Electronic Supplementary Material (ESI) for RSC Advances.

TABLE S1. The calculated bond lengths (R), vibrational frequencies (ω_e), binding energies (E_b), and corresponding experimental values for the ground electronic states of the Au_2, CO, AuH, NO, and OH molecules.

molecule	method	R (Å)	w_e (cm^{-1})	E_b (eV)
Au_2	In this work	2.564	173	2.07
	BP	2.563	172.9	1.964
	PW91	2.561	174.2	2.093
	Expt.	2.472 [a]	191 [a]	2.29±0.02 [a]
CO	In this work	1.142	2089.8	11.969
	BP	1.142	2110.5	11.794
	PW91	1.141	2117.0	11.991
	Expt.	1.120 [b]	2082.07 [b]	11.109±0.004 [c]
AuH	In this work	1.545	2191.4	2.925
	BP	1.545	2324.6	3.027
	PW91	1.544	2331.4	3.087
	Expt.	1.524 [b]	2305.01 [b]	3.1 [b]
NO	In this work	1.164	1890.6	7.609
	BP	1.165	1887.2	7.396
	PW91	1.163	1893.7	7.596
	Expt.	1.151 [b]	1904.03 [b]	6.49 [b]
OH	In this work	0.985	3631.6	5.005
	BP	0.984	3632.7	4.988
	PW91	0.984	3630.9	5.031
	Expt.	0.971 [b]	3735.21 [b]	4.39±0.22 [c]

[a] Taken from Ref. 36

[b] Taken from Ref. 37

[c] Taken from Ref. 38

Noting that the references are the same as in the manuscript.

TABLE S2. The ionization potential, IP (eV), of Au, C, O, and N atoms.

Atom	Method			
	In this work	BP	PW91	Expt.
Au	9.572	9.584	9.650	9.225
C	11.610	11.643	11.685	11.261
O	13.643	13.602	13.502	13.61
N	14.856	14.903	14.945	14.533