Supporting Information

Of

Noble Gas Decorated Planar Tetracoordinate Oxygen

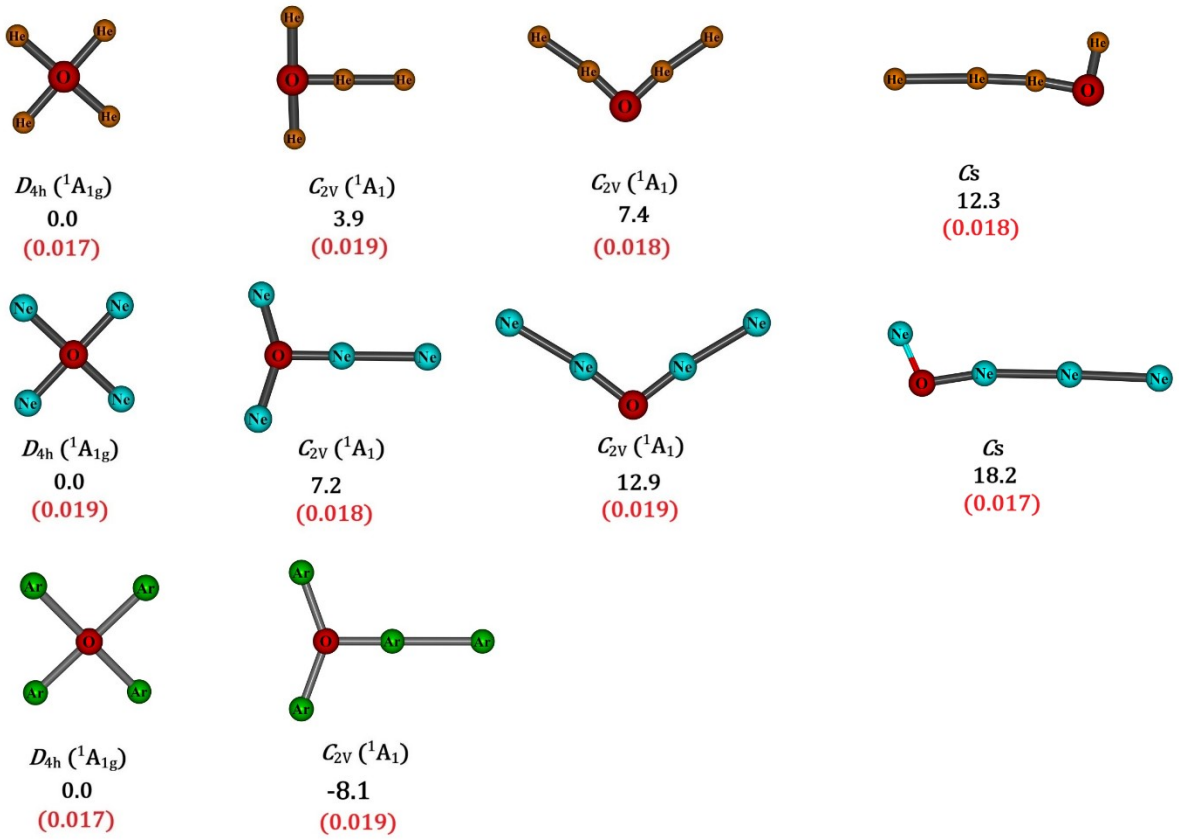


Fig S1. Relative energies (kcal/mol) of the low-lying isomers of He_4O^{2+}, Ne_4O^{2+} and Ar_4O^{2+} calculated at CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ including zero-point correction to Gibbs free energy from M06-2X/aug-cc-pVTZ. T_1 diagnostic values of the converged CCSD wavefunction are shown within parenthesis.

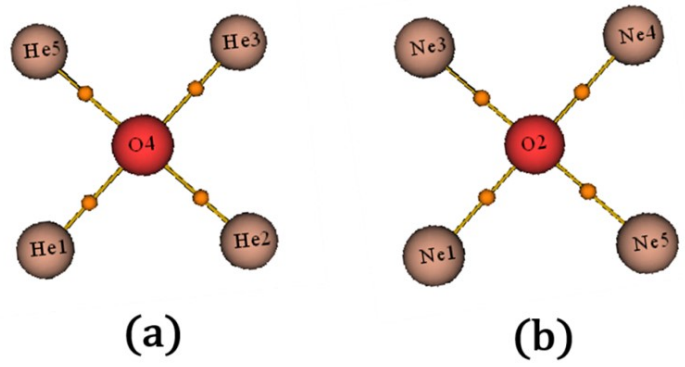


Fig S2. Molecular graph of (a) He_4O^{2+} and (b) Ne_4O^{2+} showing bond path and (3, -1) bond critical point.

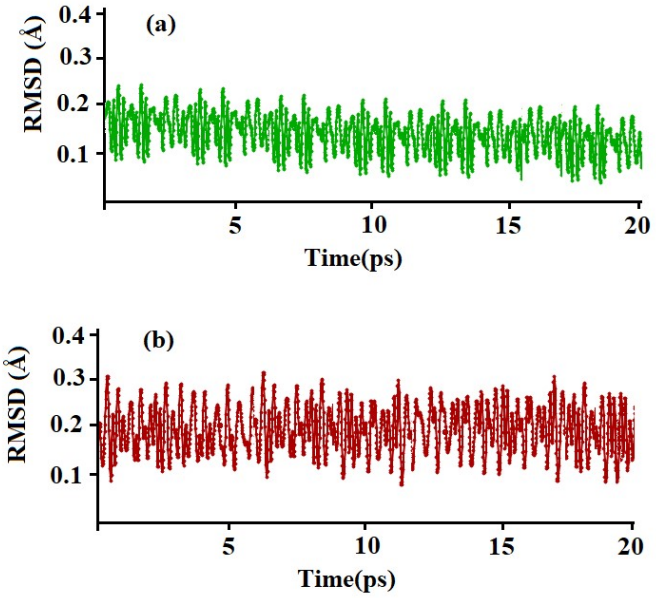


Fig S3. Root-mean-square deviations (RMSD) of the D_{4h} structures of (a) He_4O^{2+} and (b) Ne_4O^{2+} at 350 K during 20 ps Born-Oppenheimer molecular dynamics simulations.

Table S1. Electron density (ρ), Laplacian of electron density (∇^2_ρ) and electronic energy density H(r) at the O-He and O-Ne bond critical points.

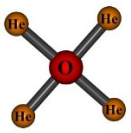
	Bond	ρ	∇^2_ρ	H(r)
He_4O^{2+}	O-He	0.13	0.39	-0.032
Ne_4O^{2+}	O-Ne	0.11	0.44	-0.016

Table S2. Fragmentation energies (kcal/mol) of He_4O^{2+} and Ne_4O^{2+} clusters calculated at M06-2X/aug-cc-pVTZ including zero-point correction. Fragments were considered at their lowest energy structures.

Pathway	Dissociation energies
$He_4O^{2+} \rightarrow He_2O^{2+}$ (Triplet) + 2He	7.9
$He_4O^{2+} \rightarrow HeO^{2+}$ (Triplet) + 3He	41.8
$Ne_4O^{2+} \rightarrow Ne_2O^{2+}$ (Singlet) + 2Ne	43.9
$He_4O^{2+} \rightarrow NeO^{2+}$ (Singlet) + 3Ne	121.6

Cartesian coordinates of the optimized geometries shown in Fig S1 calculated at M06-2X/aug-cc-pVTZ.

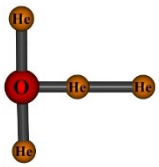
He_4O^{2+}



D_{4h} ($^1A_{1g}$)

He	-0.879674000	-1.108273000	-0.000794000
He	1.108270000	-0.879673000	0.000121000
He	0.879676000	1.108259000	-0.000738000
O	0.000000000	0.000005000	0.000324000
He	-1.108275000	0.879666000	0.000116000

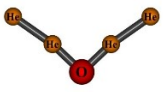
He_4O^{2+}



C_{2V} ($^1A_1$)

He	0.457174000	1.414204000	0.000006000
He	-0.699162000	0.000025000	0.000354000
He	0.457100000	-1.414257000	0.000073000
O	0.474325000	0.000000000	-0.000104000
He	-2.112413000	0.000029000	-0.000016000

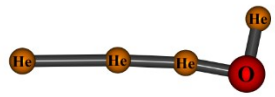
He_4O^{2+}



C_{2V} ($^1A_1$)

He	0.848556000	-0.202111000	0.000020000
He	1.993698000	-0.999202000	0.000016000
He	-0.848521000	-0.202120000	-0.000202000
O	0.000010000	0.600646000	0.000018000
He	-1.993775000	-0.999150000	0.000095000

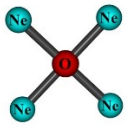
He_4O^{2+}



C_s

He	-0.220051000	-0.012891000	0.000755000
He	-3.424407000	0.031407000	-0.000352000
He	1.257264000	0.883812000	-0.000127000
O	0.987678000	-0.236877000	-0.000129000
He	-1.563517000	0.045180000	0.000238000

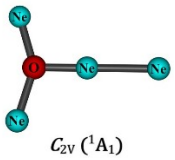
Ne_4O^{2+}



$D_{4h}\ (^1A_{1g})$

Ne	-0.588183000	-1.612870000	-0.000051000
O	0.000291000	0.000155000	0.000010000
Ne	-1.613050000	0.587820000	0.000083000
Ne	0.587916000	1.613171000	0.000036000
Ne	1.613084000	-0.588244000	-0.000076000

Ne_4O^{2+}

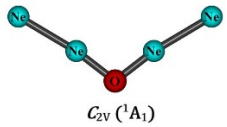


$C_{2v}\ (^1A_1)$

Ne	-1.404974000	1.616127000	0.000016000
Ne	0.695933000	-0.000002000	0.000029000
Ne	-1.404908000	-1.616154000	0.000016000
O	-0.918716000	0.000004000	-0.000065000

Ne	2.848922000	0.000026000	-0.000009000

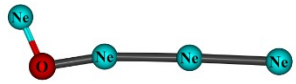
Ne_4O^{2+}



C_{2v} ($^1A_1$)

Ne	-1.237038000	0.296163000	-0.000005000
Ne	-3.079428000	-0.796514000	-0.000013000
Ne	1.237034000	0.296167000	0.000014000
O	0.000006000	1.250876000	0.000037000
Ne	3.079428000	-0.796517000	-0.000027000

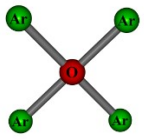
Ne_4O^{2+}



C_S

Ne	0.624337000	0.218051000	-0.000261000
Ne	-3.895482000	-0.141284000	0.001218000
Ne	3.063093000	-0.617814000	0.000235000
O	2.281467000	0.667183000	0.000725000
Ne	-1.617122000	0.007301000	-0.001772000

Ar_4O^{2+}

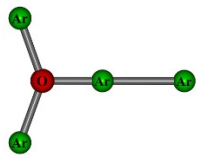


D_{4h} ($^1A_{1g}$)

Ar	1.810672000	1.035879000	-0.000079000
O	-0.000317000	0.000048000	0.000012000

Ar	1.035867000	-1.810678000	0.000153000
Ar	-1.810587000	-1.035796000	-0.000107000
Ar	-1.035812000	1.810574000	0.000028000

Ar_4O^{2+}



C_{2V} ($^1A_1$)

Ar	-1.798011000	-1.902901000	0.000314000
Ar	0.751829000	-0.000551000	-0.000380000
Ar	-1.797841000	1.903402000	0.000274000
O	-1.111620000	-0.000417000	0.000209000
Ar	3.338077000	0.000236000	-0.000302000