Bio-Inspired CO₂ Reduction by a Rhenium Tricarbonyl Bipyridine Based Catalyst Appended to Amino Acids and Peptidic Platforms: Incorporating Proton Relays and Hydrogen-Bonding Functional Groups

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Supporting Information

 Table S1: Crystal data for complex 1.

Complex	1
Empirical formula	C16H13CIN3O4Re
Formula weight	532.94
Temperature/K	273.15
Crystal system	monoclinic
Space group	P21/c
a/Å	11.1768(8)
b/Å	17.5414(15)
c/Å	9.0952(7)
α/°	90.00
β/°	92.607(4)
V/°	90.00
Volume/Å ³	1781.3(2)
z	4
ρ_{calc} (mg/mm ³)	1.987
Absorption coefficient mm ⁻¹	6.997
F(000)	1016.0
20 range for data collection	3.64 to 52.86°
Index ranges	-13 ≤ h ≤ 13, -21 ≤ k ≤ 19, -11 ≤ l ≤ 11
Reflections collected	9078
Independent reflections	3558 [Rint = 0.0645, Rsigma = 0.0922]
Data/restraints/parameters	3558/0/203
Goodness-of-fit on F ²	1.043
Final R indexes [I>=2o (I)]	R1 = 0.0643, wR2 = 0.1264
Final R indexes [all data]	R1 = 0.1196, wR2 = 0.1466
Largest diff. peak and hole (e Å-3)	2.88, -1.59