E_{H2} is the energy of a hydrogen molecule (-6.76 eV).

We began by constructing the Cu-DAN surface with two *CO adsorbates (*CO coverage = 2/10 ML). To investigate the influence of *CO coverage on the formation of *COH–CO we added more *CO molecules on the surface to gradually increase the *CO coverage from 2/10 to 5/10 ML as is shown in Figure S15. We found volcano-type relationships between *CO coverage and formation energy of *COH–CO (Figure S16). With the increase of *CO coverage, the formation energy of *COH–CO increases first and reaches a peak at 3/10 ML. This is consistent with experimental observations that a higher *CO coverage promotes C–C coupling.

As the *CO coverage increases further, the formation energy of *COH–CO decreases. This is because the steric hindrance of O atom caused by excessive *CO adsorption destabilizes the dimer intermediate *COH–CO.

Supplementary Note 4

***COH–CHO formation on planar Cu (100)**

*COH–CHO is the precursor of glycolaldehyde (CH_2OH–CHO). Two mechanisms have been hypothesized toward its formation on planar Cu surface.[1] These are: 1) *COH–CO + H → *COH–CHO, and; 2) *CHO + *COH → *COH–CHO. On planar Cu (100) surface *COH–COH prevails over *COH–CHO. The reason is discussed in detail.

For the first mechanism Cheng et al.[1] hypothesized a pathway on planar Cu (100) facets in which *COH–CO formation is followed by hydrogenation of βO atoms. This rules out the possibility of hydrogenation of βC to *COH–CHO. We attribute this to the instability of intermediate *COH–CHO. The structures of *COH–CHO and *COH–COH are tautomeric. The former is comparatively unstable because it is vertically adsorbed on surface via a double bond, and because it has a free radical on the C atom. We computed *COH–CHO to be 0.26 eV less stable than *COH–COH on planar Cu (100) surface.

This finding means the bulk of *COH–CHO are spontaneously tautomerized to *COH–COH, despite being formed first. Because *COH–CHO is not a stable molecular compound with a significant concentration on planar Cu (100) surface, the *COH–CHO pathway is blocked. Additionally if the formation of *COH–CHO follows the second mechanism, it is difficult for it to proceed on a planar surface. *COH and *CHO are preferably, respectively, stabilized on Cu (111) and Cu (100) surface.[4]

It is reportedly rare for those two adsorbates to simultaneously attain the kinetically reactable concentration on a homogeneous facet. This is the reason why we record a high-level barrier of 0.72 eV at 0 V vs RHE for *COH–CHO formation on planar Cu (100) surface.

We conclude therefore that on a planar Cu (100) surface *COH–CHO is not favored and the pathway is blocked.

Table S1. Free energy for gas phase species.

Gas Molecule	***E*** **(eV)**	***ZPE*** **(eV)**	***–TS*** **(eV)**	***G*** **(eV)**
H_2 (g)	–6.75	0.27	–0.41	–6.89
H_2O (g)	–14.22	0.56	–0.67	–14.33
CO (g)	–14.80	0.13	–0.61	-14.70
CO_2 (g)	–23.01	0.31	–0.66	–23.36
C_2H_4 (g)	–31.97	1.37	–0.55	–31.15
C_2H_5OH (g)	–46.88	2.13	–0.60	–45.35
$(CH_2OH)_2$ (g)	–53.31	2.27	–0.65	–51.69

Table S2. Summary of elementary reaction steps, hydrogen transfer model, reaction barriers at various electrode potentials and involved parameter for computation. $\Delta G(0V)$ and $\Delta G^{\neq}(0V)$ are the free energy change and reaction barrier without potential bias, $\Delta G^{\neq}(U^0)$ is the reaction barrier under U^0. U^0 is the equilibrium potential for the reductive adsorption of one proton in the system, and β' is the reaction symmetry factor, as defined in the manuscript. The two hydrogen models considered were, 1) Langmuir-Hinshelwood (LH) mechanism (i.e. direct transfer of an adsorbed *H), and 2) Eley-Rideal (ER) mechanism (i.e. water molecule shuttles an adsorbed *H). Adding hydrogen to carbon species via LH mechanism always gives lower kinetic barriers, compared with hydrogen transfer via ER mechanism. ER mechanism contributed to a lower kinetic barrier when hydrogen is added to oxygen species.[5,6] For all steps computed with H-shuttling, one H_2O molecule was included in the computation.

No.	Catalyst	Reaction Steps	Model	$\Delta G(0V)$	$\Delta G^{\ddagger}(U^0)$	U^0 [a]	β' [b]	$\Delta G^{\ddagger}(0V)$
1a	Cu-DAN	*CO+*CO+H^++e^-→*COH–CO	H-shuttling	0.79	1.07	–0.12	0.49	1.13
1b	Cu-SAN		H-shuttling	0.94	1.50	–0.25	0.49	1.63
2	Cu-DAN	*COH–CO+ H^++e^-→*COH–COH	H-shuttling	0.24	0.76	–0.17	0.49	0.84
3a	Cu-DAN	*COH–CO+ H^++e^-→*C–CO + H_2O	H-shuttling	–0.99	0.72	–0.21	0.49	0.82
3b	Cu-DAN		surface *H transfer	–1.25	1.66	–0.39	0.49	1.86
4a	Cu-DAN	*COH–CO+ H^++e^-→*COH–CHO	surface *H transfer	–0.21	0.41	–0.10	0.49	0.45
4b	Cu(100)		surface *H transfer	–0.04	0.69	–0.05	0.49	0.72
5	Cu-DAN	*COH–CHO+ H^++e^-→*CHOH–CHO	surface *H transfer	–0.38	0.52	–0.08	0.49	0.56
6	Cu-DAN	*COH–CHO+ H^++e^-→*C–CHO	surface *H transfer	0.04	1.02	–0.11	0.49	1.07
7	Cu-DAN	*CHOH–CHO+ H^++e^-→*CH_2OH–CHO	surface *H transfer	–0.27	0.25	0.04	0.49	0.23
8	Cu-DAN	*CH_2OH–CHO+ H^++e^-→*CH_2OH–CH_2O	surface *H transfer	–0.29	0.39	–0.08	0.49	0.43
9	Cu-DAN	*CH_2OH–CH_2O+ H^++e^-→CH_2OH–CH_3+*O	surface *H transfer	–0.58	0.98	–0.15	0.49	1.05
10	Cu-DAN	*CH_2OH–CH_2O+ H^++e^-→*CH_2OH–CH_2OH	H-shuttling	–0.19	0.73	–0.18	0.49	0.82

[a] U^0 is the potential where reaction *A+H^++e^-→*A+*H possess zero free energy change i.e. G(*A+*H) + eU^0 – G(*A) – 1/2H_2 = 0, where *A means the system with A adsorbed on the surface.

[b] β' is the reaction symmetry factor, which is approximated as 0.49 for all elementary steps.[7]

Table S3. Atomic coordinates of initial state (IS), transition state (TS), and final state (FS) of Reaction 1a listed in Table S1.

Reaction 1a: *CO+*CO+ H^{+}+e^{-} →*COH–CO on Cu-DAN via H-shuttling.

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  3
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
 0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
 0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
 0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
 0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
 0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
 0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
 0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
 0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
 0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
 0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
 0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
 0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
 0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
 0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
 0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
 0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
 0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
 0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
 0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
 0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
 0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
 0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
 0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
 0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
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 0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
 0.8587517665096048  0.3369126022125444  0.1288542110224797 T T T
 0.2673107969312974  0.7323697467352438  0.1328570400956452 T T T
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 0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
 0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
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 0.4688531600558845  0.3377931505960579  0.1335124512974523 T T T
 0.2652459217657827  0.3252916947539419  0.1326304864369880 T T T
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 0.0750432236247554  0.5203415532732601  0.3534734654023226 T T T
 0.2054810037805627  0.2816122894957866  0.4024585066221745 T T T
```

TS

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Cu  C  H  O
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  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  3
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
 0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
 0.0000000000000000  0.3 999999999999986  0.0000000000000000  F  F  F
 0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
 0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
 0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
 0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
 0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
 0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
 0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
 0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
 0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
 0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
 0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
 0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
 0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
 0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
 0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
 0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
 0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
 0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
 0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
 0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
 0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
 0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
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 0.6666644456031534  0.5333340047990589  0.1368027475005462  T  T  T
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 0.6666644456031534  0.7333340047990546  0.1368027475005462  T  T  T
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 0.4714711369717424  0.6624165318745637  0.4983866899032818  T  T  T
 0.1974724511719206  0.4169857562681114  0.3133159876282083  T  T  T
 0.1487678283928907  0.4618144575424958  0.2467042156132055  T  T  T
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 0.1182104312546736  0.1858927512169251  0.1794875275188736  T  T  T
 0.0359435015453488  0.4065354029343360  0.2294403723717657  T  T  T
 0.1227808175756999  0.3074926090646437  0.3496004291861500  T  T  T
```

FS

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Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  3
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
 0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
 0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
 0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
 0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
 0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
 0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
 0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
 0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
 0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
 0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
 0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
 0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
 0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
 0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
 0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
 0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
 0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
 0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
 0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
 0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
 0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
 0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
 0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
 0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
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 0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
 0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
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 0.2666548723923730  0.7338547123876894  0.1303586864887370 T T T
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 0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
 0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
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 0.1568421647179248  0.4688717419132175  0.2447163349009794 T T T
 0.0402129468101246  0.3405310331728101  0.3525643085812615 T T T
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 0.1208990886922510  0.1854463305528166  0.2030307059661308 T T T
 0.0405684917239722  0.4097960821227892  0.2326101652874483 T T T
 0.1189878580029992  0.3643200633339206  0.3798766154856253 T T T
```

Table S4. Atomic coordinates of IS, TS, and FS of Reaction 1b listed in Table S1.

Reaction 1b: *CO+*CO+ H^++e^-→*COH–CO on Cu-SAN via H-shuttling

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2781713742405466  0.9232736646864270  0.1334675070203859 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8608168405116802  0.3383705232036037  0.1287910777447995 T T T
  0.2675101587519791  0.7263712996367083  0.1347911413219611 T T T
  0.4761965227769058  0.9349936774286948  0.1340783519541450 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
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  0.2622036449511278  0.5270552565275325  0.1302665396273993 T T T
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  0.0322244313096630  0.3570798390862418  0.5261692711456819 T T T
  0.0756956245153165  0.6133076455880032  0.3658885271834095 T T T
  0.3389762906524047  0.9308740666329433  0.4498159328679205 T T T
```

TS

```
Cu  C  H  O
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  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2783873916485336  0.9275281115388972  0.1281277979589293  T  T  T
  0.4645692318962702  0.7323670548956187  0.1354057277978384  T  T  T
  0.6662002356971897  0.5338169553963326  0.1358095665998107  T  T  T
  0.8614943482297626  0.3375885859910882  0.1259431139605189  T  T  T
  0.2647073752363598  0.7287292205703846  0.1294622219763576  T  T  T
  0.4780965449700690  0.9368078844213678  0.1295463279222082  T  T  T
  0.4657270387003507  0.5320977479026254  0.1346313791995470  T  T  T
  0.6657510079991198  0.7327853666011066  0.1349863735969024  T  T  T
  0.8664329469018256  0.5332869701675668  0.1290283040895703  T  T  T
  0.6667612273759520  0.3345429816646794  0.1300800898255548  T  T  T
  0.2607430715802793  0.5247128770550800  0.1283930810090224  T  T  T
  0.4673909960366869  0.3331494006990769  0.1291942303696207  T  T  T
  0.2711834484776260  0.3349396910449310  0.1270883766527399  T  T  T
  0.6763060332669681  0.9413661619574479  0.1281313314783594  T  T  T
  0.8611589073832124  0.7309979628830492  0.1331216668749192  T  T  T
  0.8666113672291268  0.9311479124514984  0.1243083134367012  T  T  T
  0.3567881048269144  0.8612401320109135  0.2599398067120629  T  T  T
  0.5296525373004926  0.6640206900000720  0.2689701485971625  T  T  T
  0.3044046074378170  0.6398325027807998  0.2602307093677210  T  T  T
  0.5326928650501128  0.4591883111431778  0.2651453474565855  T  T  T
  0.3387914807791660  0.4595143797966413  0.2657134204713398  T  T  T
  0.5616469221640331  0.8772745282487266  0.2622723185162716  T  T  T
  0.7205881888802885  0.6614023225002197  0.2744889594999732  T  T  T
  0.7496633050788375  0.8702296112120280  0.2579945027244480  T  T  T
  0.7350269814763948  0.4725272336872526  0.2589192882804509  T  T  T
  0.4460956362498132  0.8030086568117158  0.3977108125654101  T  T  T
  0.3645090220552314  0.5862964967468515  0.3928438498553001  T  T  T
  0.6335379945814071  0.7957473383677766  0.3894484287774286  T  T  T
  0.5439150305360235  0.5670119758342237  0.3995952015073908  T  T  T
  0.5043432079384352  0.6873227519553563  0.5079265701981914  T  T  T
  0.3070746502358982  0.8342810541658814  0.3801915158326334  T  T  T
  0.2564968387795805  0.6602739253742683  0.3786313093800443  T  T  T
  0.1178297339510612  0.5250643289614290  0.4356620215454704  T  T  T
  0.9926619666032525  0.3322083320773632  0.4451014973126790  T  T  T
  0.1285087395850572  0.3707498066926874  0.4378409539475828  T  T  T
  0.0727620715414432  0.3927682764322704  0.4640718532483881  T  T  T
  0.1565130895185713  0.6153211778889837  0.4231926653263935  T  T  T
  0.2572498024076048  0.8617803921903634  0.4333807013306434  T  T  T
```

FS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2791554626737874  0.9271617504996736  0.1325692200874938 T T T
  0.4629978217000001  0.7316418424999966  0.1343579629999994 T T T
  0.6658520781999968  0.5341791682999997  0.1350646809000011 T T T
  0.8612533056452588  0.3400411119091570  0.1289789960082511 T T T
  0.2638780217162340  0.7286711196464688  0.1333415773895474 T T T
  0.4756963312307834  0.9365787896217104  0.1342596486729646 T T T
  0.4650239835999983  0.5311705551999992  0.1330028530000007 T T T
  0.6650659298000008  0.7323738879000032  0.1336240931000034 T T T
  0.8669008927108031  0.5358006293217177  0.1321842064057241 T T T
  0.6673093272410257  0.3375933696474878  0.1346265931703926 T T T
  0.2625139712363505  0.5262575409971320  0.1309940157198037 T T T
  0.4665512971025032  0.3325004612184439  0.1316402639515181 T T T
  0.2697878367673198  0.3351702921777122  0.1320653906482623 T T T
  0.8599938610757893  0.7314435265328054  0.1382410162763697 T T T
  0.8689165231372130  0.9328252369087676  0.1275099162905208 T T T
  0.3563975324814424  0.8532483625193893  0.2687254563242980 T T T
  0.5268934517999995  0.6620365268000015  0.2654936388000024 T T T
  0.3011471294477961  0.6375709591416200  0.2636805931066236 T T T
  0.5327234443271590  0.4571442296816284  0.2646404400488176 T T T
  0.3411157017640520  0.4628012432476342  0.2673955950278046 T T T
  0.5581121420201568  0.8727260335752981  0.2651624392487927 T T T
  0.7180449979782720  0.6603559098522268  0.2769927930456657 T T T
  0.7474097807438934  0.8674448149942438  0.2569134880340316 T T T
  0.7368059863854634  0.4774864429669193  0.2621422235730532 T T T
  0.4655281122060988  0.8209172660383157  0.4078030398043653 T T T
  0.3686389184751044  0.5984607700535707  0.3978216401318439 T T T
  0.6373393903430410  0.7863056091284745  0.3882490064518874 T T T
  0.5356517432955212  0.5615413491809571  0.3973590610078179 T T T
  0.5135313462457620  0.6901583548485293  0.5106571314273624 T T T
  0.2954057906979471  0.7861644422126015  0.3925887121963051 T T T
  0.2469803934712830  0.6549857978734962  0.3849587192991351 T T T
  0.1104682528824686  0.5038108215020743  0.4274641637754976 T T T
  0.9828423867862420  0.2863248866269069  0.4640024924788302 T T T
  0.0010831920880507  0.3778656667380190  0.5367683234185990 T T T
  0.0412273605829685  0.3640668916733043  0.4879188581374252 T T T
  0.1361193241016149  0.5901831120039787  0.4212226351954583 T T T
  0.2488641751469659  0.8410265269215254  0.4255409914963029 T T T
```

Table S5. Atomic coordinates of IS, TS, and FS of Reaction 2a listed in Table S1.

Reaction 2: *CO-COH+ H^++e^-→*COH–COH on Cu-DAN via H-shuttling.

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2835502922722780  0.9342747891772436  0.1319146728921217 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.9136136382241256  0.3860781389677790  0.1434650844879624 T T T
  0.2562335090357815  0.7284156988889460  0.1332433033892266 T T T
  0.4758481046697432  0.9355328846303884  0.1332868994508577 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8641457753245826  0.5423124521639792  0.1294354325990739 T T T
  0.6778934104712169  0.3393174330706111  0.1328922161884148 T T T
  0.2577558360131925  0.5249245762240896  0.1337967542621427 T T T
  0.4666868242519626  0.3363107069761908  0.1354591639721820 T T T
  0.2660059241603797  0.3294905368891279  0.1241126730267999 T T T
  0.6751160710588726  0.9398987043257256  0.1302285815846208 T T T
  0.8613753602157161  0.7350931323516167  0.1367776748547810 T T T
  0.8678697105792029  0.9341158001817512  0.1280052400387505 T T T
  0.3577600288954836  0.8535702620914803  0.2638304255268804 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3020759451455687  0.6405257097111191  0.2685269376990197 T T T
  0.5453286065120457  0.4636308358708069  0.2689065113254756 T T T
  0.3387047774911725  0.4156755497522417  0.2620817394175483 T T T
  0.5626595788420253  0.8770658925817201  0.2647468309001976 T T T
  0.7287511528164691  0.6662386056414704  0.2758859215898822 T T T
  0.7488481359246552  0.8697778566060876  0.2604410210721365 T T T
  0.7433386803634637  0.4784198409643872  0.2620719113375907 T T T
  0.4311407404758031  0.7635837125944975  0.3860952219541567 T T T
  0.3575006803438855  0.5377258137531022  0.3843006990163961 T T T
  0.6365037421000918  0.7989653989205500  0.3937687017705365 T T T
  0.5738010246767696  0.5795554274850822  0.4011280088441613 T T T
  0.4855227558485977  0.6647637134214995  0.4984617777439444 T T T
  0.2024434792603950  0.4273295416347467  0.3153335902283774 T T T
  0.1580906540985562  0.4655192038783846  0.2430408514807233 T T T
  0.0397555716120231  0.3371257039511362  0.3508369397944492 T T T
  0.0571045643292034  0.5865855822376161  0.2386268995324084 T T T
  0.0328742704738582  0.6889942618238053  0.2074936753679775 T T T
  0.3028879969680451  0.7496614238664289  0.3456536897162604 T T T
  0.1176840759660155  0.3508890625754952  0.3739940694702909 T T T
  0.0415455012628862  0.4248852794336532  0.2376432356656975 T T T
  0.0956302343597504  0.6748940771351921  0.2322907042597538 T T T
```

TS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2779455656897309  0.9295960235720864  0.1313142688210651  T  T  T
  0.4666644456098155  0.7333340047990546  0.1368027474949471  T  T  T
  0.6666644456098112  0.5333340047990589  0.1368027474949471  T  T  T
  0.8724444846941888  0.3491438192389205  0.1319717726102385  T  T  T
  0.2635151243749909  0.7323790592435730  0.1318317351849264  T  T  T
  0.4776402902196143  0.9394419802653150  0.1339479250019352  T  T  T
  0.4666644456098155  0.5333340047990589  0.1368027474949471  T  T  T
  0.6666644456098112  0.7333340047990546  0.1368027474949471  T  T  T
  0.8685578260115528  0.5379945479432033  0.1274368038962395  T  T  T
  0.6707719542425775  0.3402707231930604  0.1358441947905093  T  T  T
  0.2551701275493903  0.5236335584084898  0.1334786092455027  T  T  T
  0.4646096539117688  0.3362373644834863  0.1360486250710114  T  T  T
  0.2655580435582382  0.3313228667977165  0.1259230082635669  T  T  T
  0.6736219596012564  0.9406921078031253  0.1317007387293935  T  T  T
  0.8611209008010134  0.7312280408313447  0.1369082085708132  T  T  T
  0.8658332425606766  0.9314835424371285  0.1281676803004135  T  T  T
  0.3500244482020876  0.8479905746065853  0.2634200585805256  T  T  T
  0.5333313180097790  0.6666662410030355  0.2736054949898943  T  T  T
  0.3132359929670718  0.6454371477716326  0.2625746855299592  T  T  T
  0.5580063369420402  0.4566956793750671  0.2698404790882278  T  T  T
  0.3538096990481284  0.4072639257823029  0.2655943950342262  T  T  T
  0.5542932067354300  0.8727024378495978  0.2658034674527213  T  T  T
  0.7280832730829411  0.6682512877707601  0.2769403785715870  T  T  T
  0.7455037383526721  0.8706058746161622  0.2605571749617737  T  T  T
  0.7618642086301018  0.4933270176905362  0.2618537343647314  T  T  T
  0.4295362879553933  0.7598493261944923  0.3871416774204932  T  T  T
  0.3553152493296443  0.5370194205531169  0.3812740196989704  T  T  T
  0.6370413361810955  0.7928890525261297  0.3947662731363703  T  T  T
  0.5678632268589742  0.5714950195412650  0.3984533093248877  T  T  T
  0.4830381123642439  0.6576074316016135  0.4982609426706787  T  T  T
  0.2119245464882060  0.4084635171636491  0.3107137293471379  T  T  T
  0.1714986820070377  0.4734801447383217  0.2552915437486925  T  T  T
  0.0497313042405485  0.3219724448128812  0.3473127112246813  T  T  T
  0.0578366140322912  0.5679263497869494  0.2682001659844938  T  T  T
  0.0228619602304507  0.6662450617955663  0.2369347852564271  T  T  T
  0.1943722072250951  0.7236918845637723  0.2486868614852565  T  T  T
  0.1248100463613042  0.3217329226212039  0.3620670736294938  T  T  T
  0.0595383060380262  0.4446526600368031  0.2578101016258156  T  T  T
  0.0741993084292500  0.6539812068256405  0.2789980266785403  T  T  T
```

FS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2775500050716046  0.9303139179094220  0.1326916034017981 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8630007317752241  0.3408958891126946  0.1298305367030093 T T T
  0.2693676970648352  0.7366196943778275  0.1306997882781857 T T T
  0.4769941652552201  0.9389523224533096  0.1329389971400161 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
  0.8672946208409289  0.5355451576020245  0.1280545827415542 T T T
  0.6672328164292048  0.3383098757276715  0.1352077831132083 T T T
  0.2549370537992985  0.5253884487477735  0.1374106826332533 T T T
  0.4635984560227422  0.3364319878776870  0.1359923875959986 T T T
  0.2657963278267210  0.3319501139633022  0.1254726353937373 T T T
  0.6739621380783565  0.9408547923033490  0.1318082958277499 T T T
  0.8607009195042434  0.7311604362123854  0.1366844684035086 T T T
  0.8663088942032635  0.9312754386397296  0.1281374507559500 T T T
  0.3562380773407067  0.8605866555724276  0.2652281687232057 T T T
  0.5333313179997745  0.6666662410030355  0.2736054950010853 T T T
  0.3194814679040059  0.6564779088817901  0.2640512622929446 T T T
  0.5551653960604628  0.4589077260567607  0.2696546190196086 T T T
  0.3519137247435537  0.4117970128219803  0.2651912124528561 T T T
  0.5526237748648817  0.8704368508761507  0.2652055782253372 T T T
  0.7293560439890621  0.6681914538530680  0.2766745517750628 T T T
  0.7453611353173032  0.8700648564978183  0.2601941256637296 T T T
  0.7546967494084782  0.4858255589942364  0.2615486101522623 T T T
  0.4320561159744617  0.7666200060248543  0.3902385260215490 T T T
  0.3574360238493586  0.5423879207060736  0.3819299163764152 T T T
  0.6379014972504718  0.7943269323535470  0.3945705193136908 T T T
  0.5695522987486519  0.5743148382348380  0.3991200959121098 T T T
  0.4852580757185387  0.6613046616518690  0.4990418442552703 T T T
  0.2110930012744050  0.4124854214112594  0.3117034838271494 T T T
  0.1805237963426727  0.4901859204576344  0.2660755730053772 T T T
  0.0493607536379949  0.3244479493615915  0.3522875764199763 T T T
  0.0527961617522649  0.5318705642457534  0.2699043948444215 T T T
  0.9983381883586280  0.6723388401265855  0.2499338703092511 T T T
  0.1344662571912320  0.7241939169072963  0.2723928301314573 T T T
  0.1233855612120618  0.3197518515299390  0.3587732268159530 T T T
  0.0620884505032217  0.4584308543935757  0.2733050009380276 T T T
  0.0526646557553851  0.6603494023167612  0.2888136207561173 T T T
```

Table S6. Atomic coordinates of IS, TS, and FS of Reaction 3a listed in Table S1.

Reaction 3a: *COH–CO+ H^++e^-→*C–CO + H_2O on Cu-DAN via H-shuttling

IS

```
Cu C H O
1.00000000000000
12.8585004805000001 0.0000000000000000 0.0000000000000000
-6.4291002405000004 11.1357880710000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.2994003295999992
Cu C H O
55 2 4 3
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2000000000000028 0.0000000000000000 F F F
0.0000000000000000 0.3999999999999986 0.0000000000000000 F F F
0.0000000000000000 0.6000000000000014 0.0000000000000000 F F F
0.0000000000000000 0.7999999999999972 0.0000000000000000 F F F
0.2000000000000028 0.0000000000000000 0.0000000000000000 F F F
0.2000000000000028 0.2000000000000028 0.0000000000000000 F F F
0.2000000000000028 0.3999999999999986 0.0000000000000000 F F F
0.2000000000000028 0.6000000000000014 0.0000000000000000 F F F
0.2000000000000028 0.7999999999999972 0.0000000000000000 F F F
0.3999999999999986 0.0000000000000000 0.0000000000000000 F F F
0.3999999999999986 0.2000000000000028 0.0000000000000000 F F F
0.3999999999999986 0.3999999999999986 0.0000000000000000 F F F
0.3999999999999986 0.6000000000000014 0.0000000000000000 F F F
0.3999999999999986 0.7999999999999972 0.0000000000000000 F F F
0.6000000000000014 0.0000000000000000 0.0000000000000000 F F F
0.6000000000000014 0.2000000000000028 0.0000000000000000 F F F
0.6000000000000014 0.3999999999999986 0.0000000000000000 F F F
0.6000000000000014 0.6000000000000014 0.0000000000000000 F F F
0.6000000000000014 0.7999999999999972 0.0000000000000000 F F F
0.7999999999999972 0.0000000000000000 0.0000000000000000 F F F
0.7999999999999972 0.2000000000000028 0.0000000000000000 F F F
0.7999999999999972 0.3999999999999986 0.0000000000000000 F F F
0.7999999999999972 0.6000000000000014 0.0000000000000000 F F F
0.7999999999999972 0.7999999999999972 0.0000000000000000 F F F
0.2754853223973319 0.9280542119740220 0.1321050992058303 T T T
0.4666644456031577 0.7333340047990546 0.1368027475005462 T T T
0.6666644456031534 0.5333340047990589 0.1368027475005462 T T T
0.9148840435160694 0.3929005659329380 0.1418594404705856 T T T
0.2657420588702997 0.7332813529504331 0.1304389382652731 T T T
0.4741852410382195 0.9369321166432620 0.1336590460086046 T T T
0.4666644456031577 0.5333340047990589 0.1368027475005462 T T T
0.6666644456031534 0.7333340047990546 0.1368027475005462 T T T
0.8689739798321495 0.5503257444040384 0.1318670190409217 T T T
0.6810023127692383 0.3429524475393212 0.1329783987262073 T T T
0.2554994795859796 0.5247714509766100 0.1337815173310091 T T T
0.4706228454925862 0.3357591357267293 0.1337186116044826 T T T
0.2724162563437057 0.3345251642184403 0.1291092241241057 T T T
0.6705103970574626 0.9385017892242716 0.1325544778275857 T T T
0.8615657789221387 0.7386133438463136 0.1375829405649014 T T T
0.8660202490703673 0.9348352038262692 0.1291917255091476 T T T
0.3515268595702523 0.8559791901326022 0.2646143106998788 T T T
0.5333313179997745 0.6666662410030355 0.2736054950010853 T T T
0.3024080918916358 0.6474429079468154 0.2636411558646067 T T T
0.5422227549871768 0.4634972219223635 0.2680778031855087 T T T
0.3429008566790230 0.4408863331893378 0.2708616790423115 T T T
0.5494226515305862 0.8688780568293838 0.2679776089179000 T T T
0.7268393318207258 0.6658184685287586 0.2758578135854551 T T T
0.7410033700217820 0.8680209527206089 0.2611271031844126 T T T
0.7417995616102280 0.4788628266180843 0.2627524974422909 T T T
0.4199930313257727 0.7675017991715182 0.3912758324158004 T T T
0.3326257673607005 0.5511734291025511 0.3961446476130203 T T T
0.6305695713035999 0.7939000299613547 0.3974806687305341 T T T
0.5540743993567845 0.5730892511733611 0.4025654818151094 T T T
0.4819548441992225 0.6678088245021883 0.5079311926994450 T T T
0.1948979619679175 0.4354987649826234 0.3187145500790093 T T T
0.1520632172441079 0.4693876247846010 0.2423382806841823 T T T
0.0299071774453494 0.3327213129785165 0.3418969059994203 T T T
0.1216140089162640 0.6403281611538626 0.6049935409320039 T T T
0.0548303461594674 0.5658161727860495 0.5243887781969900 T T T
0.3468346232764675 0.6561279919594573 0.4748624442031349 T T T
0.1062979769565863 0.3514217476198621 0.3713175605133378 T T T
0.0360737784583452 0.4173627581253126 0.2318436661195032 T T T
0.0459516610100328 0.6085433142975686 0.5736921802055815 T T T
```

TS

```
Cu C H O
1.00000000000000
12.8585004805000001 0.0000000000000000 0.0000000000000000
-6.4291002405000004 11.1357880710000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.2994003295999992
Cu C H O
55 2 4 3
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2000000000000028 0.0000000000000000 F F F
0.0000000000000000 0.3999999999999986 0.0000000000000000 F F F
0.0000000000000000 0.6000000000000014 0.0000000000000000 F F F
0.0000000000000000 0.7999999999999972 0.0000000000000000 F F F
0.2000000000000028 0.0000000000000000 0.0000000000000000 F F F
0.2000000000000028 0.2000000000000028 0.0000000000000000 F F F
0.2000000000000028 0.3999999999999986 0.0000000000000000 F F F
0.2000000000000028 0.6000000000000014 0.0000000000000000 F F F
0.2000000000000028 0.7999999999999972 0.0000000000000000 F F F
0.3999999999999986 0.0000000000000000 0.0000000000000000 F F F
0.3999999999999986 0.2000000000000028 0.0000000000000000 F F F
0.3999999999999986 0.3999999999999986 0.0000000000000000 F F F
0.3999999999999986 0.6000000000000014 0.0000000000000000 F F F
0.3999999999999986 0.7999999999999972 0.0000000000000000 F F F
0.6000000000000014 0.0000000000000000 0.0000000000000000 F F F
0.6000000000000014 0.2000000000000028 0.0000000000000000 F F F
0.6000000000000014 0.3999999999999986 0.0000000000000000 F F F
0.6000000000000014 0.6000000000000014 0.0000000000000000 F F F
0.6000000000000014 0.7999999999999972 0.0000000000000000 F F F
0.7999999999999972 0.0000000000000000 0.0000000000000000 F F F
0.7999999999999972 0.2000000000000028 0.0000000000000000 F F F
0.7999999999999972 0.3999999999999986 0.0000000000000000 F F F
0.7999999999999972 0.6000000000000014 0.0000000000000000 F F F
0.7999999999999972 0.7999999999999972 0.0000000000000000 F F F
0.2779467328907058 0.9274786982060373 0.1328680434655334 T T T
0.4666644456031577 0.7333340047990546 0.1368027475005462 T T T
0.6666644456031534 0.5333340047990589 0.1368027475005462 T T T
0.8717571811346642 0.3463703330189130 0.1335636207064972 T T T
0.2674400484483616 0.7319499330193718 0.1308969524243295 T T T
0.4765484565139981 0.9383210172820501 0.1340200845263425 T T T
0.4666644456031577 0.5333340047990589 0.1368027475005462 T T T
0.6666644456031534 0.7333340047990546 0.1368027475005462 T T T
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0.2732318904629051 0.3334434117114330 0.1294872382279098 T T T
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0.8601118087533485 0.7320625544692392 0.1374244291348447 T T T
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0.4321037077929593 0.7624078311912311 0.3877804613338307 T T T
0.2968202780735863 0.5354555102654469 0.4015468424941161 T T T
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0.4681485590556491 0.6633578456454501 0.5053766494427947 T T T
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0.9758340433608577 0.3491031599363528 0.2377360539017425 T T T
0.1066593371177582 0.5912176135088791 0.5556790224022721 T T T
```

FS

```
Cu C H O
1.00000000000000
12.8585004805000001 0.0000000000000000 0.0000000000000000
-6.4291002405000004 11.1357880710000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 15.2994003295999992
Cu C H O
55 2 4 3
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.2000000000000028 0.0000000000000000 F F F
0.0000000000000000 0.3999999999999986 0.0000000000000000 F F F
0.0000000000000000 0.6000000000000014 0.0000000000000000 F F F
0.0000000000000000 0.7999999999999972 0.0000000000000000 F F F
0.2000000000000028 0.0000000000000000 0.0000000000000000 F F F
0.2000000000000028 0.2000000000000028 0.0000000000000000 F F F
0.2000000000000028 0.3999999999999986 0.0000000000000000 F F F
0.2000000000000028 0.6000000000000014 0.0000000000000000 F F F
0.2000000000000028 0.7999999999999972 0.0000000000000000 F F F
0.3999999999999986 0.0000000000000000 0.0000000000000000 F F F
0.3999999999999986 0.2000000000000028 0.0000000000000000 F F F
0.3999999999999986 0.3999999999999986 0.0000000000000000 F F F
0.3999999999999986 0.6000000000000014 0.0000000000000000 F F F
0.3999999999999986 0.7999999999999972 0.0000000000000000 F F F
0.6000000000000014 0.0000000000000000 0.0000000000000000 F F F
0.6000000000000014 0.2000000000000028 0.0000000000000000 F F F
0.6000000000000014 0.3999999999999986 0.0000000000000000 F F F
0.6000000000000014 0.6000000000000014 0.0000000000000000 F F F
0.6000000000000014 0.7999999999999972 0.0000000000000000 F F F
0.7999999999999972 0.0000000000000000 0.0000000000000000 F F F
0.7999999999999972 0.2000000000000028 0.0000000000000000 F F F
0.7999999999999972 0.3999999999999986 0.0000000000000000 F F F
0.7999999999999972 0.6000000000000014 0.0000000000000000 F F F
0.7999999999999972 0.7999999999999972 0.0000000000000000 F F F
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0.6666644456031534 0.5333340047990589 0.1368027475005462 T T T
0.8777576134271079 0.3515309694160303 0.1346822972908201 T T T
0.2666048300313900 0.7335834981613010 0.1301761024445074 T T T
0.4745407560315668 0.9379265828528840 0.1337459772896743 T T T
0.4666644456031577 0.5333340047990589 0.1368027475005462 T T T
0.6666644456031534 0.7333340047990546 0.1368027475005462 T T T
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0.2622532498248409 0.5278208214523722 0.1342726410511423 T T T
0.4685263025065909 0.3350024299494282 0.1333734119339760 T T T
0.2721500916272092 0.3331579644641910 0.1284828945220616 T T T
0.6706103343121271 0.9385633358758662 0.1331608093891978 T T T
0.8602451692886606 0.7322910333966455 0.1374410415587587 T T T
0.8635210769997296 0.9306271705389524 0.1302661439093837 T T T
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0.5333313179997745 0.6666662410030355 0.2736054950010853 T T T
0.3171141202310075 0.6578289987268154 0.2626393219444799 T T T
0.5351891432324477 0.4612477584400704 0.2672863958469836 T T T
0.3390573677271339 0.4490365333504341 0.2669853258955897 T T T
0.5455141686826148 0.8676977395463875 0.2670019164774842 T T T
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0.4203835746834200 0.7754145642038496 0.3924705580488284 T T T
0.3115998945871231 0.5483228439766182 0.3929997520121437 T T T
0.6197480358023882 0.7833418224340384 0.3997337600019402 T T T
0.5064427242322260 0.5491262981284272 0.3998077152763629 T T T
0.4577938451979691 0.6600196115028965 0.5034607420002999 T T T
0.2017419951583855 0.4796043147600400 0.2878442797819495 T T T
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0.9575504127459556 0.3267717907606929 0.4742459420470073 T T T
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0.0788650181234323 0.3995233385597401 0.4255570187039974 T T T
0.0933522887661183 0.5389955278993832 0.5288406015456194 T T T
0.0417849486807895 0.3857000176821640 0.4836203904516509 T T T
0.9849399689309276 0.3604719042692881 0.2422250092697757 T T T
0.1332636009250236 0.6252216887110227 0.5431219664371980 T T T
```

Table S7. Atomic coordinates of IS, TS, and FS of Reaction 3b listed in Table S1.

Reaction 3b: *COH–CO+ H^++e^-→*C–CO + H_2O on Cu-DAN via surface *H transfer

IS

```
Cu C H O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu C H O
55  2  5  2
Selective
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
 0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
 0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
 0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
 0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
 0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
 0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
 0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
 0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
 0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
 0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
 0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
 0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
 0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
 0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
 0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
 0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
 0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
 0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
 0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
 0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
 0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
 0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
 0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
 0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
 0.2752053958105344  0.9339439589761694  0.1327670696624419 T T T
 0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
 0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
 0.9102105890265042  0.3684869562188853  0.1436267400812801 T T T
 0.2640084312338805  0.7324654224752489  0.1277175090534191 T T T
 0.4727051250732295  0.9330780525467548  0.1334889884629417 T T T
 0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
 0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
 0.8717735845097668  0.5382143799940207  0.1289171270272521 T T T
 0.6785653253105682  0.3422523273193867  0.1341273253941728 T T T
 0.2477907084217909  0.5256224929232950  0.1339067486259621 T T T
 0.4616251920961347  0.3378668945654455  0.1375267820476050 T T T
 0.2545863581217992  0.3376575447231827  0.1315045518840904 T T T
 0.6697290446791372  0.9385423379270396  0.1324561431277958 T T T
 0.8627709831984931  0.7314896965716159  0.1347630218409190 T T T
 0.8636861106498250  0.9309436314968084  0.1295527729413490 T T T
 0.3376756246337181  0.8572032306723175  0.2653428931031695 T T T
 0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
 0.3111338473132184  0.6526303185607582  0.2630663753300698 T T T
 0.5581294652948900  0.4659464274831417  0.2718448985462245 T T T
 0.3528770182459049  0.4067714450049785  0.2711019715667438 T T T
 0.5429170065121565  0.8672547529853452  0.2685154323681632 T T T
 0.7326360558265756  0.6715886588173202  0.2724439713953231 T T T
 0.7364443251447784  0.8710149056858995  0.2614121622517396 T T T
 0.7575375311771058  0.4899374496393202  0.2616536383231379 T T T
 0.4108278119102587  0.7569425423433168  0.3949785249229972 T T T
 0.3622578115283588  0.5438237276776903  0.3799756615266006 T T T
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 0.5844222992818175  0.5879826871336482  0.4020482153950768 T T T
 0.4816708519180253  0.6590139467013927  0.5009420032674186 T T T
 0.2056445540343730  0.4071932828588076  0.3075310875910325 T T T
 0.1486522525363599  0.4060366934049549  0.2248036335478256 T T T
 0.0468107870493780  0.3306116326002592  0.3525109881295637 T T T
 0.2779164418935965  0.9403804602137472  0.2395338777622968 T T T
 0.1963965594648570  0.6144200045825042  0.1913983494226776 T T T
 0.2893761197383481  0.7440543424158584  0.3406825034212908 T T T
 0.3456372728707347  0.6316951974031232  0.4678288473353099 T T T
 0.1275809400186538  0.3534499251203177  0.3755849822832679 T T T
 0.0322154251444465  0.3554680308979235  0.2221100895220382 T T T
```

TS

```
Cu C H O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
  Cu   C   H   O
  55   2   5   2
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
 0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
 0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
 0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
 0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
 0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
 0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
 0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
 0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
 0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
 0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
 0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
 0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
 0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
 0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
 0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
 0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
 0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
 0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
 0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
 0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
 0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
 0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
 0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
 0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
 0.2774982481182827  0.9354884448322739  0.1329477155694769  T  T  T
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 0.6666644456098112  0.5333340047990589  0.1368027474949471  T  T  T
 0.9007223515121709  0.3658418985977799  0.1427679051892002  T  T  T
 0.2662541670287100  0.7331485566375998  0.1274757468213157  T  T  T
 0.4750414662286031  0.9346744188913859  0.1329483286072327  T  T  T
 0.4666644456098155  0.5333340047990589  0.1368027474949471  T  T  T
 0.6666644456098112  0.7333340047990546  0.1368027474949471  T  T  T
 0.8701259946768864  0.5395360414207374  0.1297078836318406  T  T  T
 0.6773308631856756  0.3405063651678481  0.1332151652333212  T  T  T
 0.2354843020731359  0.5153230415825005  0.1372082025447597  T  T  T
 0.4653581309603667  0.3365351750960127  0.1349948850031779  T  T  T
 0.2646092271826690  0.3363928013807855  0.1278492189900385  T  T  T
 0.6728247724267694  0.9394092289996248  0.1319635286257767  T  T  T
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 0.5333313180097790  0.6666662410030355  0.2736054949898943  T  T  T
 0.3080357857629651  0.6525935692435644  0.2642256395240517  T  T  T
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 0.7264944204977748  0.6658376054046979  0.2759342377610673  T  T  T
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 0.7493015837535477  0.4827523357739296  0.2611099287241918  T  T  T
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 0.3463966307119719  0.5477506688880425  0.3847793362525636  T  T  T
 0.6223475698054410  0.7970668628766425  0.3968795590981641  T  T  T
 0.5607559580644494  0.5749599544572633  0.4007495255625768  T  T  T
 0.4732109073934367  0.6606487788709074  0.5024867163153246  T  T  T
 0.2010129379630213  0.4192742070413628  0.3087012158925224  T  T  T
 0.1311237832861465  0.4132812835590142  0.2354065190013193  T  T  T
 0.0552793351659478  0.3587456466031958  0.3899922197670536  T  T  T
 0.2878295783873985  0.9481175115174425  0.2395225580296755  T  T  T
 0.1955829467265681  0.6168592419222305  0.1910893205382998  T  T  T
 0.2935840567295274  0.7489015871697543  0.3427520778048979  T  T  T
 0.2255896914902443  0.4505774013271088  0.4412649723606199  T  T  T
 0.1333341442832632  0.3607737919126963  0.3914767424607822  T  T  T
 0.0160986675899098  0.3648527187402158  0.2340971901011210  T  T  T
```

FS

```
Cu C H O
1.0
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu C H O
55  2  5  2
Selective
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
 0.0000000000000000  0.2000000000000030  0.0000000000000000 F F F
 0.0000000000000000  0.3999999999999990  0.0000000000000000 F F F
 0.0000000000000000  0.6000000000000010  0.0000000000000000 F F F
 0.0000000000000000  0.7999999999999970  0.0000000000000000 F F F
 0.2000000000000030  0.0000000000000000  0.0000000000000000 F F F
 0.2000000000000030  0.2000000000000030  0.0000000000000000 F F F
 0.2000000000000030  0.3999999999999990  0.0000000000000000 F F F
 0.2000000000000030  0.6000000000000010  0.0000000000000000 F F F
 0.2000000000000030  0.7999999999999970  0.0000000000000000 F F F
 0.3999999999999990  0.0000000000000000  0.0000000000000000 F F F
 0.3999999999999990  0.2000000000000030  0.0000000000000000 F F F
 0.3999999999999990  0.3999999999999990  0.0000000000000000 F F F
 0.3999999999999990  0.6000000000000010  0.0000000000000000 F F F
 0.3999999999999990  0.7999999999999970  0.0000000000000000 F F F
 0.6000000000000010  0.0000000000000000  0.0000000000000000 F F F
 0.6000000000000010  0.2000000000000030  0.0000000000000000 F F F
 0.6000000000000010  0.3999999999999990  0.0000000000000000 F F F
 0.6000000000000010  0.6000000000000010  0.0000000000000000 F F F
 0.6000000000000010  0.7999999999999970  0.0000000000000000 F F F
 0.7999999999999970  0.0000000000000000  0.0000000000000000 F F F
 0.7999999999999970  0.2000000000000030  0.0000000000000000 F F F
 0.7999999999999970  0.3999999999999990  0.0000000000000000 F F F
 0.7999999999999970  0.6000000000000010  0.0000000000000000 F F F
 0.7999999999999970  0.7999999999999970  0.0000000000000000 F F F
 0.2754785041014220  0.9346477123971870  0.1319474087029630 T T T
 0.4666644456031580  0.7333340047990550  0.1368027475005460 T T T
 0.6666644456031530  0.5333340047990590  0.1368027475005460 T T T
 0.8795853102034310  0.3535464450022020  0.1344318105018020 T T T
 0.2650038568977710  0.7304563758970271  0.1276427338019130 T T T
 0.4735059615993860  0.9334180497982980  0.1325727993976220 T T T
 0.4666644456031580  0.5333340047990590  0.1368027475005460 T T T
 0.6666644456031530  0.7333340047990550  0.1368027475005460 T T T
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 0.6717288015992650  0.3387514112022100  0.1333126033021020 T T T
 0.2618586349985180  0.5261256970988550  0.1367820835991370 T T T
 0.4683740083990880  0.3362468962974600  0.1337736493005080 T T T
 0.2703869120018250  0.3307954519979650  0.1273849746012200 T T T
 0.6705988258026350  0.9386255072975160  0.1335289338986390 T T T
 0.8615832712012120  0.7324887824995659  0.1363858865019050 T T T
 0.8637590566978660  0.9315684116973700  0.1302542951009970 T T T
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 0.3135840463020050  0.6629872780020490  0.2640669819969120 T T T
 0.5390479424052400  0.4626556214029450  0.2688265743032260 T T T
 0.3420350012947040  0.4435534365962890  0.2641533464015000 T T T
 0.5427583814999440  0.8675087142020740  0.2689453753974430 T T T
 0.7243744524994820  0.6635763254011380  0.2764048854005380 T T T
 0.7356356616027140  0.8661251495992131  0.2632147045991640 T T T
 0.7376270041990550  0.4766004875956110  0.2634005536023100 T T T
 0.4114909273967410  0.7721433918980690  0.3973085689992500 T T T
 0.3345007450996960  0.5506958747958000  0.3883820922970360 T T T
 0.2912995514023460  0.7573862270030250  0.3392410654983920 T T T
 0.1487918408246570  0.3700218268728220  0.4506394668202200 T T T
 0.0858280746966855  0.2896785044967490  0.4240040507959930 T T T
 0.9906429924986140  0.3683237032034940  0.2416208720970590 T T T
```

Table S8. Atomic coordinates of IS, TS, and FS of Reaction 4a listed in Table S1.

Reaction 4a: *COH–CO+ H^++e^-→*COH–CHO on Cu-DAN via surface *H transfer

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2796943016308203  0.9317068161380664  0.1305827619309295 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.9175099794238600  0.3880853146057087  0.1458854691989256 T T T
  0.2533085952427774  0.7253665194305916  0.1314481873374182 T T T
  0.4783399481237271  0.9416495440184156  0.1337600702483050 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8699855904405507  0.5453100802765608  0.1308272382140089 T T T
  0.6818592220855718  0.3421351895945606  0.1332703604629227 T T T
  0.2561416618033415  0.5192572985736794  0.1321778646330710 T T T
  0.4686727974263157  0.3372659541589615  0.1358728079260946 T T T
  0.2670523026740779  0.3267528222889919  0.1240424656338551 T T T
  0.6716969466481695  0.9379332295917626  0.1323399691318839 T T T
  0.8619109667243207  0.7353853970291550  0.1360476120099854 T T T
  0.8650197910289508  0.9327456683779652  0.1290444473648214 T T T
  0.3507161948570421  0.8462644079096314  0.2584714235710577 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.2908024755522102  0.6341065172237058  0.2643686007126078 T T T
  0.5458464122683822  0.4650277933084669  0.2696768657316754 T T T
  0.3373781858032339  0.4118079536463745  0.2626068858683608 T T T
  0.5502983817159030  0.8714685655960007  0.2677671763920775 T T T
  0.7290881567137978  0.6671477434291664  0.2744070680336458 T T T
  0.7411578783569842  0.8680250205903626  0.2623892239779709 T T T
  0.7455109565654552  0.4812121052110473  0.2617164809868030 T T T
  0.4125213788326579  0.7598964598455814  0.3909939830361572 T T T
  0.3622578115319257  0.5438237276787249  0.3799756615237435 T T T
  0.6216535681157477  0.7985975633158312  0.3948803250730785 T T T
  0.5762445455244836  0.5833255631365809  0.4014170577646454 T T T
  0.4816708519165286  0.6590139467039255  0.5009420032697598 T T T
  0.2047180917904713  0.4306545357868545  0.3191541795883955 T T T
  0.1557958774749468  0.4516815445865356  0.2406408540963999 T T T
  0.0420343146968721  0.3377012990390427  0.3544548036668936 T T T
  0.2041709945575623  0.6173878941678945  0.4702911504705081 T T T
  0.1872849022577914  0.6964500126003027  0.4019932208269788 T T T
  0.2180635253554659  0.7176041731062375  0.2465285302907642 T T T
  0.1208635771727074  0.3628179368423970  0.3821124431768357 T T T
  0.0393589120680367  0.3982318888203152  0.2320645108510543 T T T
  0.2310222580275883  0.7013226336985462  0.4558456108992784 T T T
```

TS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2728232980128804  0.9289203393505542  0.1306950360003955  T  T  T
  0.4666644456187115  0.7333340047990546  0.1368027474874722  T  T  T
  0.6666644456187072  0.5333340047990589  0.1368027474874722  T  T  T
  0.8944044523014442  0.3667593351122457  0.1395120083341442  T  T  T
  0.2606745712737109  0.7307482473791244  0.1328530754242690  T  T  T
  0.4716970210869418  0.9358193342744222  0.1331945540447110  T  T  T
  0.4666644456187115  0.5333340047990589  0.1368027474874722  T  T  T
  0.6666644456187072  0.7333340047990546  0.1368027474874722  T  T  T
  0.8695077886097431  0.5424524584191067  0.1304016820028025  T  T  T
  0.6772975941506491  0.3402118101477879  0.1330212619263656  T  T  T
  0.2512805645492763  0.5213260569319559  0.1366960736788470  T  T  T
  0.4674056166090474  0.3356631973370561  0.1343919758865350  T  T  T
  0.2685596828047868  0.3330084830999249  0.1263944918334683  T  T  T
  0.6678193031184636  0.9372940399213858  0.1338942002980632  T  T  T
  0.8607393887905028  0.7339120813908122  0.1369627368592458  T  T  T
  0.8618669230981428  0.9311895415565369  0.1305459826073564  T  T  T
  0.3461391458659135  0.8658276638154017  0.2631055776282937  T  T  T
  0.5333313180231087  0.6666662410030355  0.2736054949749445  T  T  T
  0.3317095097561940  0.6704470806974940  0.2624157016483607  T  T  T
  0.5441465780692447  0.4620701176442590  0.2681219684497911  T  T  T
  0.3419374848654747  0.4299754471741756  0.2652035972477771  T  T  T
  0.5393587131770825  0.8662659667988604  0.2700202428739741  T  T  T
  0.7248271423278452  0.6647139113646018  0.2760743178111921  T  T  T
  0.7339154106428359  0.8652626521129144  0.2645594668667074  T  T  T
  0.7452272738740533  0.4800562274070552  0.2610593869639999  T  T  T
  0.4051452680660595  0.7729831462623321  0.4006149400711324  T  T  T
  0.3348440041259860  0.5472402711340377  0.3819020057979962  T  T  T
  0.6107176323322914  0.7930376726618975  0.3974673025187130  T  T  T
  0.5488976836399643  0.5702401343250676  0.4007720647824234  T  T  T
  0.4640681246685778  0.6546150553182071  0.5008895418501699  T  T  T
  0.1902802064495621  0.4198058753987398  0.3134140527561339  T  T  T
  0.1323867339777658  0.4338454108453548  0.2359658458285511  T  T  T
  0.0306582970082497  0.2974800241276276  0.3440386537931097  T  T  T
  0.2146796787154242  0.6841859461963091  0.5042376236146758  T  T  T
  0.2020909788827947  0.7671856853669379  0.4364053415692032  T  T  T
  0.2021167872110124  0.5919335356926260  0.2038442145595609  T  T  T
  0.1122618027033370  0.3290827368801025  0.3682538051379341  T  T  T
  0.0186106060586901  0.3780375329417323  0.2273503701688108  T  T  T
  0.2574560251108374  0.7649003548664119  0.4791788882818100  T  T  T
```

FS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2729929277172859  0.9297772274426410  0.1303624970686971 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8763302222758490  0.3480499878659764  0.1367199227794972 T T T
  0.2632528336438612  0.7320122100427358  0.1310551650781501 T T T
  0.4724672958381290  0.9375115904095712  0.1339604219939373 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
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  0.6695979998212085  0.3344441805028023  0.1311932916691460 T T T
  0.2630024879128680  0.5319940128653448  0.1320851954940759 T T T
  0.4693380537603241  0.3361998894363065  0.1340762146762512 T T T
  0.2719868866967235  0.3372022547287425  0.1295261834299136 T T T
  0.6662839443765669  0.9351314581265198  0.1348008844516944 T T T
  0.8617447072442188  0.7323946671200590  0.1355517970872361 T T T
  0.8603403726474588  0.9289641138007266  0.1326634739992980 T T T
  0.3413787839789078  0.8625602381081479  0.2615905859582662 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3326355253160293  0.6687060112976141  0.2613052940847528 T T T
  0.5273354950788235  0.4652634918392893  0.2693340670326633 T T T
  0.3265617026237381  0.4617753832798963  0.2654949335693352 T T T
  0.5352061688015421  0.8668710122799136  0.2720857173377234 T T T
  0.7246466891405701  0.6614912851850313  0.2714003959526963 T T T
  0.7265021148722226  0.8601810089293906  0.2685437365384400 T T T
  0.7219078882703610  0.4632966554492442  0.2614698036955323 T T T
  0.3887391598520006  0.7776479447184177  0.3979788481618768 T T T
  0.2771877113899249  0.5369733390800261  0.3929443525832658 T T T
  0.5871625032142173  0.7825152397749671  0.4019081421640222 T T T
  0.4778224321698687  0.5447083317272042  0.3997196185675860 T T T
  0.4258947263493524  0.6522795539252482  0.5027346650835467 T T T
  0.1550538427350676  0.4070576127933664  0.3155892641847701 T T T
  0.0796452971650534  0.4273284003171841  0.2573422711969393 T T T
  0.0220766247906616  0.2471247877565359  0.3194676099531389 T T T
  0.2036528195659758  0.6878443661784567  0.4981184559168570 T T T
  0.1857147513203133  0.7744052756524745  0.4375231712145397 T T T
  0.1116551529887108  0.5206065411396487  0.2354004671430756 T T T
  0.1019999065025345  0.2914223480294780  0.3475671965606031 T T T
  0.9739232450350146  0.3420127999871758  0.2349742154017027 T T T
  0.2414465449383610  0.7720313578417725  0.4798846608306375 T T T
```

Table S9. Atomic coordinates of IS, TS, and FS of Reaction 4c listed in Table S1.

Reaction 4b: *COH–CO+ H^++e^-→*COH–CHO on planar Cu (100) via surface *H transfer

IS

Cu C H O
1.00000000000000
10.9033256753999996 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.9033256753999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.6344418917999999
Cu C H O
36 2 2 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.1661041259954941 0.0008695378088244 0.1619882777796406 T T T
0.9995854207921430 0.1670516348230785 0.1649245184631450 T T T
0.1666666666666643 0.1666666666666643 0.0000000000000000 F F F
0.0000000000000000 0.3333333333333357 0.0000000000000000 F F F
0.1664415101985676 0.3332290967530651 0.1617822724428833 T T T
0.9997562743553990 0.4997578192274045 0.1622764859777086 T T T
0.1666666666666643 0.5000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.6666666666666643 0.0000000000000000 F F F
0.1639901206847034 0.6682089858481457 0.1611648800777758 T T T
0.9991196295680950 0.8338781576929283 0.1620198075772152 T T T
0.1666666666666643 0.8333333333333357 0.0000000000000000 F F F
0.3333333333333357 0.0000000000000000 0.0000000000000000 F F F
0.5002715303656241 0.0002944146804081 0.1623122392668561 T T T
0.3336233147562353 0.1663903303844037 0.1621524171165534 T T T
0.5000000000000000 0.1666666666666643 0.0000000000000000 F F F
0.3333333333333357 0.3333333333333357 0.0000000000000000 F F F
0.5025121458238192 0.3314724932912396 0.1678101234102215 T T T
0.3318164580322804 0.5016036180781258 0.1692018541826215 T T T
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.3333333333333357 0.6666666666666643 0.0000000000000000 F F F
0.4981462177966607 0.6681366770134289 0.1692124547645107 T T T
0.3317795142791436 0.8361575700248703 0.1611647837928961 T T T
0.5000000000000000 0.8333333333333357 0.0000000000000000 F F F
0.6666666666666643 0.0000000000000000 0.0000000000000000 F F F
0.8329676755448812 0.0002971881994578 0.1649166396738098 T T T
0.6682781463880616 0.1644864174007575 0.1651160889588236 T T T
0.8333333333333357 0.1666666666666643 0.0000000000000000 F F F
0.6666666666666643 0.3333333333333357 0.0000000000000000 F F F
0.8354067672288140 0.3318334795686460 0.1649933419499269 T T T
0.6684751656146590 0.4976723635318578 0.1677835236298524 T T T
0.8333333333333357 0.5000000000000000 0.0000000000000000 F F F
0.6666666666666643 0.6666666666666643 0.0000000000000000 F F F
0.8336080645684568966 0.6664258514133563 0.1621331480542856 T T T
0.6666895664454081 0.8334454813277262 0.1617969452907017 T T T
0.8333333333333357 0.8333333333333357 0.0000000000000000 F F F
0.4554538836332186 0.5444410637074751 0.3044095668841552 T T T
0.5514402691501205 0.4484101218772729 0.3139921071042192 T T T
0.4611097447278152 0.5393161924450083 0.4832854698334224 T T T
0.8309714754755351 0.1695980991580818 0.2185727790337578 T T T
0.4146957401267218 0.5849918964564399 0.4185270683446837 T T T
0.5901722201266092 0.4102828789059565 0.4167617771546612 T T T

TS

Cu C H O
1.00000000000000
10.9033256753999996 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.9033256753999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.6344418917999999
Cu C H O
36 2 2 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.1660864284965375 0.0006090524000273 0.1627564135632032 T T T
0.9996828870111660 0.1668916261782245 0.1626618321231320 T T T
0.1666666666876395 0.1666666666876395 0.0000000000000000 F F F
0.0000000000000000 0.3333333333123605 0.0000000000000000 F F F
0.1658222599191973 0.3326776229563612 0.1619516827540445 T T T
0.9997830061794007 0.4998960179630280 0.1625296523692658 T T T
0.1666666666876395 0.5000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.6666666666876395 0.0000000000000000 F F F
0.1633564751298621 0.6681582706254641 0.1617415544105775 T T T
0.9993978075783454 0.8339086054070536 0.1627536257032900 T T T
0.1666666666876395 0.8333333333123605 0.0000000000000000 F F F
0.3333333333123605 0.0000000000000000 0.0000000000000000 F F F
0.5001249938557017 0.0002197588932932 0.1625404939251031 T T T
0.3328861589628708 0.1657047200658749 0.1619740438635099 T T T
0.5000000000000000 0.1666666666876395 0.0000000000000000 F F F
0.3333333333123605 0.3333333333123605 0.0000000000000000 F F F
0.5006357921907516 0.3309144818895444 0.1663883799392043 T T T
0.3334125651700385 0.4995335749729921 0.1678294464889087 T T T
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.3333333333123605 0.6666666666876395 0.0000000000000000 F F F
0.5001992639966042 0.6667820022390294 0.1680663349987641 T T T
0.3318355744755442 0.8366914310170881 0.1617232703452010 T T T
0.5000000000000000 0.8333333333123605 0.0000000000000000 F F F
0.6666666666876395 0.0000000000000000 0.0000000000000000 F F F
0.8330999758248234 0.0003237298301323 0.1626557912014171 T T T
0.6674386438918012 0.1649206114047846 0.1634686225089745 T T T
0.8333333333123605 0.1666666666876395 0.0000000000000000 F F F
0.6666666666876395 0.3333333333123605 0.0000000000000000 F F F
0.8351419044383710 0.3325601912296752 0.1634518135231096 T T T
0.6689797095209409 0.4993305772400200 0.1665047791496560 T T T
0.8333333333123605 0.5000000000000000 0.0000000000000000 F F F
0.6666666666876395 0.6666666666876395 0.0000000000000000 F F F
0.8342751768706803 0.6671091429721240 0.1619770986975105 T T T
0.6673077023610385 0.8341505597131198 0.1619687885209637 T T T
0.8333333333123605 0.8333333333123605 0.0000000000000000 F F F
0.4315929954476401 0.5676622453318021 0.3126968767666341 T T T
0.5127388659590715 0.4918038624039694 0.3746750242326554 T T T
0.3773172475163558 0.6196597526995888 0.4842695374618884 T T T
0.6272254083304288 0.3726698310489057 0.2440934425380004 T T T
0.3583034425455959 0.6391831356396294 0.3964899238392943 T T T
0.5604084871526547 0.4478124346847349 0.4646995466481276 T T T

FS

Cu C H O
1.00000000000000
10.9033256753999996 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.9033256753999996 0.0000000000000000
0.0000000000000000 0.0000000000000000 10.6344418917999999
Cu C H O
36 2 2 2
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.1656183641702520 0.0009120206962821 0.1625777155000722 T T T
0.9996863978847994 0.1668664325953029 0.1627126800127553 T T T
0.1666666667033496 0.1666666667033496 0.0000000000000000 F F F
0.0000000000000000 0.3333333332966504 0.0000000000000000 F F F
0.1665743031880270 0.3330611318288907 0.1619518881803572 T T T
0.9991427312927184 0.4993331392748290 0.1625478197274055 T T T
0.1666666667033496 0.5000000000000000 0.0000000000000000 F F F
0.0000000000000000 0.6666666667033496 0.0000000000000000 F F F
0.1622367575357500 0.6677071395809152 0.1622162458447615 T T T
0.9991126624570652 0.8342478379006895 0.1625551841130585 T T T
0.1666666667033496 0.8333333332966504 0.0000000000000000 F F F
0.3333333332966504 0.0000000000000000 0.0000000000000000 F F F
0.5006544469543923 0.0008257786984203 0.1626075557627554 T T T
0.3329985705370204 0.1657798649206059 0.1628190670802992 T T T
0.5000000000000000 0.1666666667033496 0.0000000000000000 F F F
0.3333333332966504 0.3333333332966504 0.0000000000000000 F F F
0.5001192642486006 0.3299752870446936 0.1618319291567784 T T T
0.3334353045168431 0.4990121075085339 0.1676474627907450 T T T
0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
0.3333333332966504 0.6666666667033496 0.0000000000000000 F F F
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0.5000000000000000 0.8333333332966504 0.0000000000000000 F F F
0.6666666667033496 0.0000000000000000 0.0000000000000000 F F F
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0.6670816427661515 0.1661724664039810 0.1625402005455117 T T T
0.8333333332966504 0.1666666667033496 0.0000000000000000 F F F
0.6666666667033496 0.3333333332966504 0.0000000000000000 F F F
0.8337281909035029 0.3329582240493775 0.1625430453029703 T T T
0.6698268903690056 0.4999588078432516 0.1617648901991565 T T T
0.8333333332966504 0.5000000000000000 0.0000000000000000 F F F
0.6666666667033496 0.6666666667033496 0.0000000000000000 F F F
0.8341611197343570 0.6669487047425560 0.1627844198494415 T T T
0.6667821242038060 0.8332780704974725 0.1619951397918860 T T T
0.8333333332966504 0.8333333332966504 0.0000000000000000 F F F
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0.4841703392037808 0.5201356331287620 0.3972210108965136 T T T
0.3444777582969926 0.6509239316088790 0.4660718536578153 T T T
0.5514938920491012 0.4553852717559961 0.3518780932489524 T T T
0.3274867100251982 0.6671011635961941 0.3754455049486158 T T T
0.4749276522117104 0.5311597608130554 0.5130415835288753 T T T

Table S10. Atomic coordinates of IS, TS, and FS of Reaction 6 listed in Table S1.

Reaction 5: *COH–CHO+ H^++e^-→*CHOH–CHO on Cu-DAN via surface *H transfer

IS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  3  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2749572387050879  0.9309358175651332  0.1307200272892057 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8751501080392288  0.3456020029828772  0.1357551308583945 T T T
  0.2634815931144797  0.7336465136383843  0.1299711893578452 T T T
  0.4739818706573261  0.9374439313533059  0.1337955913696540 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8627555964959942  0.5345343412852757  0.1332729969493650 T T T
  0.6690931560936799  0.3343155246559910  0.1311943589054069 T T T
  0.2626812230223050  0.5320342042619988  0.1315451986884447 T T T
  0.4691716079585302  0.3362475670303962  0.1340905848774796 T T T
  0.2718924470193333  0.3378054394829134  0.1299484369986734 T T T
  0.6696488612914034  0.9358158570144874  0.1334306696769441 T T T
  0.8619844817741069  0.7316301092606330  0.1352203887486433 T T T
  0.8616993367101874  0.9290779634566980  0.1321924273005906 T T T
  0.3487031337339976  0.8666911791373820  0.2626600332986361 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3270136069881073  0.6682509215751307  0.2582034379080965 T T T
  0.5258094641424575  0.4654854835422800  0.2699303932074159 T T T
  0.3237140244110364  0.4614854223111029  0.2667075981255879 T T T
  0.5448858786777627  0.8715671824697988  0.2703917919363797 T T T
  0.7246765428582623  0.6607565931524024  0.2710393068565731 T T T
  0.7311235721136649  0.8605993506756376  0.2680183003764355 T T T
  0.7207303941835592  0.4627082748066372  0.2619705153250779 T T T
  0.4043436858119964  0.7693529867835289  0.3925332188421380 T T T
  0.2643794497590707  0.5400342043884944  0.3907244453060288 T T T
  0.5991413867677747  0.7827393555644692  0.4029587445011084 T T T
  0.4653714224704237  0.5410732536101805  0.3978640343613609 T T T
  0.4274329279271105  0.6530773893959864  0.5043931175693327 T T T
  0.1516565105472588  0.3984066741818298  0.3134586437001274 T T T
  0.0755438136805919  0.4183180571402835  0.2556512097609271 T T T
  0.0229727937080223  0.2359409269719859  0.3139386914057656 T T T
  0.2621399879992259  0.6715647057225248  0.3624420414101656 T T T
  0.1065282206019879  0.5118506484214487  0.2352913199894024 T T T
  0.1012729559487974  0.2824485251211821  0.3439176856858405 T T T
  0.9700699706660176  0.3330894831738468  0.2325332523352996 T T T
```

TS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  3  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2745307534447609  0.9298615095608592  0.1309321554590475  T  T  T
  0.4666644456187115  0.7333340047990546  0.1368027474874722  T  T  T
  0.6666644456187072  0.5333340047990589  0.1368027474874722  T  T  T
  0.8764478190503052  0.3482321636408392  0.1359267878986532  T  T  T
  0.2630953566803464  0.7323686092923913  0.1308908454540787  T  T  T
  0.4722172662871298  0.9366122270742764  0.1344089232323916  T  T  T
  0.4666644456187115  0.5333340047990589  0.1368027474874722  T  T  T
  0.6666644456187072  0.7333340047990546  0.1368027474874722  T  T  T
  0.8617433249048382  0.5347563643495657  0.1338672991999574  T  T  T
  0.6689819345952859  0.3339665236884587  0.1312835406777208  T  T  T
  0.2631513669131710  0.5324724753512612  0.1308226213865315  T  T  T
  0.4695337808317065  0.3365088954526411  0.1342129052315802  T  T  T
  0.2724905011652489  0.3384957840906558  0.1304537453366072  T  T  T
  0.6674108453579601  0.9353434886998487  0.1344972299225069  T  T  T
  0.8615102481353439  0.7323146450823637  0.1353568477072525  T  T  T
  0.8608358436417799  0.9291054021357308  0.1324960602512162  T  T  T
  0.3428225009847072  0.8618567717248081  0.2646348124972653  T  T  T
  0.5333313180231087  0.6666662410030355  0.2736054949749445  T  T  T
  0.3316553813241094  0.6682028583502269  0.2585970803972064  T  T  T
  0.5236197407222551  0.4652037606364730  0.2707541823322207  T  T  T
  0.3225122283220377  0.4646858744092153  0.2672150837109139  T  T  T
  0.5397395889743234  0.8684213109217959  0.2710582739617974  T  T  T
  0.7241555910629394  0.6601422972662520  0.2717666323089726  T  T  T
  0.7291023793183443  0.8595838509271293  0.2681348719960618  T  T  T
  0.7161362877696540  0.4604728123941494  0.2626990162062761  T  T  T
  0.3993094549602701  0.7736079410141741  0.3933126451651265  T  T  T
  0.2706285958830123  0.5408098449356201  0.3967147580905991  T  T  T
  0.5962160482939394  0.7801986035602223  0.4031410513077281  T  T  T
  0.4665785637422857  0.5449306454520448  0.3996123318659107  T  T  T
  0.4255346470464081  0.6583142936579496  0.5055330531912018  T  T  T
  0.1514108077489530  0.4070519444255158  0.3216997063256145  T  T  T
  0.0734494975317682  0.4285339992330197  0.2650052332992077  T  T  T
  0.0168623305830347  0.2493232267963118  0.3332586587035923  T  T  T
  0.1449965222050245  0.5204368281214775  0.4115591152718436  T  T  T
  0.1023278448725197  0.5227139395564944  0.2483799283185678  T  T  T
  0.1014423500522688  0.2929797104309962  0.3530695524907151  T  T  T
  0.9744353972614448  0.3420535793512579  0.2361307660873716  T  T  T
```

FS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  3  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2715003010494951  0.9267470601173382  0.1305958371233524 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8854925864756757  0.3584626882077612  0.1381377935205611 T T T
  0.2609672462036827  0.7285108702576125  0.1308641027294543 T T T
  0.4697196902106006  0.9353155085750878  0.1345632605051716 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8661339508299709  0.5401873980953772  0.1326392935679157 T T T
  0.6733705730926021  0.3377098542206333  0.1320968696936541 T T T
  0.2621232210770117  0.5286982534360950  0.1307874916080362 T T T
  0.4705838244007388  0.3371550897602982  0.1345849529866167 T T T
  0.2706427422541151  0.3364491697463526  0.1301755418519660 T T T
  0.6653122867565464  0.9353583694023820  0.1348431000932789 T T T
  0.8633471678512129  0.7342849411670848  0.1350017022026100 T T T
  0.8591208991520473  0.9290516775848724  0.1333393279338262 T T T
  0.3356673867822670  0.8548841632160956  0.2631420888549333 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3223541356273887  0.6559672015897690  0.2591199776152909 T T T
  0.5327029086500313  0.4686016386819827  0.2715563329194058 T T T
  0.3343236368247049  0.4627197970938926  0.2636587631058437 T T T
  0.5336770292007164  0.8660304875780103  0.2705636088116523 T T T
  0.7288041854313724  0.6661898199484104  0.2697720847736219 T T T
  0.7248038354040672  0.8612572139197083  0.2691747153781587 T T T
  0.7309323156604179  0.4718176755690248  0.2615816036231264 T T T
  0.3880036425476195  0.7703267915496561  0.3909219761730294 T T T
  0.2565943078318819  0.5285378264110914  0.3883273317117349 T T T
  0.5851913621810022  0.7804995176203077  0.4037801913148893 T T T
  0.4570065048601006  0.5405790081257892  0.3976162538796837 T T T
  0.4133944194189720  0.6523824029256242  0.5007014391540586 T T T
  0.0720475180117184  0.4076334290490687  0.3819724008632919 T T T
  0.0221089733606538  0.4327233689726996  0.3072964203584352 T T T
  0.0254269973788378  0.2539632798219378  0.3326842166971006 T T T
  0.0613943106499491  0.4436675579005697  0.4445334496969669 T T T
  0.0251686380002753  0.5200633870353409  0.3049942173581585 T T T
  0.0538045319981566  0.2919510883861496  0.3902116132352266 T T T
  0.9739612498582289  0.3563564328914799  0.2451775995757434 T T T
```

Table S11. Atomic coordinates of IS, TS, and FS of Reaction 5 listed in Table S1.

Reaction 6: *COH–CHO+ H^++e^-→*C–CHO on Cu-DAN via surface *H transfer

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2749572387050879  0.9309358175651332  0.1307200272892057 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8751501080392288  0.3456020029828772  0.1357551308583945 T T T
  0.2634815931144797  0.7336465136383843  0.1299711893578452 T T T
  0.4739818706573261  0.9374439313533059  0.1337955913696540 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8627555964959942  0.5345343412852757  0.1332729969493650 T T T
  0.6690931560936799  0.3343155246559910  0.1311943589054069 T T T
  0.2626812230223050  0.5320342042619988  0.1315451986884447 T T T
  0.4691716079585302  0.3362475670303962  0.1340905848774796 T T T
  0.2718924470193333  0.3378054394829134  0.1299484369986734 T T T
  0.6696488612914034  0.9358158570144874  0.1334306696769441 T T T
  0.8619844817741069  0.7316301092606330  0.1352203887486433 T T T
  0.8616993367101874  0.9290779634566980  0.1321924273005906 T T T
  0.3487031337339976  0.8666911791373820  0.2626600332986361 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3270136069881073  0.6682509215751307  0.2582034379080965 T T T
  0.5258094641424575  0.4654854835422800  0.2699303932074159 T T T
  0.3237140244110364  0.4614854223111029  0.2667075981255879 T T T
  0.5448858786777627  0.8715671824697988  0.2703917919363797 T T T
  0.7246765428582623  0.6607565931524024  0.2710393068565731 T T T
  0.7311235721136649  0.8605993506756376  0.2680183003764355 T T T
  0.7207303941835592  0.4627082748066372  0.2619705153250779 T T T
  0.4043436858119964  0.7693529867835289  0.3925332188421380 T T T
  0.2643794497590707  0.5400342043884944  0.3907244453060288 T T T
  0.5991413867677747  0.7827393555644692  0.4029587445011084 T T T
  0.4653714224704237  0.5410732536101805  0.3978640343613609 T T T
  0.4274329279271105  0.6530773893959864  0.5043931175693327 T T T
  0.1516565105472588  0.3984066741818298  0.3134586437001274 T T T
  0.0755438136805919  0.4183180571402835  0.2556512097609271 T T T
  0.0229727937080223  0.2359409269719859  0.3139386914057656 T T T
  0.2621399879992259  0.6715647057225248  0.3624420414101656 T T T
  0.1065282206019879  0.5118506484214487  0.2352913199894024 T T T
  0.1012729559487974  0.2824485251211821  0.3439176856858405 T T T
  0.9700699706660176  0.3330894831738468  0.2325332523352996 T T T
```

TS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2766753296932336  0.9305738362641733  0.1285479763820661  T  T  T
  0.4666644456031577  0.7333340047990546  0.1368027475005462  T  T  T
  0.6666644456031534  0.5333340047990589  0.1368027475005462  T  T  T
  0.8825178758874870  0.3525854871721421  0.1335193707457805  T  T  T
  0.2690355179355564  0.7354193947586154  0.1284383926880395  T  T  T
  0.4765384801487045  0.9401663796921227  0.1286946936902424  T  T  T
  0.4666644456031577  0.5333340047990589  0.1368027475005462  T  T  T
  0.6666644456031534  0.7333340047990546  0.1368027475005462  T  T  T
  0.8638458349467797  0.5362156394479385  0.1276778718818434  T  T  T
  0.6696596500683327  0.3353545623732757  0.1293389679103782  T  T  T
  0.2639728315250096  0.5288142885091887  0.1356974297276992  T  T  T
  0.4658965399515722  0.3313891099007478  0.1275101511184360  T  T  T
  0.2692722121463973  0.3344301523069930  0.1259006510015723  T  T  T
  0.6745982153229093  0.9406879577370759  0.1293720044095323  T  T  T
  0.8612692360833023  0.7316951596723982  0.1324398654829437  T  T  T
  0.8633699998491053  0.9307900696719642  0.1257579365707784  T  T  T
  0.3564710867139240  0.8679721741541542  0.2603397457550969  T  T  T
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  0.3339550799094866  0.4461779770324981  0.2651353759580388  T  T  T
  0.5501988717313040  0.8747227463490361  0.2592893325191525  T  T  T
  0.7217316969738050  0.6580612293872363  0.2755505595713146  T  T  T
  0.7395279193836402  0.8645719492200001  0.2622387331190765  T  T  T
  0.7379710274147797  0.4708707395894365  0.2600035579334374  T  T  T
  0.4642805678061777  0.7611929955249082  0.3894082494869124  T  T  T
  0.3012876970598128  0.5412287359158725  0.3903915345975264  T  T  T
  0.6588894853183263  0.7503228439989940  0.3985042999028963  T  T  T
  0.4988640785229919  0.5297027037692956  0.3908878612524163  T  T  T
  0.5004604734743765  0.6566398811214782  0.5042387037989258  T  T  T
  0.2097052112319146  0.4936707765450665  0.2717356574268423  T  T  T
  0.0834071252601503  0.4478571288219834  0.2686715299041044  T  T  T
  0.1918767416035243  0.5286409430758371  0.5672485571991110  T  T  T
  0.2920395873934075  0.6558292586785712  0.5331759729430655  T  T  T
  0.0445501097416646  0.4832109567453968  0.3175952775914572  T  T  T
  0.2645936488524119  0.5697032612334356  0.5315001253576105  T  T  T
  0.0110513984104420  0.3722935983693709  0.2125094123339619  T  T  T
```

FS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  3  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2731829895066407  0.9333091507936000  0.1304414487981246 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8844839633723388  0.3595133270023359  0.1386039072340100 T T T
  0.2662556927913377  0.7382295295453830  0.1288687148043082 T T T
  0.4713733706479514  0.9377636340362704  0.1334800918747687 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
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  0.6741852037629568  0.3372542021662746  0.1319746830994769 T T T
  0.2584246429098896  0.5264021517941578  0.1381397102527550 T T T
  0.4706689109523867  0.3358123845465387  0.1341964295244632 T T T
  0.2727390620021706  0.3345459689412506  0.1285262544267302 T T T
  0.6670577816128642  0.9378383417611704  0.1343091345522208 T T T
  0.8619190900230567  0.7343465570564935  0.1354399438248876 T T T
  0.8597123765888207  0.9301310706927138  0.1322659704099688 T T T
  0.3425843518699067  0.8685008147625205  0.2638015242913752 T T T
  0.5333313179997745  0.6666662410030355  0.2736054950010853 T T T
  0.3136308030884463  0.6680522452827820  0.2611681577493407 T T T
  0.5363043209664436  0.4647364600803867  0.2696437845320231 T T T
  0.3380988002768040  0.4498551122022579  0.2671475477334174 T T T
  0.5342127015013701  0.8657100163737939  0.2676594962445215 T T T
  0.7261449591691064  0.6641469536817476  0.2721246778975461 T T T
  0.7264964611795538  0.8624672713139764  0.2665104916905593 T T T
  0.7320931981736686  0.4705343972802679  0.2613948335366666 T T T
  0.4018171688233069  0.7803846943536763  0.3948180766515512 T T T
  0.3096123553011442  0.5559887384203561  0.3872244870182152 T T T
  0.5954475503560787  0.7853106338933865  0.4002240261359933 T T T
  0.4981028920281349  0.5508356344133490  0.4025813884328926 T T T
  0.4410876152178007  0.6620346869033661  0.5055085191585839 T T T
  0.2113095020164276  0.4929046182056642  0.2752435683784388 T T T
  0.0842445696412110  0.4249913725959378  0.2790954520835555 T T T
  0.0985740452177204  0.2976842838054491  0.5087917202980373 T T T
  0.9978521539811700  0.2808425083522703  0.5717209242337030 T T T
  0.0419807250117815  0.4134863955495169  0.3444463004654241 T T T
  0.0783814346865220  0.3397494110207233  0.5524948175668991 T T T
  0.0144483761403342  0.3754435910716315  0.2137013755827944 T T T
```

Table S12. Atomic coordinates of IS, TS, and FS of Reaction 7 listed in Table S1.

Reaction 7: *CHOH–CHO+ H^++e^-→*CH_2OH–CHO on Cu-DAN via surface *H transfer

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2768842633337026  0.9263701058982168  0.1319859884029393 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8814619781179763  0.3538842400109978  0.1368996987185896 T T T
  0.2601853987481614  0.7264692982260241  0.1290711299568778 T T T
  0.4747730081179445  0.9368374878746980  0.1346797826198278 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8637377554744010  0.5373618089428061  0.1333510255940112 T T T
  0.6708415204181082  0.3353572229363184  0.1315163021463490 T T T
  0.2614728532354219  0.5264142527478071  0.1290610850474772 T T T
  0.4705794933891757  0.3372568091794533  0.1350712605420796 T T T
  0.2711203734909837  0.3345145866781458  0.1300078827152449 T T T
  0.6703683354619134  0.9365236828446027  0.1338531443911362 T T T
  0.8628075100594271  0.7327259958495609  0.1352999237448195 T T T
  0.8621631386896529  0.9295123641366068  0.1317377457786914 T T T
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  0.3322299850869059  0.4608413538336575  0.2627001221647493 T T T
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  0.7353947009884829  0.8614700864028313  0.2679330252108892 T T T
  0.7239013618062736  0.4657516328293147  0.2620240526413571 T T T
  0.4065910308329426  0.7437584063430558  0.3873051505200079 T T T
  0.2423698948233720  0.5118004580200001  0.3870726091475440 T T T
  0.6081705903289361  0.7786286038786671  0.4047143548916508 T T T
  0.4487997989080419  0.5456829510160216  0.3977033782873480 T T T
  0.4425630559563447  0.6638301335319416  0.5139817829856133 T T T
  0.0584748752810936  0.3934315041799267  0.3828325202740581 T T T
  0.0103772485872298  0.4204575313371999  0.3081850986977471 T T T
  0.0107704016584024  0.2398159629369817  0.3326331272267211 T T T
  0.0141451595957280  0.5081606975800880  0.3065001061184824 T T T
  0.0474033490884412  0.4288318861851282  0.4455934243544923 T T T
  0.2874916578510464  0.7388447914169152  0.3390496791716815 T T T
  0.0384597508792987  0.2768717907704269  0.3904907920686352 T T T
  0.9631232522787602  0.3452687933413510  0.2450947157266563 T T T
```

TS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2762090528019860  0.9268521388648761  0.1317638917295824  T  T  T
  0.4666644456187115  0.7333340047990546  0.1368027474874722  T  T  T
  0.6666644456187072  0.5333340047990589  0.1368027474874722  T  T  T
  0.8703264889433930  0.3422857941158472  0.1328180779170704  T  T  T
  0.2630095656856550  0.7287482023117032  0.1316052816097734  T  T  T
  0.4755908123507301  0.9371001799443269  0.1334545252434286  T  T  T
  0.4666644456187115  0.5333340047990589  0.1368027474874722  T  T  T
  0.6666644456187072  0.7333340047990546  0.1368027474874722  T  T  T
  0.8646315669923613  0.5357049709345892  0.1321531409356810  T  T  T
  0.6680686702925908  0.3362511172446067  0.1324603522328909  T  T  T
  0.2637944727791444  0.5295598182287081  0.1324323410466271  T  T  T
  0.4674579154400220  0.3348801756254912  0.1329276312739459  T  T  T
  0.2710199210436064  0.3370806584627956  0.1307955722180187  T  T  T
  0.6726075397700411  0.9377534037223337  0.1322131141472142  T  T  T
  0.8616954165280170  0.7314932845908612  0.1372380002863965  T  T  T
  0.8648828255616996  0.9303254275175301  0.1300873386837008  T  T  T
  0.3534834312713863  0.8588307018021855  0.2626842587247638  T  T  T
  0.5333313180231087  0.6666662410030355  0.2736054949749445  T  T  T
  0.3159687633997231  0.6519072136302236  0.2627231830978201  T  T  T
  0.5312770310423403  0.4611885128658791  0.2679304296801592  T  T  T
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  0.5533085711333935  0.8744891349460522  0.2676977154254172  T  T  T
  0.7220897885771906  0.6607956461423442  0.2744100787988743  T  T  T
  0.7399278882453902  0.8642613896619945  0.2639810933742229  T  T  T
  0.7315433240487996  0.4713090904572151  0.2621592205727845  T  T  T
  0.4211720736183301  0.7730206848275349  0.3907187982000820  T  T  T
  0.3145664627405325  0.5548241431310460  0.3996842103816325  T  T  T
  0.6208620112734150  0.7899764210842715  0.3983080798040624  T  T  T
  0.4990293754584899  0.5480678754139806  0.4003350428801752  T  T  T
  0.4709809576730417  0.6730474276637771  0.5079214703528898  T  T  T
  0.0518748909469833  0.3664581257071153  0.3646459738246945  T  T  T
  0.0153949889783266  0.4021616606732116  0.2909944989881934  T  T  T
  0.9645742853723148  0.2058045596393630  0.3278408266958671  T  T  T
  0.0452496395252894  0.4978086066043228  0.2816615093411201  T  T  T
  0.0976276306173631  0.4260435523418025  0.4197619576974912  T  T  T
  0.2748063932238528  0.6610658254367560  0.3716693985659347  T  T  T
  0.0124707919147178  0.2484965739910724  0.3797247140322691  T  T  T
  0.9420286545880943  0.3207529033713045  0.2354140146984040  T  T  T
```

FS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  4  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2743659231457726  0.9251492809960306  0.1320908533464791 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8629821939165943  0.3368582690513640  0.1299021977515819 T T T
  0.2632242062210838  0.7272196741781962  0.1342780815550796 T T T
  0.4719085474449865  0.9356854878291168  0.1340998310271381 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8629579665638079  0.5338672105917504  0.1332002780098050 T T T
  0.6662190354911330  0.3365108783142655  0.1332405896921454 T T T
  0.2610460080355665  0.5297801602350909  0.1324718059937467 T T T
  0.4675323230089852  0.3378386289051335  0.1354040497204658 T T T
  0.2689612785744467  0.3356469257745357  0.1291832879302558 T T T
  0.6701235750021315  0.9391753506313359  0.1324182377192616 T T T
  0.8622207895055293  0.7325079704610094  0.1355079402532195 T T T
  0.8644301717613339  0.9311563892425198  0.1290514155560016 T T T
  0.3467311223532172  0.8524901290073614  0.2662337317267019 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3260430621395171  0.6520693875442434  0.2669808236040775 T T T
  0.5318989195102770  0.4692809868689175  0.2724424401526956 T T T
  0.3306874904437209  0.4594102559123397  0.2607151231805501 T T T
  0.5474397320411839  0.8731070523906956  0.2667127510620786 T T T
  0.7304338420316236  0.6676956653392224  0.2724625767460152 T T T
  0.7408172829563247  0.8694043965865339  0.2604004569777698 T T T
  0.7274325932197885  0.4719892652468760  0.2640083623697005 T T T
  0.4232049117006613  0.7766828230537903  0.3963612748069681 T T T
  0.3914115100534463  0.5719566652479930  0.3940603934536772 T T T
  0.6287234739144756  0.8090938234778821  0.3937976938634589 T T T
  0.5968728549970976  0.6031995480160363  0.4053099994577300 T T T
  0.5090284357727921  0.6919901526091011  0.5122887127973696 T T T
  0.0090509658467734  0.3420127886697791  0.3849727770203366 T T T
  0.9831454433678312  0.3800863533159702  0.3000203163938397 T T T
  0.9116481838910628  0.1792635980116119  0.3422959442962076 T T T
  0.0232692632539337  0.4777496885958367  0.2876739370030019 T T T
  0.9796156728810628  0.3820705262083626  0.4371362649340806 T T T
  0.1087519519254265  0.3881817541679150  0.3909951857726459 T T T
  0.9562496071253208  0.2174950510887692  0.3959795911433197 T T T
  0.9180357014301158  0.3043672677706052  0.2449108564294740 T T T
```

Table S13. Atomic coordinates of IS, TS, and FS of Reaction 8 listed in Table S1.

Reaction 8: *$CH_2OH–CHO$+ H^++e^-→*$CH_2OH–CH_2O$ on Cu-DAN via surface *H transfer

IS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  5  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2761236519117876  0.9278198311943484  0.1327233204184499 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8618793007888876  0.3358245339651861  0.1301661018757480 T T T
  0.2663797728966663  0.7316795867060356  0.1327196913245399 T T T
  0.4736200859267635  0.9371571497732512  0.1343784281192424 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
  0.8608241542170086  0.5325903660902195  0.1341499003968534 T T T
  0.6654347127332602  0.3354039902319105  0.1327416466842824 T T T
  0.2580862789839746  0.5286763141635877  0.1315618197512199 T T T
  0.4679771093216881  0.3380139687097364  0.1360827147416684 T T T
  0.2706183363415890  0.3338187958699417  0.1285086055384095 T T T
  0.6712073760819974  0.9398540937026104  0.1319600995990565 T T T
  0.8618965699893191  0.7326850497112367  0.1354466818458297 T T T
  0.8655734476262216  0.9315875326188950  0.1286367334122483 T T T
  0.3486553999039206  0.8521218609935657  0.2661965272922538 T T T
  0.5333313179997745  0.6666662410030355  0.2736054950010853 T T T
  0.3218100110889323  0.6490240545779831  0.2677532909866263 T T T
  0.5254655764253243  0.4677396782528800  0.2740325986736656 T T T
  0.3274513065068088  0.4576459046113668  0.2606002569263587 T T T
  0.5492292418175059  0.8720095173576039  0.2660660684965180 T T T
  0.7297906026016708  0.6663681231691140  0.2722053247047242 T T T
  0.7422064188342645  0.8689042619638054  0.2596890268135197 T T T
  0.7163182955247975  0.4655079784876336  0.2650235004820248 T T T
  0.4258278598243272  0.7722354840751254  0.3945604981629520 T T T
  0.3952751333454403  0.5669082310967621  0.3951111664309668 T T T
  0.6320991481058638  0.8077789158225698  0.3937363048430915 T T T
  0.5997808732466814  0.6021882778262472  0.4056268948864898 T T T
  0.5100882853944445  0.6922356688235982  0.5122924292638521 T T T
  0.0044120868068559  0.3336351872336645  0.3859114966795592 T T T
  0.9755782631689500  0.3739633513463833  0.3030003725794074 T T T
  0.9132259228097204  0.1727097351220463  0.3385035666934232 T T T
  0.0087904226688885  0.4712156363937767  0.2947161736355418 T T T
  0.9719418128100494  0.3675794954906367  0.4402202063617894 T T T
  0.1041213090469381  0.3853504643949608  0.3919455029446464 T T T
  0.2202473190227991  0.4992604912413686  0.2407693439332338 T T T
  0.9575643503406566  0.2092846050273173  0.3925855583352295 T T T
  0.9150496520480716  0.3003870233457944  0.2452865406171894 T T T
```

TS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  5  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2775545662328540  0.9228353890411592  0.1334078947563524  T  T  T
  0.4666644456120537  0.7333340047990546  0.1368027474930713  T  T  T
  0.6666644456120494  0.5333340047990589  0.1368027474930713  T  T  T
  0.8766927727345930  0.3510556565244288  0.1331325732304071  T  T  T
  0.2648729348551537  0.7254605100439412  0.1330072391554513  T  T  T
  0.4759588283108025  0.9367565272308778  0.1347475904347542  T  T  T
  0.4666644456120537  0.5333340047990589  0.1368027474930713  T  T  T
  0.6666644456120494  0.7333340047990546  0.1368027474930713  T  T  T
  0.8609806949994184  0.5361187899933771  0.1352096266764411  T  T  T
  0.6698400569350571  0.3354758913144252  0.1322387688301181  T  T  T
  0.2580313665427508  0.5250541138666838  0.1304666244418921  T  T  T
  0.4706105520417468  0.3379498967701501  0.1361263964225759  T  T  T
  0.2709567471192422  0.3299415327180311  0.1270319169408700  T  T  T
  0.6730893532603237  0.9392623732461318  0.1316530609758570  T  T  T
  0.8625463761826326  0.7344449829522599  0.1351547786709444  T  T  T
  0.8678127304746265  0.9334117848891652  0.1280401907030244  T  T  T
  0.3524658750469685  0.8422290569421838  0.2654845081550919  T  T  T
  0.5333313180131043  0.6666662410030355  0.2736054949861355  T  T  T
  0.3163405704100769  0.6354528395215183  0.2669589426113659  T  T  T
  0.5192818215193151  0.4658614035200854  0.2741301145886325  T  T  T
  0.3145102151645132  0.4459560153075279  0.2588234654275842  T  T  T
  0.5570203490055783  0.8745887183917127  0.2666081550271251  T  T  T
  0.7299583364776656  0.6645144376746327  0.2705412604259360  T  T  T
  0.7482071725670791  0.8687095265079027  0.2593829218781218  T  T  T
  0.7115645522470216  0.4615233739177669  0.2651769516457628  T  T  T
  0.4301472165473186  0.7594956688857349  0.3900674571405083  T  T  T
  0.3979607366568985  0.5521108543447543  0.3919903912994750  T  T  T
  0.6396697650242156  0.8064107883244881  0.3939088857384734  T  T  T
  0.6061485052120664  0.6001554652616332  0.4041791024556071  T  T  T
  0.5118291308632839  0.6829481273736832  0.5087997574788410  T  T  T
  0.0344981605311752  0.3716649705200400  0.3768977972915147  T  T  T
  0.0410840671689165  0.4205863157855325  0.2852852448429355  T  T  T
  0.9514395137327949  0.2162987871934216  0.3230013068056860  T  T  T
  0.0566984090896981  0.5132862484437531  0.2818366431018423  T  T  T
  0.9661350278320844  0.3860750059098446  0.4113100781732704  T  T  T
  0.1195337104765877  0.4221502106707982  0.4128366275776555  T  T  T
  0.1801799245763534  0.4674033825845426  0.2564780213834455  T  T  T
  1.0002619952624454  0.2489367332468920  0.3760657999682075  T  T  T
  0.9682359748813840  0.3414592732540453  0.2300538329162405  T  T  T
```

FS

```
Cu  C  H  O
  1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu  C  H  O
55  2  5  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2756720025716634  0.9236044371451840  0.1325433991272673 T T T
  0.4666644456187115  0.7333340047990546  0.1368027474874722 T T T
  0.6666644456187072  0.5333340047990589  0.1368027474874722 T T T
  0.8616335111293771  0.3387953289014125  0.1301854000956983 T T T
  0.2636079854157238  0.7255383613534767  0.1342986623259290 T T T
  0.4740902423861987  0.9364123258434672  0.1342768273690592 T T T
  0.4666644456187115  0.5333340047990589  0.1368027474874722 T T T
  0.6666644456187072  0.7333340047990546  0.1368027474874722 T T T
  0.8707147581596307  0.5436122895935079  0.1321671123730218 T T T
  0.6558759480025973  0.3314017074198691  0.1301412957587763 T T T
  0.2603223349461531  0.5278145711324801  0.1322920356853330 T T T
  0.4649121274882424  0.3375837405774271  0.1360433389855049 T T T
  0.2681237888407114  0.3342116179046336  0.1288233898106571 T T T
  0.6722276497998285  0.9404802202511902  0.1320909311300175 T T T
  0.8618263001920708  0.7347778079194587  0.1351792693694261 T T T
  0.8662293243010195  0.9328247647625436  0.1285594946636733 T T T
  0.3500751541295435  0.8500544612779126  0.2655051150450474 T T T
  0.5333313180231087  0.6666662410030355  0.2736054949749445 T T T
  0.3254414398205130  0.6472590874364180  0.2665086584928069 T T T
  0.5378148315121434  0.4682748703729230  0.2714752004652617 T T T
  0.3342537775339245  0.4557777477332600  0.2607159580251618 T T T
  0.5528228697605423  0.8750010902902119  0.2663701473952645 T T T
  0.7303288189889073  0.6654770881367615  0.2720240561334797 T T T
  0.7447796791025745  0.8690325285354404  0.2599969937825141 T T T
  0.7320878058340610  0.4672836818856664  0.2647205284984930 T T T
  0.4274317016763530  0.7743306999848463  0.3934279115376569 T T T
  0.3897252700263955  0.5677033790421474  0.3941047115411169 T T T
  0.6335321588178053  0.8084807887630396  0.3935434452485014 T T T
  0.5957476555672943  0.6000402952215469  0.4047642382871205 T T T
  0.5101260044072872  0.6906780731063347  0.5108601492892423 T T T
  0.9395633605272764  0.3595203960751032  0.3579163096785259 T T T
  0.9711799291867348  0.4661808479222064  0.2988164674761227 T T T
  0.8403444230093896  0.2132014517223341  0.2885433844531506 T T T
  0.9870831449397820  0.5445342485872543  0.3387246249737805 T T T
  0.8590990469942943  0.3385062581709525  0.3971160737122768 T T T
  0.0147609949917773  0.3834348237471397  0.4032952411090668 T T T
  0.0548272655391017  0.4904722369423264  0.2625338783565703 T T T
  0.9224743084262468  0.2561018844129628  0.3106071311647022 T T T
  0.8752071997042600  0.4376734745491226  0.2375647728796312 T T T
```

Table S14. Atomic coordinates of IS, TS, and FS of Reaction 9 listed in Table S1.

Reaction 9: $*CH_2OH–CH_2O+ H^+ + e^- \rightarrow CH_2OH–CH_3 + *O$ on Cu-DAN via surface *H transfer

IS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  6  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2744366393428607  0.9257087469915096  0.1320078141484228 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8582300728614861  0.3360903791083737  0.1301203999752996 T T T
  0.2645728620329414  0.7283313265232871  0.1337608814578433 T T T
  0.4720536622179538  0.9361657049862592  0.1336345825205599 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
  0.8694984896194502  0.5402863602253558  0.1309881900118947 T T T
  0.6515068779775574  0.3263117390964216  0.1323757735330723 T T T
  0.2612344478221794  0.5301123289773310  0.1330959665057073 T T T
  0.4617934197909201  0.3336845062759491  0.1414202176278924 T T T
  0.2690660870073077  0.3367342231745249  0.1293377488107725 T T T
  0.6706932676348192  0.9398997095808946  0.1327215686746877 T T T
  0.8623396892252876  0.7333617280805175  0.1348631903820176 T T T
  0.8640994974575894  0.9305563927154455  0.1294337164755407 T T T
  0.3460413838375380  0.8540087823658735  0.2655669290765321 T T T
  0.5333313179997745  0.6666662410030355  0.2736054950010853 T T T
  0.3275412939960604  0.6525984182022815  0.2667653491838564 T T T
  0.5423787208358840  0.4746344586181326  0.2740828674486979 T T T
  0.3372378832549888  0.4603540068482996  0.2622890860764242 T T T
  0.5466501736429041  0.8742852579349778  0.2658945953359768 T T T
  0.7323516432707685  0.6690013203240841  0.2718395771708835 T T T
  0.7396158168906993  0.8679148603763950  0.2611620657756177 T T T
  0.7433739395951015  0.4794614628248251  0.2658602189489243 T T T
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  0.3932716519111416  0.5774732192184687  0.3950767601211713 T T T
  0.6250131702393575  0.8146463828715327  0.3937545023568692 T T T
  0.6007007757116833  0.6125485886106884  0.4068252135890286 T T T
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  0.9437351048668278  0.3584963890562798  0.3610434801424955 T T T
  0.9732371361510824  0.4604827819219401  0.2976746049752621 T T T
  0.8441195367581296  0.2126925864953398  0.2916542506525999 T T T
  0.5228901283418337  0.2580227114329180  0.1837016055680720 T T T
  0.9943041349470728  0.5424839246110167  0.3347514371056869 T T T
  0.8660726739853926  0.3416884233845601  0.4020985768816490 T T T
  0.0215803039641006  0.3856958202172941  0.4044674846096891 T T T
  0.0536924231353299  0.4794671559045026  0.2590905723363494 T T T
  0.9233889503498970  0.2507998946860574  0.3188118177430584 T T T
  0.8739342189570407  0.4314289074205752  0.2392251491843614 T T T
```

TS

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Cu   C   H   O
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  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  6  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
  0.0000000000000000  0.2000000000000028  0.0000000000000000  F  F  F
  0.0000000000000000  0.3999999999999986  0.0000000000000000  F  F  F
  0.0000000000000000  0.6000000000000014  0.0000000000000000  F  F  F
  0.0000000000000000  0.7999999999999972  0.0000000000000000  F  F  F
  0.2000000000000028  0.0000000000000000  0.0000000000000000  F  F  F
  0.2000000000000028  0.2000000000000028  0.0000000000000000  F  F  F
  0.2000000000000028  0.3999999999999986  0.0000000000000000  F  F  F
  0.2000000000000028  0.6000000000000014  0.0000000000000000  F  F  F
  0.2000000000000028  0.7999999999999972  0.0000000000000000  F  F  F
  0.3999999999999986  0.0000000000000000  0.0000000000000000  F  F  F
  0.3999999999999986  0.2000000000000028  0.0000000000000000  F  F  F
  0.3999999999999986  0.3999999999999986  0.0000000000000000  F  F  F
  0.3999999999999986  0.6000000000000014  0.0000000000000000  F  F  F
  0.3999999999999986  0.7999999999999972  0.0000000000000000  F  F  F
  0.6000000000000014  0.0000000000000000  0.0000000000000000  F  F  F
  0.6000000000000014  0.2000000000000028  0.0000000000000000  F  F  F
  0.6000000000000014  0.3999999999999986  0.0000000000000000  F  F  F
  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
  0.6000000000000014  0.7999999999999972  0.0000000000000000  F  F  F
  0.7999999999999972  0.0000000000000000  0.0000000000000000  F  F  F
  0.7999999999999972  0.2000000000000028  0.0000000000000000  F  F  F
  0.7999999999999972  0.3999999999999986  0.0000000000000000  F  F  F
  0.7999999999999972  0.6000000000000014  0.0000000000000000  F  F  F
  0.7999999999999972  0.7999999999999972  0.0000000000000000  F  F  F
  0.2757634503209447  0.9245244526846964  0.1288281706361248  T  T  T
  0.4666644456000029  0.7333340047999997  0.1368027474999991  T  T  T
  0.6666644455999986  0.5333340047999968  0.1368027474999991  T  T  T
  0.8699991874356819  0.3308794638099289  0.1221901425777182  T  T  T
  0.2643744093620456  0.7266162447145027  0.1306106128498220  T  T  T
  0.4732084320997345  0.9347574707548032  0.1307713339885007  T  T  T
  0.4666644456000029  0.5333340047999968  0.1368027474999991  T  T  T
  0.6666644455999986  0.7333340047999997  0.1368027474999991  T  T  T
  0.8646574515717305  0.5338546104564008  0.1300109292731049  T  T  T
  0.6601977965049272  0.3313730691987100  0.1308974591233575  T  T  T
  0.2609859799947373  0.5275077939893738  0.1291156382887337  T  T  T
  0.4666214349245646  0.3375582070534683  0.1305974812837548  T  T  T
  0.2681334454766005  0.3340860664619403  0.1254219706502784  T  T  T
  0.6727551964288868  0.9385887390036880  0.1293371853950349  T  T  T
  0.8617806718055266  0.7311866356730008  0.1314128111247255  T  T  T
  0.8657276713809261  0.9308600764553980  0.1254077219649425  T  T  T
  0.3502503196643935  0.8487757465695928  0.2631042664245554  T  T  T
  0.5333313180000019  0.6666662410000015  0.2736054949999982  T  T  T
  0.3213998514535610  0.6448498094384922  0.2649010357572685  T  T  T
  0.5330364037059596  0.4678189402460641  0.2702545826234437  T  T  T
  0.3309150050279610  0.4550486986664333  0.2588456980323056  T  T  T
  0.5552382164472981  0.8781285715214756  0.2650464411121765  T  T  T
  0.7300792026479522  0.6614231789655369  0.2728590654772008  T  T  T
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  0.7472654048985021  0.4666630220487892  0.2816881954318803  T  T  T
  0.4282743903988565  0.7712515438693422  0.3902541592434516  T  T  T
  0.3888080913863791  0.5642681794322457  0.3928604119077492  T  T  T
  0.6353609794893820  0.8100774766063001  0.3931605367392632  T  T  T
  0.5967451160429079  0.6012096049537409  0.4043938605837564  T  T  T
  0.5101395985739186  0.6888790484745534  0.5088779024639463  T  T  T
  0.7838693930862850  0.3325954469970556  0.4240954507872289  T  T  T
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  0.8060502644819487  0.3013098322486332  0.3018625196682708  T  T  T
  0.7234173148610431  0.5219481698259989  0.3608139391638432  T  T  T
  0.8023652414301948  0.5033192708825294  0.4610442024463445  T  T  T
  0.6880586006467192  0.2779769592043795  0.4432742875685116  T  T  T
  0.8362860872408505  0.3384826412653301  0.4835010252729776  T  T  T
  0.9091918510904911  0.5172088926765318  0.3802856430883975  T  T  T
  0.8144029416534045  0.2726808632188301  0.3601990738603820  T  T  T
  0.7997731351685335  0.3782489437909359  0.2103970927387993  T  T  T
```

FS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  6  2
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2775379839499419  0.9233865078508138  0.1330000619368655 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8635210701849614  0.3330009994386119  0.1266835065177122 T T T
  0.2632422750338969  0.7246379508662281  0.1344226265725328 T T T
  0.4759155207694119  0.9370793779099720  0.1344045719731181 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
  0.8668362197742544  0.5371993444258868  0.1339337158697246 T T T
  0.6598085826974381  0.3316231819964185  0.1338496263362990 T T T
  0.2593984124177633  0.5270074817571568  0.1315513592063421 T T T
  0.4665002368143330  0.3378635497964166  0.1350331963905259 T T T
  0.2673618317007911  0.3328800053235535  0.1279915233198526 T T T
  0.6738789839808194  0.9416251210983836  0.1316126413220370 T T T
  0.8623759090583770  0.7326146733952241  0.1347455268055910 T T T
  0.8672362485932450  0.9324144496009684  0.1277953729220505 T T T
  0.3526993334296759  0.8482798978495998  0.2653854651469106 T T T
  0.5333313179997745  0.6666662410030355  0.2736054950010853 T T T
  0.3236377489369072  0.6439590768945407  0.2664515945783989 T T T
  0.5326518646139627  0.4687878444001297  0.2719851620886350 T T T
  0.3301298694514506  0.4530429090371841  0.2590454927636089 T T T
  0.5573861922523281  0.8773018085774157  0.2662989776086173 T T T
  0.7313751546650880  0.6671224664744804  0.2714970606287361 T T T
  0.7473462455059243  0.8694813364933890  0.2586910712662308 T T T
  0.7268350721723220  0.4726826566520535  0.2716280289181344 T T T
  0.4323719429785368  0.7696326923892878  0.3915437291312154 T T T
  0.3924180194187462  0.5618607314836839  0.3928584244097783 T T T
  0.6404394387499245  0.8103129319755967  0.3937299039933084 T T T
  0.6019562611125300  0.5997232266545831  0.4032875728441005 T T T
  0.5144142786038537  0.6857572384206611  0.5087350916187374 T T T
  0.8906491994459922  0.1901027322087174  0.4655302985440436 T T T
  0.9278020482013972  0.2930992493231870  0.4016511442491482 T T T
  0.8039089215643681  0.0661825062119152  0.3754601816164663 T T T
  0.8542926470777089  0.2761246685192176  0.3564165031508429 T T T
  0.9518179057257986  0.3769641410225075  0.4367449254538479 T T T
  0.8152070368931169  0.1795056405609469  0.5067382812544913 T T T
  0.9652459557473704  0.2073862549541124  0.5096412478398552 T T T
  0.0058541626334373  0.3078856210735467  0.3626182614955770 T T T
  0.8593249286250998  0.0780870076710802  0.4232642250024882 T T T
  0.8029121628213129  0.3917128436138595  0.2164642966482045 T T T
```

Table S15. Atomic coordinates of IS, TS, and FS of Reaction 10 listed in Table S1.

Reaction 10: $*CH_2OH–CH_2O + H^+ + e^- \rightarrow *CH_2OH–CH_2OH$ on Cu-DAN via H-shuttling

IS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
  -6.4291002405000004  11.1357880710000003   0.0000000000000000
   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
55  2  8  3
Selective dynamics
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000 F F F
  0.0000000000000000  0.2000000000000028  0.0000000000000000 F F F
  0.0000000000000000  0.3999999999999986  0.0000000000000000 F F F
  0.0000000000000000  0.6000000000000014  0.0000000000000000 F F F
  0.0000000000000000  0.7999999999999972  0.0000000000000000 F F F
  0.2000000000000028  0.0000000000000000  0.0000000000000000 F F F
  0.2000000000000028  0.2000000000000028  0.0000000000000000 F F F
  0.2000000000000028  0.3999999999999986  0.0000000000000000 F F F
  0.2000000000000028  0.6000000000000014  0.0000000000000000 F F F
  0.2000000000000028  0.7999999999999972  0.0000000000000000 F F F
  0.3999999999999986  0.0000000000000000  0.0000000000000000 F F F
  0.3999999999999986  0.2000000000000028  0.0000000000000000 F F F
  0.3999999999999986  0.3999999999999986  0.0000000000000000 F F F
  0.3999999999999986  0.6000000000000014  0.0000000000000000 F F F
  0.3999999999999986  0.7999999999999972  0.0000000000000000 F F F
  0.6000000000000014  0.0000000000000000  0.0000000000000000 F F F
  0.6000000000000014  0.2000000000000028  0.0000000000000000 F F F
  0.6000000000000014  0.3999999999999986  0.0000000000000000 F F F
  0.6000000000000014  0.6000000000000014  0.0000000000000000 F F F
  0.6000000000000014  0.7999999999999972  0.0000000000000000 F F F
  0.7999999999999972  0.0000000000000000  0.0000000000000000 F F F
  0.7999999999999972  0.2000000000000028  0.0000000000000000 F F F
  0.7999999999999972  0.3999999999999986  0.0000000000000000 F F F
  0.7999999999999972  0.6000000000000014  0.0000000000000000 F F F
  0.7999999999999972  0.7999999999999972  0.0000000000000000 F F F
  0.2752303944766232  0.9263359656921808  0.1301153490706918 T T T
  0.4666644456031577  0.7333340047990546  0.1368027475005462 T T T
  0.6666644456031534  0.5333340047990589  0.1368027475005462 T T T
  0.8545743282796847  0.3333469135437325  0.1303676321528229 T T T
  0.2682822594659300  0.7326501781691810  0.1365413568420741 T T T
  0.4741982126658023  0.9344004380957902  0.1324216036979791 T T T
  0.4666644456031577  0.5333340047990589  0.1368027475005462 T T T
  0.6666644456031534  0.7333340047990546  0.1368027475005462 T T T
  0.8652753651327058  0.5374113739578591  0.1310545448074178 T T T
  0.6468236552719199  0.3226605321043938  0.1330326819259660 T T T
  0.2615767367688727  0.5322797571850801  0.1331806255079303 T T T
  0.4593307370485910  0.3313632145452218  0.1410923288964443 T T T
  0.2685007721007158  0.3375545346299040  0.1294594853564495 T T T
  0.6742603994476639  0.9414422909065310  0.1322231547749926 T T T
  0.8620180535622982  0.7335269980148659  0.1351635213331809 T T T
  0.8670747331774857  0.9319923705029102  0.1281968981917073 T T T
  0.3583994239358973  0.8682957235667612  0.2696506011080131 T T T
  0.5333313179997745  0.6666662410030355  0.2736054950010853 T T T
  0.3312343802005254  0.6602757896688132  0.2677177967682297 T T T
  0.5381304692258596  0.4712494010898286  0.2721503981390175 T T T
  0.3343107668208665  0.4627393952531190  0.2611976837157955 T T T
  0.5546520437929250  0.8733061963723471  0.2658291367501808 T T T
  0.7300267009014604  0.6664417888046522  0.2722637038914287 T T T
  0.7475123838235719  0.8698902985245337  0.2594737651793512 T T T
  0.7352320553837279  0.4732795317225998  0.2666569122243488 T T T
  0.4352855329002502  0.7815409247424704  0.3969439205760735 T T T
  0.3915240303180250  0.5741833506062360  0.3951781868567371 T T T
  0.6377237258320959  0.8089669945556817  0.3928927745611411 T T T
  0.5965327898524324  0.6003238797633668  0.4053270733379669 T T T
  0.5162015444752682  0.6942264241604830  0.5117621525768934 T T T
  0.9402511749769648  0.3528227385312556  0.3564602049625749 T T T
  0.9662361837111290  0.4588663669934679  0.2984018110398110 T T T
  0.8475504677588446  0.2077069938537733  0.2839572390554156 T T T
  0.4405736584575494  0.1075672672590930  0.2762459783700361 T T T
  0.5013302300109148  0.0681642421409062  0.3465346431851808 T T T
  0.9811818533647404  0.5359868164690105  0.3392387244268551 T T T
  0.8595226364499621  0.3274178060902465  0.3967153320490787 T T T
  0.0169653532968931  0.3800841891648614  0.4010093553690381 T T T
  0.0490835787479282  0.4858107595994356  0.2603808129015729 T T T
  0.5132122262278708  0.2462520026865973  0.1799104008608621 T T T
  0.9283129749168602  0.2519666002883865  0.3085105608505694 T T T
  0.8677634096021904  0.4292733607225207  0.2391139970147138 T T T
  0.4227370165011188  0.0488325778579263  0.3234360195027663 T T T
```

TS

```
Cu   C   H   O
   1.00000000000000
  12.8585004805000001   0.0000000000000000   0.0000000000000000
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   0.0000000000000000   0.0000000000000000  15.2994003295999992
Cu   C   H   O
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Selective dynamics
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  0.6000000000000014  0.6000000000000014  0.0000000000000000  F  F  F
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Cu   C   H   O
55  2  8  3
Selective dynamics
Direct
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Supplementary References

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