ECR Voltage Assumptions

-2V ideal case from Joshua’s recommendation (This likely comes from the direct reduction of CO2 of one-electron transfer to form the CO2 anion radical (CO2⋅–), which has a negative formal redox potential of −1.97 V against SHE)

Table of Standard Potential E0 for Products

|  |  |  |
| --- | --- | --- |
| Product | ΔH (combustion) in kJ/mol | E0in V [] |
| Acetaldehyde | -1188 | -1.176 |
| Acetic Acid | -875 | -1.131 |
| Ethanol | -1367 | -1.145 |
| Ethylene Glycol | -1184 | -1.44 [] |
| Formic Acid | -254 | -1.4 |
| Glycolaldehyde | -1042 | -1.344 [] |
| Methanol | -727 | -1.213 |
| Carbon Monoxide | -283 | -1.333 |

**According to Sun Z, Ma T, Tao H, Fan Q, Han B (2017)**. ["Fundamentals and Challenges of Electrochemical CO2 Reduction Using Two-Dimensional Materials](https://doi.org/10.1016%2Fj.chempr.2017.09.009)”

* Using catalysts, we can bypass CO2 radical formation using proton assisted multiple electron transfer.

Ethanol

2CO2+12H++12e−→C2H5OH+3H2O E0redox=−0.329V

2CO2+9H2O+12e−→C2H5OH+12OH− E0redox=−1.157V

Formic Acid

CO2+2H++2e−→HCOOH E0redox=−0.610V

CO2+2H2O+2e−→HCOOH−+OH− E0redox=−1.491V

Methanol

CO2+6H++6e−→CH3OH+H2O E0redox=−0.380V

CO2+5H2O+6e−→CH3OH+6OH− E0redox=−1.225V

Carbon Monoxide

CO2+2H++2e−→CO+H2O E0redox=−0.530V

CO2+2H2O+2e−→CO+2OH− E0redox=−1.347V

Acetaldehyde has been produced at less negative potentials than methane (which is CO2+8H++8e−→CH4+2H2O E0redox=−0.240V or CO2+6H2O+8e−→CH4+8OH− E0redox=−1.072V), especially at high pH and on copper-based catalysts.

Acetic Acid/Acetate has been reported at around -0.8 to -1.0 V on N-doped nanodiamond at 91.2-91.8% FE.

**Despite the alcohols having lower E0, due to thermodynamic barriers, simpler 1C compounds (CO/HCOOH,HCHO) are more thermodynamically favourable**

According to Huang at al. (2022) <https://doi.org/10.1002/anie.202210985>

* Faradaic efficiency of C1 CO2RR products (mainly CO) reached up to 97% FE, although potentially requiring more voltage? (-0.8 to 2.4 V stated)

According to Greenblatt, J. B., Miller, D. J., Ager, J. W., Houle, F. A. & Sharp, I. D. The Technical and Energetic Challenges of Separating (Photo)Electrochemical Carbon Dioxide Reduction Products. Joule 2, 381–420 (2018)

* Most of the C1 – C3 eCO2RR products have a general E0 of -1.06 to -1.44, with the exception of CO and formate/FA, which require an additional ~1.0V of overpotential (likely due to kinetic reaction barriers)

Moreover, if the electrolyte pH is known, the RHE can be related to the SHE scale by Nernst equation: 12,13,15 E\_SHE = E\_RHE + 0.059 · pH