

Supporting Information

Single Pt atom stabilized on nitrogen doped graphene: CO oxidation readily via the tri-molecular Eley-Rideal mechanism

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Supporting information 1:

Table S1: The vibrational frequencies of the transition states for the main reaction steps of CO oxidation.

Reaction step	Vibrational frequencies (cm ⁻¹)
$\text{O}_2 \rightarrow \text{O} + \text{O}$	i674.63, 128.03, 376.28, 499.74, 750.84, 841.50
$\text{CO} + \text{O}_2 \rightarrow \text{CO}_3$	i659.50, 24.63, 76.31, 116.23, 150.19, 175.67, 190.74, 230.94, 378.37, 448.90, 744.56, 1866.64
$2\text{CO} + \text{O}_2 \rightarrow \text{OCO-OCO}$	i1215.23, 32.09, 66.22, 106.98, 128.29, 147.79, 210.95, 292.54, 320.38, 412.63, 429.19, 447.11, 457.89, 608.17, 1028.49, 1278.35, 1919.80, 1967.44
$\text{OCO-OCO} \rightarrow 2\text{CO}_2$	i1023.34, 90.63, 131.25, 266.99, 370.35, 400.10, 443.16, 493.46, 565.60, 606.35, 693.61, 771.50, 824.38, 953.90, 1086.98, 1198.69, 1393.19, 1591.86