

Supporting Information

Spodium Bonding with Noble Gas Atoms

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Table S1. Bond dissociation energies (BDE, kcal/mol) in three different levels.

Complexes	BDE(kcal/mol) BP86-D3(BJ) /def2TZVPP	BDE (kcal/mol) MP2/def2QZVP	BDE (kcal/mol) CCSD/def2TZVP
Zn₃-Ar	1.77	1.28	1.36
Zn₃-Ar₂	3.55	2.57	2.72

Table S2: The amount of charge transferred, $|\Delta q|$ and the interaction energy (BDE) for the Be₃ complexes with noble gases at BP86-D3(BJ)/def2-TZVPP level.

Complexes	BDE	$ \Delta q $
Zn₃-Ne	0.35	0.007
Zn₃-Ar	1.77	0.025
Zn₃-Kr	2.64	0.032
Zn₃-Xe	4.11	0.048
Cd₃-Ne	0.33	0.005
Cd₃-Ar	1.87	0.018
Cd₃-Kr	2.76	0.023
Cd₃-Xe	4.23	0.033

Table S3. Bond dissociation energies (BDE, kcal/mol) of the CO@M₃ rings.

Complexes	BDE(kcal/mol) BP86-D3(BJ)/def2TZVPP
Zn₃-CO	4.57
Zn₃-(CO)₂	9.15
Cd₃-CO	4.04
Cd₃-(CO)₂	8.09
Hg₃-CO	1.96
Hg₃-(CO)₂	3.94

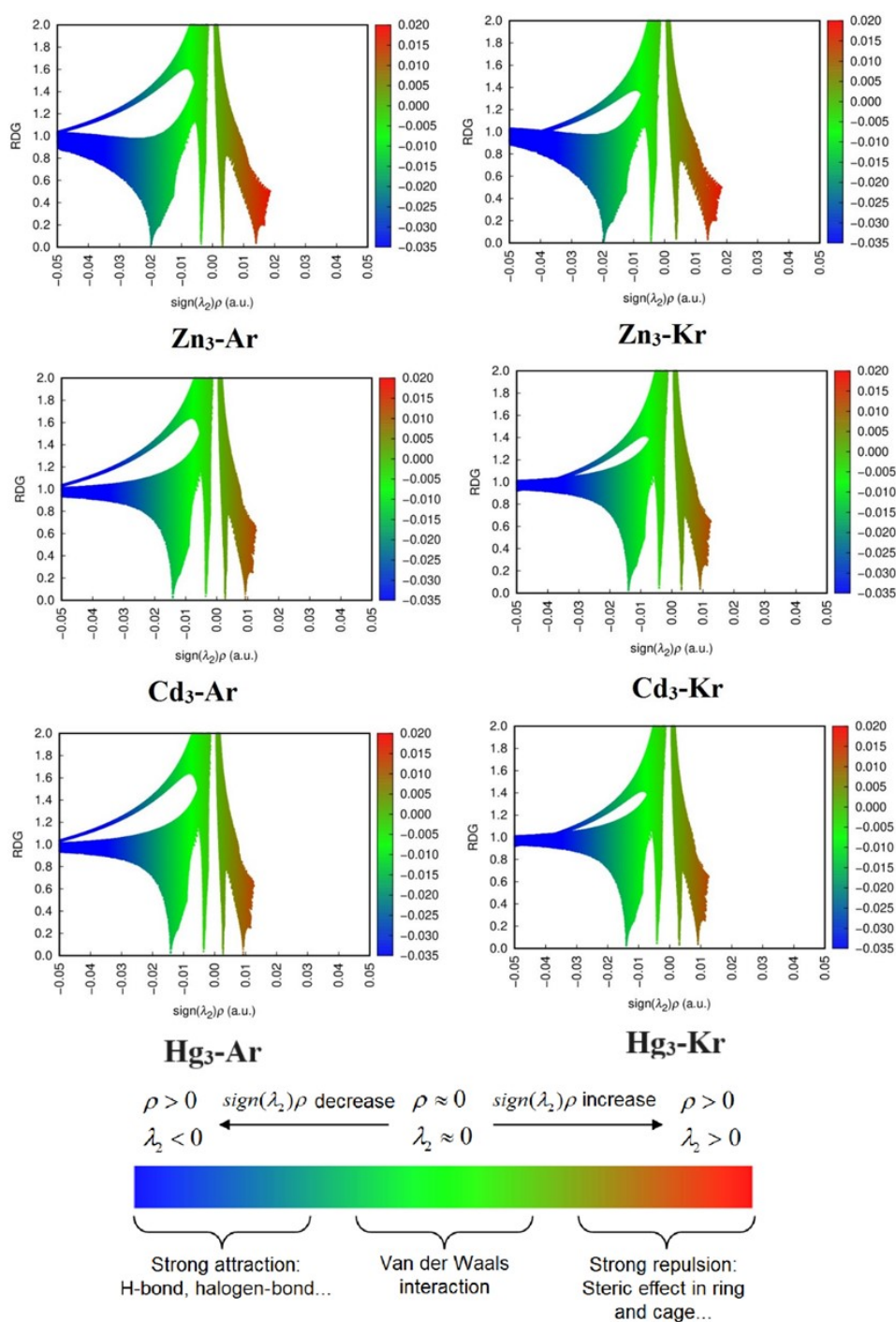


Figure S1- Reduced density gradient (RDG) color-filled scatter map of Ng@Zn₃ and Ng@Cd₃ complexes (Ng = Ar, Kr).

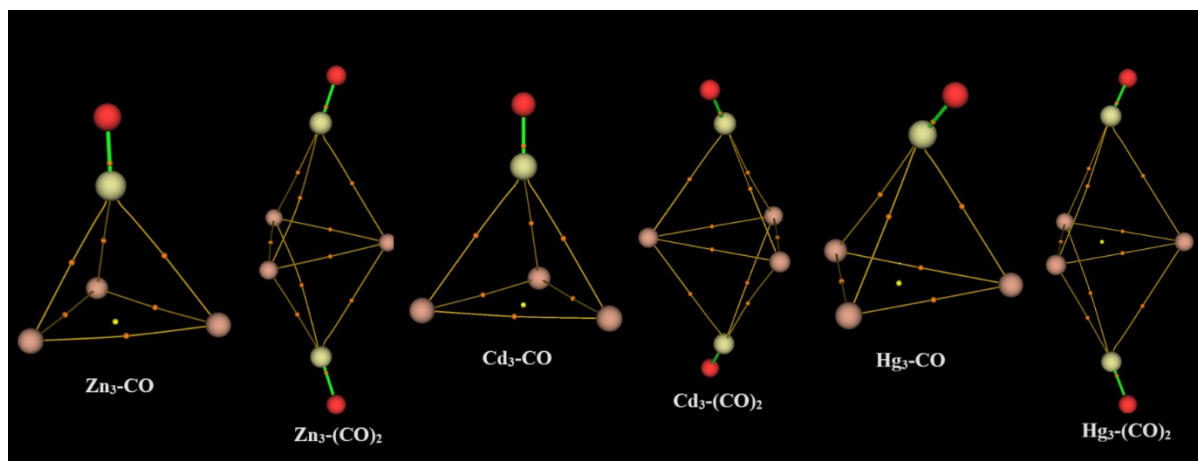


Figure S2. Molecular graph of CO@M₃ complexes. Bond critical points are shown in orange.

Cartesian coordinates of the [Zn₃-Ng] and [Cd₃-Ng] compounds and their complexes with noble gases along with their total energies calculated using BP86-D3(BJ) /def2TZVPP(au).

Zn₃

30	1.508543000	-0.870000000	0.000000000
30	-1.508543000	-0.870062000	0.000000000
30	0.000000000	1.740062000	0.000000000

Sum of electronic and zero-point Energies=	-5339.003028
Sum of electronic and thermal Energies=	-5338.998075
Sum of electronic and thermal Enthalpies=	-5338.997130
Sum of electronic and thermal Free Energies=	-5339.035474

Zn₃-Ne

30	-1.627077000	0.658906000	-0.288199000
30	1.357968000	1.077557000	-0.380838000
30	0.226336000	-1.717829000	-0.383695000
10	0.128320000	-0.055903000	3.158194000

Sum of electronic and zero-point Energies=	-5467.970097
Sum of electronic and thermal Energies=	-5467.962453
Sum of electronic and thermal Enthalpies=	-5467.961509
Sum of electronic and thermal Free Energies=	-5468.010189

Zn₃-Ne₂

30	-0.003315000	1.637253000	0.583673000
30	0.000701000	-0.318457000	-1.713620000
30	0.003452000	-1.331436000	1.127638000
10	3.488385000	0.023370000	0.003140000
10	-3.490900000	0.014547000	0.003789000

Sum of electronic and zero-point Energies=	-5596.937194
Sum of electronic and thermal Energies=	-5596.926850
Sum of electronic and thermal Enthalpies=	-5596.925905
Sum of electronic and thermal Free Energies=	-5596.984957

Zn₃-Ar

30	-0.547979000	-1.280082000	-1.190660000
30	-0.606870000	-0.381662000	1.689734000
30	-0.552838000	1.665981000	-0.527637000
18	2.846145000	-0.007062000	0.047606000

Sum of electronic and zero-point Energies=	-5866.587061
Sum of electronic and thermal Energies=	-5866.579525
Sum of electronic and thermal Enthalpies=	-5866.578581
Sum of electronic and thermal Free Energies=	-5866.626105

Zn₃-Ar₂

30	-0.001673000	0.410192000	-1.689390000
30	0.001138000	-1.673743000	0.499246000
30	0.001251000	1.264878000	1.208466000
18	3.430686000	-0.000861000	-0.016462000
18	-3.431880000	-0.001351000	-0.014074000

Sum of electronic and zero-point Energies= -6394.171106
Sum of electronic and thermal Energies= -6394.160956
Sum of electronic and thermal Enthalpies= -6394.160012
Sum of electronic and thermal Free Energies= -6394.217093

Zn₃-Kr

30	0.989724000	-1.747540000	-0.032899000
30	0.993160000	0.901297000	-1.494612000
30	0.993673000	0.844389000	1.527253000
36	-2.480464000	0.001545000	0.000215000

Sum of electronic and zero-point Energies= -8093.045417
Sum of electronic and thermal Energies= -8093.037885
Sum of electronic and thermal Enthalpies= -8093.036941
Sum of electronic and thermal Free Energies= -8093.085118

Zn₃-Kr₂

30	0.000085000	-0.954838000	1.462598000
30	-0.000383000	-0.785511000	-1.565137000

30	0.000262000	1.753571000	0.095320000
36	-3.486307000	-0.005428000	0.003098000
36	3.486338000	-0.005590000	0.002919000

Sum of electronic and zero-point Energies= -10847.087798
Sum of electronic and thermal Energies= -10847.077638
Sum of electronic and thermal Enthalpies= -10847.076693
Sum of electronic and thermal Free Energies= -10847.135408

Zn₃-Xe

30	1.328325000	1.091505000	-1.367623000
30	1.328336000	0.639119000	1.628546000
30	1.326891000	-1.731327000	-0.261033000
54	-2.213085000	0.000391000	0.000062000

Sum of electronic and zero-point Energies= -5668.509386
Sum of electronic and thermal Energies= -5668.501895
Sum of electronic and thermal Enthalpies= -5668.500951
Sum of electronic and thermal Free Energies= -5668.549216

Zn₃-Xe₂

30	0.000083000	-0.382406000	-1.713452000
30	-0.000116000	1.679680000	0.529361000
30	-0.000012000	-1.294694000	1.192867000
54	-3.562793000	-0.000733000	-0.002455000
54	3.562818000	-0.000700000	-0.002421000

Sum of electronic and zero-point Energies= -5998.015632
Sum of electronic and thermal Energies= -5998.005544

Sum of electronic and thermal Enthalpies= -5998.004600

Sum of electronic and thermal Free Energies= -5998.063275

Cd₃

48 1.699888000 -0.981081000 0.000000000

48 -1.699888000 -0.981082000 0.000000000

48 0.000000000 1.962163000 0.000000000

Sum of electronic and zero-point Energies= -503.711030

Sum of electronic and thermal Energies= -503.705836

Sum of electronic and thermal Enthalpies= -503.704892

Sum of electronic and thermal Free Energies= -503.746485

Cd₃-Ne

48 -1.963222000 -0.029251000 -0.226801000

48 0.953950000 1.717206000 -0.221653000

48 1.008326000 -1.681523000 -0.234959000

10 0.004538000 -0.030874000 3.280387000

Sum of electronic and zero-point Energies= -632.678081

Sum of electronic and thermal Energies= -632.670191

Sum of electronic and thermal Enthalpies= -632.669246

Sum of electronic and thermal Free Energies= -632.721363

Cd₃-Ne₂

48 1.906372000 -0.513658000 -0.011826000

48 -0.489619000 1.900028000 0.011304000

48	-1.383182000	-1.380277000	0.000045000
10	-0.099931000	0.004255000	-3.492511000
10	-0.061213000	-0.033504000	3.494804000

Sum of electronic and zero-point Energies=	-761.645116
Sum of electronic and thermal Energies=	-761.634549
Sum of electronic and thermal Enthalpies=	-761.633605
Sum of electronic and thermal Free Energies=	-761.695444

Cd₃-Ar

48	-1.967412000	0.158107000	-0.352038000
48	1.108946000	1.613868000	-0.406480000
48	0.831717000	-1.778356000	-0.389200000
18	0.071329000	0.017016000	3.060580000

Sum of electronic and zero-point Energies=	-1031.295220
Sum of electronic and thermal Energies=	-1031.287410
Sum of electronic and thermal Enthalpies=	-1031.286466
Sum of electronic and thermal Free Energies=	-1031.337261

Cd₃-Ar₂

48	0.000030000	1.664565000	-1.053973000
48	-0.000038000	-1.741717000	-0.915036000
48	0.000004000	0.081777000	1.965062000
18	3.448325000	-0.006212000	0.005260000
18	-3.448314000	-0.006122000	0.005269000

Sum of electronic and zero-point Energies=	-1558.879415
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Sum of electronic and thermal Energies=	-1558.868958
Sum of electronic and thermal Enthalpies=	-1558.868014
Sum of electronic and thermal Free Energies=	-1558.928716

Cd₃-Kr

48	0.698498000	-0.681331000	1.849390000
48	0.714558000	-1.254998000	-1.513865000
48	0.693642000	1.944768000	-0.329049000
36	-2.808930000	-0.011252000	-0.008635000

Sum of electronic and zero-point Energies=	-3257.753613
Sum of electronic and thermal Energies=	-3257.745797
Sum of electronic and thermal Enthalpies=	-3257.744853
Sum of electronic and thermal Free Energies=	-3257.796206

Cd₃-Kr₂

48	0.000347000	0.931360000	-1.744801000
48	-0.000749000	-1.975770000	0.069299000
48	0.000378000	1.050277000	1.677604000
36	3.516426000	-0.004328000	-0.001397000
36	-3.516393000	-0.003494000	-0.001405000

Sum of electronic and zero-point Energies=	-6011.796168
Sum of electronic and thermal Energies=	-6011.785693
Sum of electronic and thermal Enthalpies=	-6011.784749
Sum of electronic and thermal Free Energies=	-6011.846649

Cd₃-Xe

48	-0.977474000	1.658836000	-1.071784000
48	-0.980125000	-1.757192000	-0.900168000
48	-0.981419000	0.099544000	1.970452000
54	2.612461000	-0.001057000	0.001334000

Sum of electronic and zero-point Energies=	-833.217531
Sum of electronic and thermal Energies=	-833.209744
Sum of electronic and thermal Enthalpies=	-833.208800
Sum of electronic and thermal Free Energies=	-833.260383

Cd₃-Xe₂

48	0.000032000	-1.964767000	0.310149000
48	-0.000008000	1.252530000	1.544248000
48	0.000017000	0.713274000	-1.857414000
54	3.606372000	-0.000453000	0.001345000
54	-3.606409000	-0.000468000	0.001337000

Sum of electronic and zero-point Energies=	-1162.724001
Sum of electronic and thermal Energies=	-1162.713549
Sum of electronic and thermal Enthalpies=	-1162.712605
Sum of electronic and thermal Free Energies=	-1162.774833

Hg₃

80	0.000000000	-2.081725000	0.000000000
80	-1.803244000	1.041323000	0.000000000
80	1.803244000	1.040402000	0.000000000

Sum of electronic and zero-point Energies=	-461.007551
Sum of electronic and thermal Energies=	-461.002164
Sum of electronic and thermal Enthalpies=	-461.001219
Sum of electronic and thermal Free Energies=	-461.046195

Hg₃-Ar

80	0.023365000	2.086474000	-0.236929000
80	-1.820296000	-1.023541000	-0.235392000
80	1.797008000	-1.063934000	-0.235225000
18	-0.000345000	0.004450000	3.144649000

Sum of electronic and zero-point Energies=	-988.591439
Sum of electronic and thermal Energies=	-988.583407
Sum of electronic and thermal Enthalpies=	-988.582463
Sum of electronic and thermal Free Energies=	-988.636575

Hg₃-Ar₂

80	0.231544000	-2.081096000	0.009449000
80	-1.917013000	0.840513000	-0.025853000
80	1.688732000	1.239676000	0.015689000
18	0.044185000	-0.012412000	-3.378383000
18	-0.058692000	0.016443000	3.381564000

Sum of electronic and zero-point Energies=	-1516.175336
Sum of electronic and thermal Energies=	-1516.164658
Sum of electronic and thermal Enthalpies=	-1516.163714
Sum of electronic and thermal Free Energies=	-1516.226968

Hg₃-Kr

80	0.268414000	-2.078394000	-0.450757000
80	1.666448000	1.270998000	-0.451887000
80	-1.934381000	0.806553000	-0.452593000
36	-0.001071000	0.001873000	3.011637000

Sum of electronic and zero-point Energies=	-3215.049587
Sum of electronic and thermal Energies=	-3215.041543
Sum of electronic and thermal Enthalpies=	-3215.040598
Sum of electronic and thermal Free Energies=	-3215.095306

Hg₃-Kr₂

80	0.001708000	-1.954042000	-0.794380000
80	-0.001229000	0.289614000	2.090246000
80	-0.000408000	1.666323000	-1.294839000
36	-3.462027000	-0.003510000	-0.002232000
36	3.461868000	-0.000702000	-0.000050000

Sum of electronic and zero-point Energies=	-5969.091621
Sum of electronic and thermal Energies=	-5969.080915
Sum of electronic and thermal Enthalpies=	-5969.079970
Sum of electronic and thermal Free Energies=	-5969.144428

Hg₃-Xe

80	0.656327000	2.101086000	0.084444000
80	0.652485000	-0.979722000	-1.861600000
80	0.648497000	-1.124899000	1.779062000
54	-2.899717000	0.005237000	-0.002823000
Sum of electronic and zero-point Energies=	-790.512969		
Sum of electronic and thermal Energies=	-790.504933		
Sum of electronic and thermal Enthalpies=	-790.503989		
Sum of electronic and thermal Free Energies=	-790.558908		

Hg₃-Xe₂

80	0.000197000	1.530582000	1.475234000
80	-0.000136000	-2.043376000	0.587357000
80	-0.000038000	0.512656000	-2.063323000
54	3.551041000	-0.000014000	0.000482000
54	-3.551076000	0.000219000	0.000603000
Sum of electronic and zero-point Energies=	-1120.018374		
Sum of electronic and thermal Energies=	-1120.007676		
Sum of electronic and thermal Enthalpies=	-1120.006732		
Sum of electronic and thermal Free Energies=	-1120.071704		