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‘Supporting Information’

A comparative study of CO oxidation reaction over pristine and C-doped boron nitride fullerene

Mehdi D. Esrafili*, Parisa Nematollahi and Roghaye Nurazar

Laboratory of Theoretical Chemistry, Department of Chemistry, University of Maragheh, Maragheh, Iran

* Corresponding author. **Phone:** (+98) 4212237955. **Fax:** (+98) 4212276060. **P.O. Box:** 5513864596**. E-mail**: esrafili@maragheh.ac.ir (Mehdi D. Esrafili).

Figure S1. Optimized structures of the O_2-/CO-$B_{12}N_{12}$ complexes along with their corresponding electron density difference maps (0.001 au). In the EDD maps, the charge depletion and accumulation sites are displayed in red and blue, respectively. All bond distances are in Å.

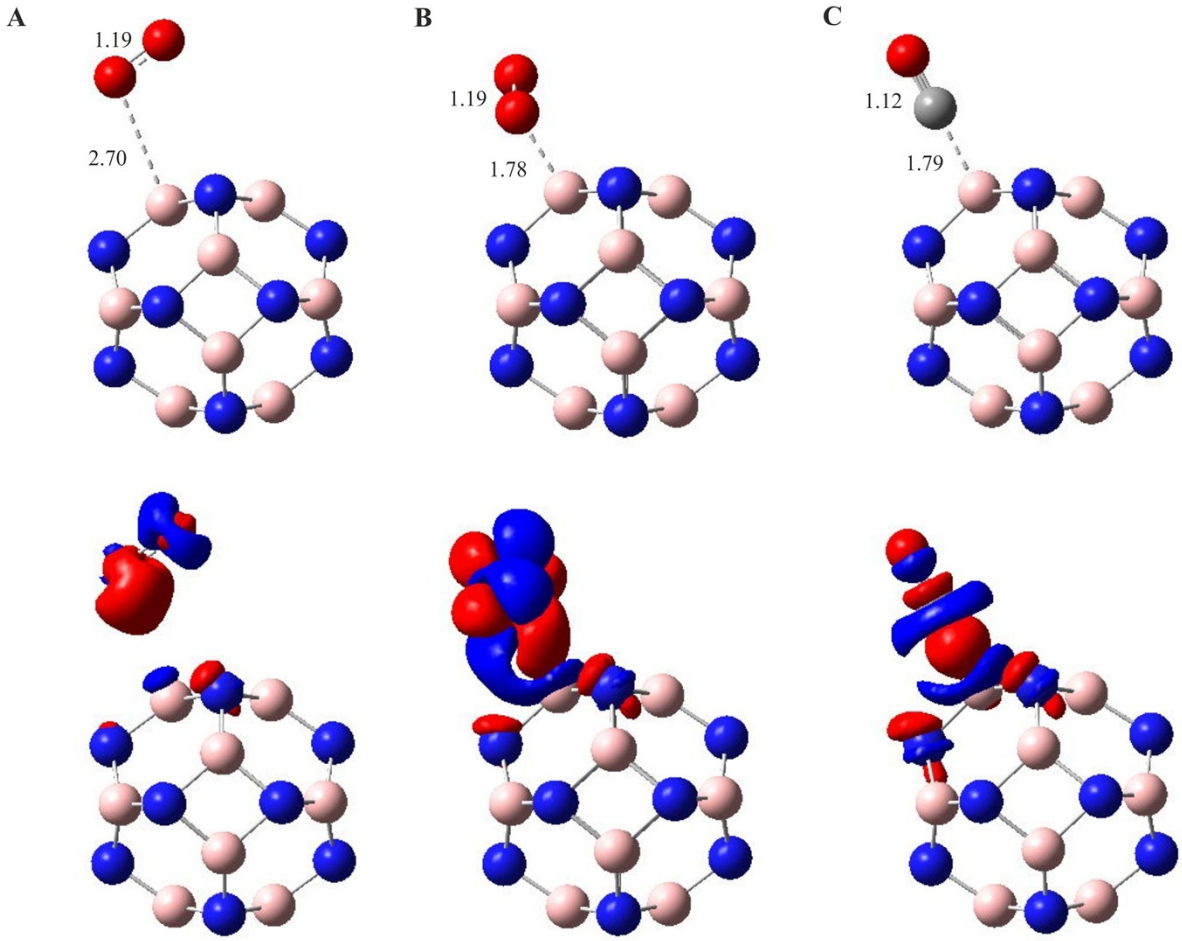


Figure S2. Optimized structures of O_2-/CO-$B_{11}N_{12}C$ complexes along with their corresponding electron density difference maps (0.001 au). In the EDD maps, the charge depletion and accumulation sites are displayed in red and blue, respectively. All bond distances are in Å.

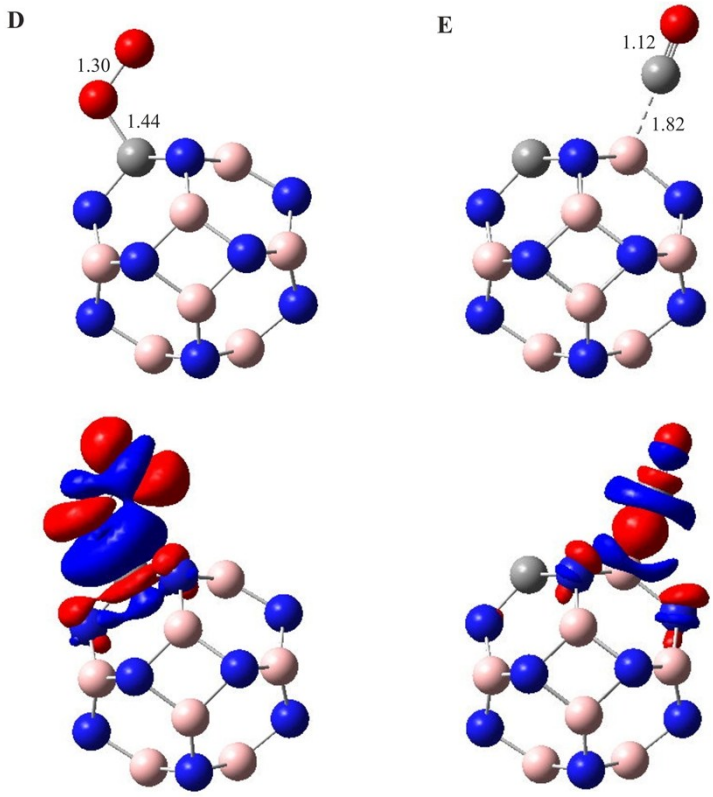


Figure S3. Schematic energy profile corresponding to local configurations along the minimum-energy pathway via (a) $O_2 + CO \rightarrow O_{ads} + CO_2$ and (b) $O_{ads} + CO \rightarrow CO_2$ over $B_{12}N_{12}$ cage. All energies are in eV.

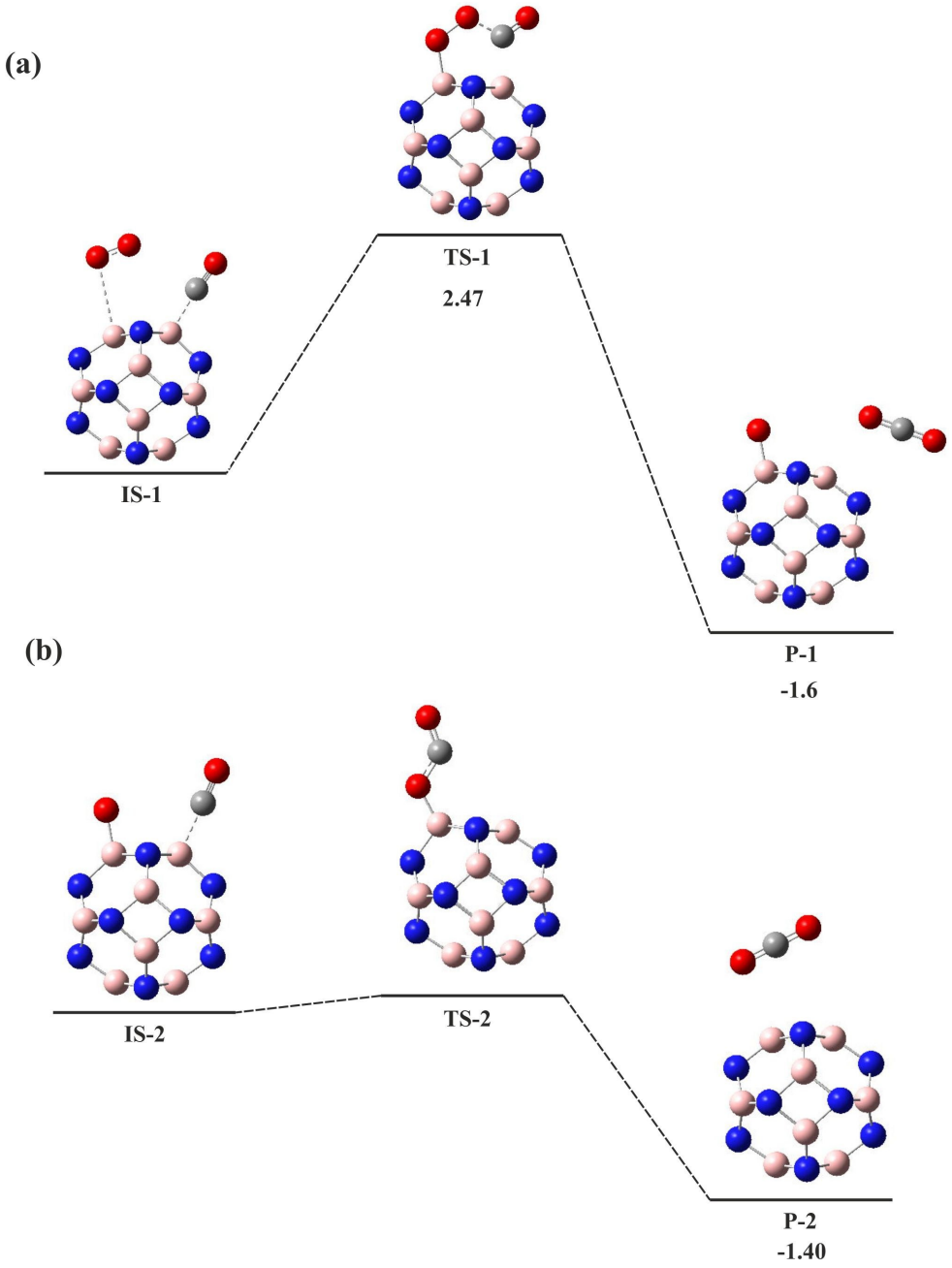
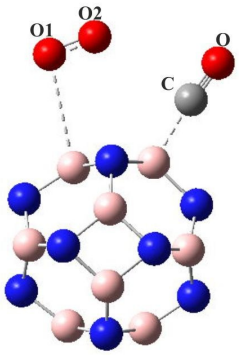
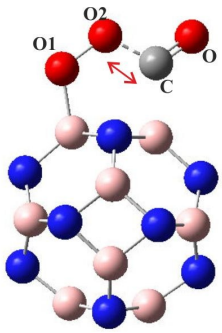


Figure S4. Local configurations of the gas molecules over the $B_{12}N_{12}$ cluster in various states, including the initial state (IS), transition state (TS) and product (P) along the minimum-energy pathway via the $O_2 + CO \rightarrow O_{ads} + CO_2$ and $O_{ads} + CO \rightarrow CO_2$ routes. The triplet ground state of O_2 molecule is considered. All bond distances are in Å.



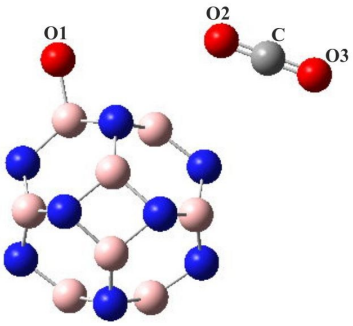
IS-1

r (B-O1)= 2.85
r (B-C)= 1.78
r (O1-O2)= 1.19
r (C-O)= 1.12
r (O2-C)= 2.84



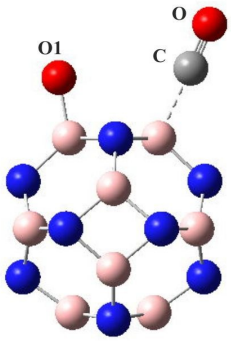
TS-1

r (B-O1)= 1.56
r (B-C)= 1.84
r (O1-O2)= 1.34
r (C-O)= 1.17
r (O2-C)= 1.42



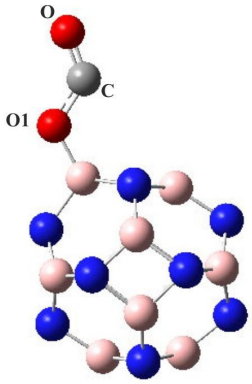
P-1

r (B-O1)= 1.43
r (N-C)= 3.01
r (O2-C)= 1.17
r (C-O3)= 1.16



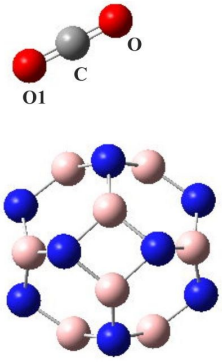
IS-2

r (B-O1)= 1.43
r (O1-C)= 3.06
r (C-O)= 1.12
r (B-C)= 1.79



TS-2

r (B-O1)= 1.43
r (O1-C)= 1.32
r (C-O)= 1.18



P-2

r (B-C)= 2.99
r (O1-C)= 1.16
r (C-O)= 1.16

Figure S5. Schematic energy profile corresponding to local configurations along the minimum-energy pathway via (a) $O_2 + CO \rightarrow O_{ads} + CO_2$ and (b) $O_{ads} + CO \rightarrow CO_2$ reaction mechanisms over $B_{12}N_{12}$ cluster. The singlet spin state of O_2 molecule is considered. All relative energies are in eV.

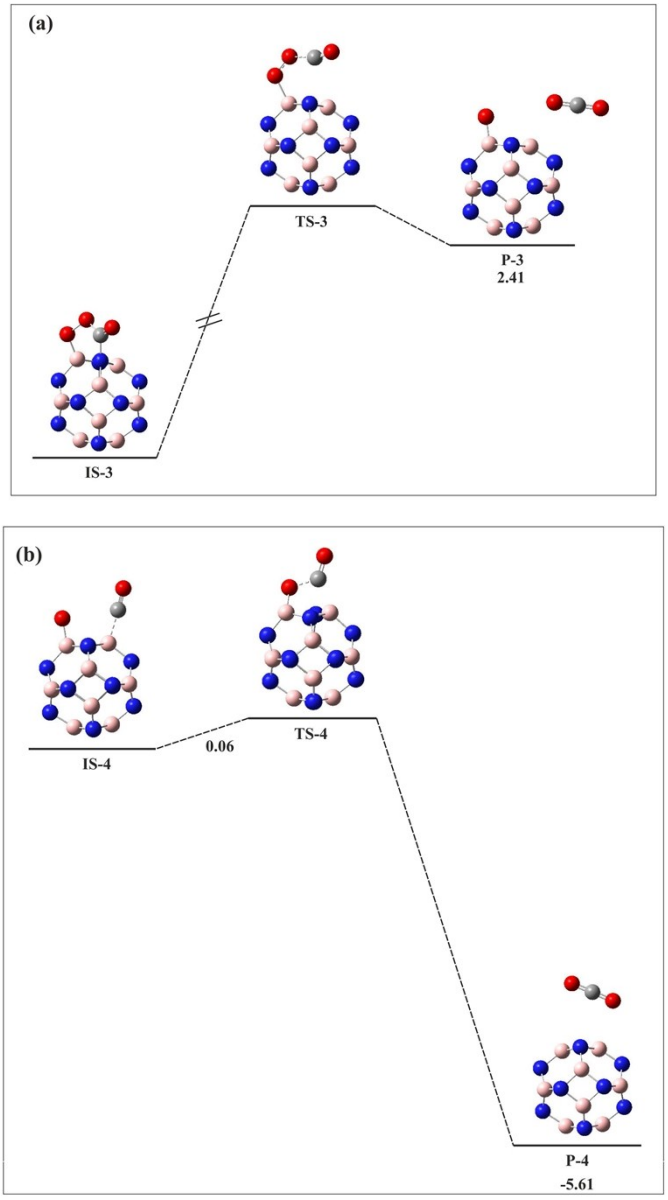
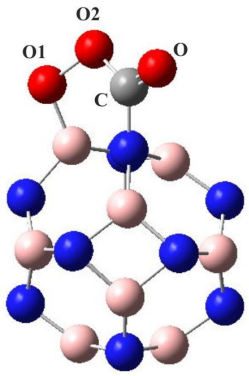
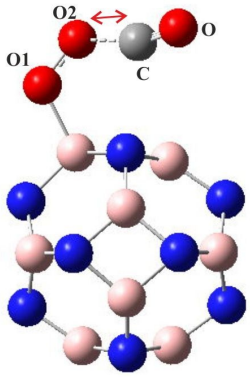


Figure S6. Local configurations of the gas molecules over the $B_{12}N_{12}$ cluster in various states, including the initial state (IS), transition state (TS) and product (P) along the minimum-energy pathway via the $O_2 + CO \rightarrow O_{ads} + CO_2$ and $O_{ads} + CO \rightarrow CO_2$ routes. The singlet spin state of O_2 molecule is considered. All bond distances are in Å.



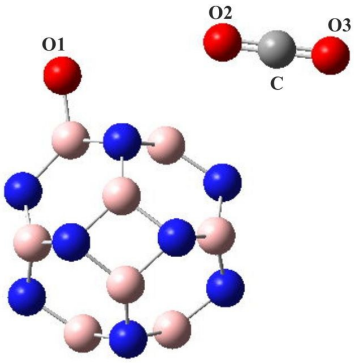
IS-3

r (B-O1)= 1.42
r (O1-O2)= 1.34
r (O2-C)= 1.35
r (C-O)= 1.17



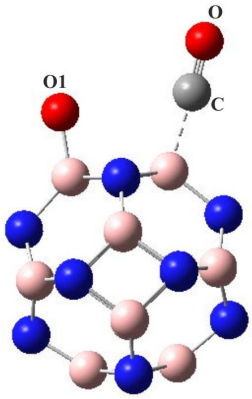
TS-3

r (B-O1)= 1.61
r (O1-O2)= 1.22
r (O2-C)= 2.03
r (C-O)= 1.12



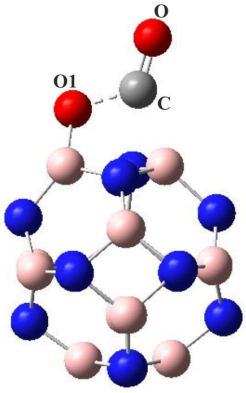
P-3

r (B-O1)= 1.38
r (N-C)= 3.04
r (O2-C)= 1.16
r (C-O3)= 1.15



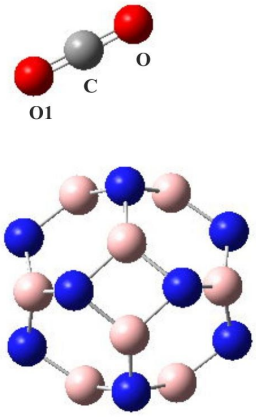
IS-4

r (B-O1)= 1.40
r (B-C)= 1.76
r (O1-C)= 2.83
r (C-O)= 1.12



TS-4

r (B-O1)= 1.41
r (O1-C)= 1.49
r (C-O)= 1.17



P-4

r (B-C)= 2.99
r (O1-C)= 1.16
r (C-O)= 1.16

Figure S7. Schematic energy profile corresponding to local configurations along the minimum-energy pathway via (a) $O_2 + CO \rightarrow O_{ads} + CO_2$ and (b) $O_{ads} + CO \rightarrow CO_2$ over $B_{11}N_{12}C$ cluster. The triplet spin state of O_2 molecule is considered .All energies are in eV.

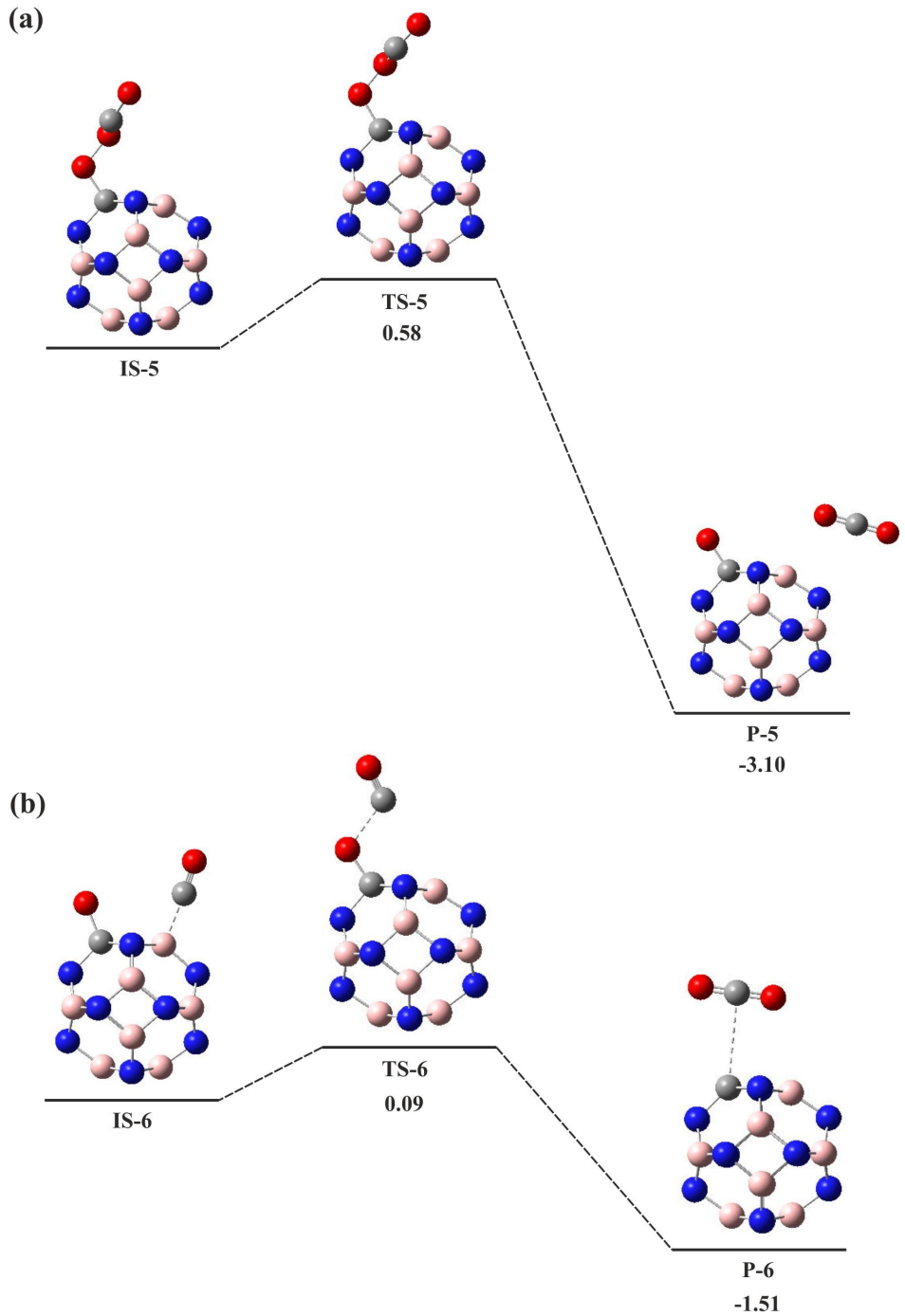
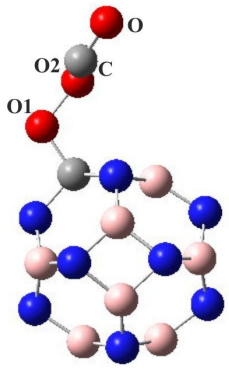
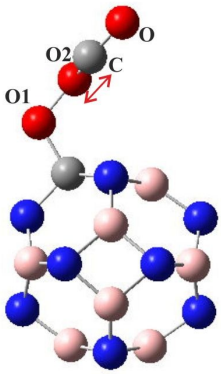


Figure S8. Local configurations of the gas molecules over the $B_{11}N_{12}C$ cluster in various states, including the initial state (IS), transition state (TS) and product (P) along the minimum-energy pathway via the $O_2 + CO \rightarrow O_{ads} + CO_2$ and $O_{ads} + CO \rightarrow CO_2$ routes. All bond distances are in Å.



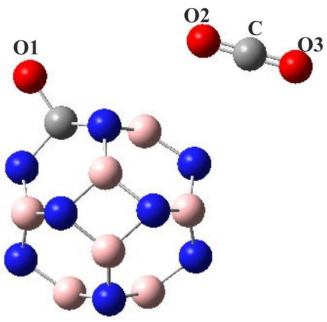
IS-5

r (C-O1)= 1.40
r (O1-O2)= 1.41
r (O2-C)= 1.35
r (C-O)= 1.18



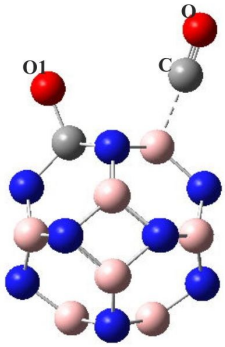
TS-5

r (C-O1)= 1.41
r (O1-O2)= 1.35
r (O2-C)= 1.77
r (C-O)= 1.14



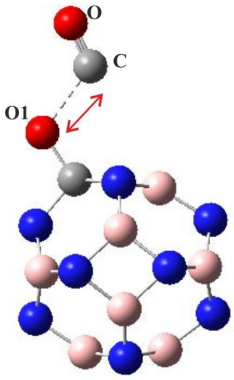
P-5

r (C-O1)= 1.35
r (N-C)= 3.02
r (O2-C)= 1.17
r (C-O3)= 1.16



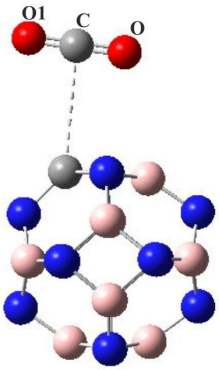
IS-6

r (C-O1)= 1.37
r (B-C)= 1.81
r (C-O)= 1.12
r (O1-C)= 3.24



TS-6

r (C-O1)= 1.36
r (O1-C)= 1.97
r (C-O)= 1.13



P-6

r (C-C)= 3.04
r (O1-C)= 1.16
r (C-O)= 1.16

Figure S9. Potential energy profiles for the minimum-energy pathway: $O_2 + CO \rightarrow O_{ads} + CO_2$ and $O_{ads} + CO \rightarrow CO_2$ reactions over $B_{11}N_{12}C$ cluster which are performed via LH and ER mechanism, respectively. The triplet spin state of O_2 molecule is considered. All relative energies are in eV.

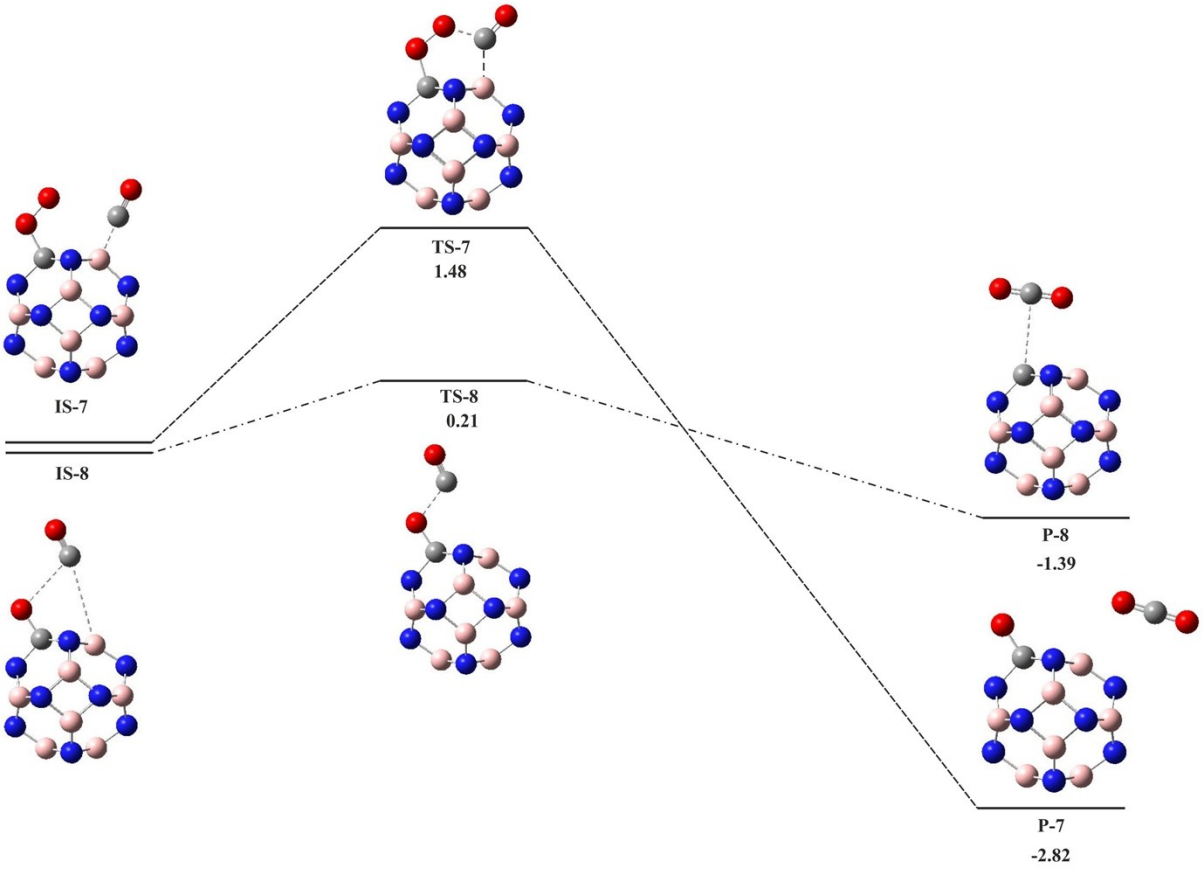
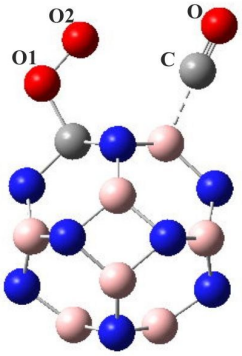
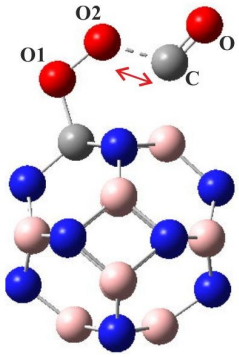


Figure S10. Optimized structures of stationary points for reaction pathways $O_2 + CO \rightarrow O_{ads} + CO_2$ and $O_{ads} + CO \rightarrow CO_2$ reactions over $B_{11}N_{12}C$ cluster. All bond distances are in Å.



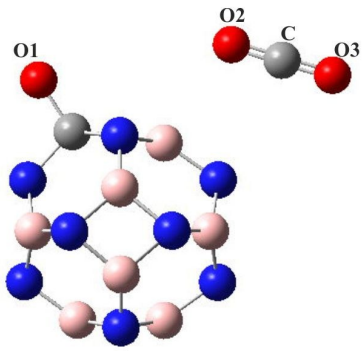
IS-7

r (C-O1)= 1.46
r (O1-O2)= 1.29
r (B-C)= 1.76
r (C-O)= 1.12



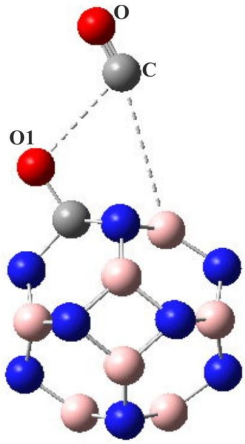
TS-7

r (C-O1)= 1.47
r (O1-O2)= 1.35
r (O2-C)= 1.59
r (C-O)= 1.15
r (B-C)= 1.82



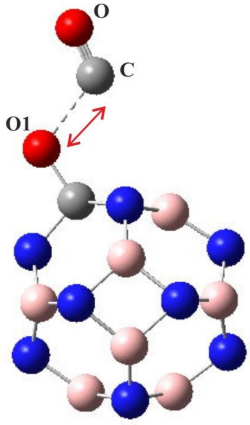
P-7

r (C-O1)= 1.35
r (N-C)= 3.02
r (O2-C)= 1.16
r (C-O3)= 1.15



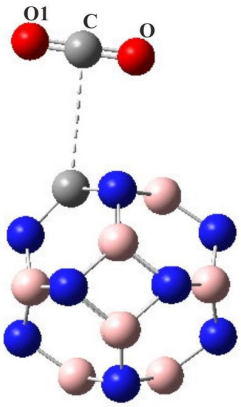
IS-8

r (C-O1)= 1.35
r (O1-C)= 2.73
r (C-O)= 1.12
r (B-C)= 3.50



TS-8

r (C-O1)= 1.36
r (O1-C)= 1.97
r (C-O)= 1.13



P-8

r (C-C)= 3.04
r (O1-C)= 1.16
r (C-O)= 1.16

Table S1. Calculated activation energy (E_{act}) and reaction energy (ΔE) for different pathways of CO oxidation over $B_{12}N_{12}$ and $B_{11}N_{12}C$ cluster. The singlet spin state is considered for the O_2 molecule in the reaction pathways performed over $B_{12}N_{12}$.

Reaction	E_{act} (eV)	ΔE (eV)
$B_{12}N_{12}$		
IS-3 → P-3	3.35	2.41
IS-4 → P-4	0.06	-5.61
$B_{12}N_{12}C$		
IS-7 → P-7	1.48	-2.82
IS-8 → P-8	0.21	-1.39