

## Supplementary

Thermodynamic data, adapted from references <sup>16, 32</sup>:

I: Thermodynamic data, gas phase

Species	Vibrational parameters	Ground state energy
CO <sub>2,g</sub>	B=0.39 cm <sup>-1</sup> , σ=2, ν=1340, 667(2), 2350 cm <sup>-1</sup>	-433 kJ·mol <sup>-1</sup>
CO <sub>g</sub>	B=1.90 cm <sup>-1</sup> , σ=1, ν=2170 cm <sup>-1</sup>	-132 kJ·mol <sup>-1</sup>

II: Thermodynamic data, adsorbed species

Copper plane	Species	Vibrational parameters	Ground state energy
111,100	CO <sub>2</sub> <sup>*</sup>	ν=410, 14(2), 1343, 667(2), 2349 cm <sup>-1</sup>	-463 kJ·mol <sup>-1</sup>
111,100	O <sup>*</sup>	ν=391, 508(2) cm <sup>-1</sup>	-243 kJ·mol <sup>-1</sup>
111,100	CO <sup>*</sup>	ν=330, 17(2), 2077 cm <sup>-1</sup>	-181 kJ·mol <sup>-1</sup>
110	CO <sub>2</sub> <sup>*</sup>	ν=410, 14(2), 1343, 667(2), 2349 cm <sup>-1</sup>	-463 kJ·mol <sup>-1</sup>
110	O <sup>*</sup>	ν=391, 508(2) cm <sup>-1</sup>	-243 kJ·mol <sup>-1</sup>
110	CO <sup>*</sup>	ν=342, 17(2), 2088 cm <sup>-1</sup>	-190 kJ·mol <sup>-1</sup>