On the Nature of the Partial Covalent Bond between Noble Gas Elements and Noble Metal Atoms

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SUPPLIMENTARY INFORMATION

Table S1. EDA results of NgMO (M = Cu, Ag, Au) complexes considering Ng as one fragment and MO as another fragment at the PBE-D3/QZ4P//CCSD(T)/VTZ level. All energy terms are in kcal/mol. (The values within the parentheses are in percentage and show the contribution toward the total attractive interaction, ΔE_{elstat} + ΔE_{orb} + ΔE_{disp}). [Reprinted from Ref. [76] with permission from John Wiley and Sons. © 2015 Wiley Periodicals, Inc.]

Systems	ΔE_{int}	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}	ΔE_{disp}
ArCuO	−6.66	−15.4 (49.3)	−15.7 (50.2)	24.6	−0.1 (0.4)
KrCuO	−8.91	−19.3 (50.3)	−18.9 (49.2)	29.5	−0.2 (0.4)
XeCuO	−12.93	−25.2 (49.9)	−25.1 (49.7)	37.5	−0.2 (0.4)
RnCuO	−14.07	−25.3 (49.6)	−25.4 (50.0)	36.9	−0.22 (0.4)
ArAgO	−4.44	−8.0 (50.6)	−7.6 (47.7)	11.4	−0.2 (1.7)
KrAgO	−6.63	−12.8 (52.9)	−11.1 (45.9)	17.5	−0.29 (1.2)
XeAgO	−10.14	−21.3 (55.5)	−16.9 (43.8)	28.3	−0.29 (0.8)
RnAgO	−11.56	−23.1 (55.8)	−17.9 (43.3)	29.9	−0.37 (0.9)
ArAuO	−6.66	−17.0 (49.3)	−17.2 (40.1)	27.7	−0.21 (0.6)
KrAuO	−9.81	−25.0 (51.4)	−23.4 (48.1)	38.8	−0.25 (0.5)
XeAuO	−14.83	−37.8 (53.4)	−32.7 (46.2)	56.0	−0.28 (0.4)
RnAuO	−16.58	−40.1 (53.8)	−34.1 (45.8)	57.8	−0.35 (0.5)

Table S2. EDA results of the NgMCN (M = Cu, Ag, Au) clusters with Ng and MCN as fragments calculated at the PBE-D3/QZ4P//CCSD(T)/def2-TZVPPD level. All energy terms are in kcal/mol. (The percentage values within the parentheses show the contribution toward the total attractive interaction, ΔE_{elstat} + ΔE_{orb} + ΔE_{disp}). [Reprinted from Ref. [75] with permission from John Wiley and Sons. © 2015 Wiley Periodicals, Inc.]

Systems	ΔE_{int}	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}	ΔE_{disp}
ArCuCN	−8.5	−11.6 (45.5)	−13.7 (53.7)	16.9	−0.2 (0.8)
KrCuCN	−11.0	−15.0 (47.0)	−16.7 (52.4)	20.9	−0.2 (0.6)
XeCuCN	−15.5	−18.7 (45.9)	−21.7 (53.3)	25.2	−0.3 (0.7)
RnCuCN	−16.6	−19.9 (46.2)	−22.9 (53.1)	26.6	−0.3 (0.7)
ArAgCN	−5.2	−7.0 (47.3)	−7.5 (50.7)	9.7	−0.3 (2.0)
KrAgCN	−7.5	−11.2 (49.8)	−10.9 (48.4)	15.0	−0.4 (1.8)
XeAgCN	−11.0	−17.1 (52.0)	−15.4 (46.8)	21.9	−0.4 (1.2)
RnAgCN	−12.4	−19.7 (52.8)	−17.1 (45.8)	24.9	−0.5 (1.3)
ArAuCN	−7.9	−16.1 (48.6)	−16.7 (50.5)	25.2	−0.3 (0.9)
KrAuCN	−11.1	−22.4 (50.7)	−21.5 (48.6)	33.2	−0.3 (0.7)
XeAuCN	−16.1	−32.3 (52.5)	−28.8 (46.8)	45.4	−0.4 (0.7)
RnAuCN	−17.8	−35.2 (53.1)	−30.6 (46.2)	48.5	−0.5 (0.8)

Table S3. Electron density descriptors (au) at the bond critical points (BCPs) in between Ng and M atoms in NgMCN obtained from the wave functions generated at the MP2/def2-TZVPPD/WTBS//CCSD(T)/def2-TZVPPD level (All electron WTBS basis set is used only for Ag, Au, Xe, and Rn). [Reprinted from Ref. [75] with permission from John Wiley and Sons. © 2015 Wiley Periodicals, Inc.]

Systems	BCP	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$G(r_c)/\rho(r_c)$
ArCuCN	Ar-Cu	0.046	0.229	0.063	−0.07	−0.007	1.37
KrCuCN	Kr-Cu	0.049	0.198	0.058	−0.067	−0.009	1.184
XeCuCN	Xe-Cu	0.052	0.132	0.047	−0.061	−0.014	0.904
RnCuCN	Rn-Cu	0.053	0.109	0.042	−0.057	−0.015	0.792
ArAgCN	Ar-Ag	0.028	0.141	0.034	−0.033	0.001	1.214
KrAgCN	Kr-Ag	0.033	0.146	0.038	−0.039	−0.001	1.152
XeAgCN	Xe-Ag	0.034	0.138	0.036	−0.037	−0.001	1.059
RnAgCN	Rn-Ag	0.036	0.13	0.035	−0.038	−0.003	0.972
ArAuCN	Ar-Au	0.046	0.244	0.062	−0.063	−0.001	1.348
KrAuCN	Kr-Au	0.05	0.222	0.06	−0.065	−0.005	1.2
XeAuCN	Xe-Au	0.046	0.195	0.052	−0.056	−0.004	1.13
RnAuCN	Rn-Au	0.046	0.175	0.048	−0.053	−0.005	1.043

Table S4. Electron density descriptors (au) at the BCPs in between Ng and M centers obtained from the wave functions generated at the MP2/cc-pVTZ/WTBS//CCSD(T)/VTZ level (All electron WTBS basis set is used only for Ag,

Au, Xe, and Rn). [Reprinted from Ref. [76] with permission from John Wiley and Sons. © 2015 Wiley Periodicals, Inc.]

Systems	BCP	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$G(r_c)/\rho(r_c)$
ArCuO	Ar-Cu	0.045	0.271	0.071	20.075	20.004	1.578
KrCuO	Kr-Cu	0.045	0.271	0.071	20.075	20.004	1.578
XeCuO	Xe-Cu	0.043	0.188	0.052	20.057	20.005	1.209
RnCuO	Rn-Cu	0.041	0.161	0.046	20.051	20.005	1.122
ArAgO	Ar-Ag	0.028	0.147	0.035	20.034	0.001	1.250
KrAgO	Kr-Ag	0.031	0.153	0.038	20.037	0.001	1.226
XeAgO	Xe-Ag	0.037	0.154	0.041	20.043	20.002	1.108
RnAgO	Rn-Ag	0.037	0.141	0.038	20.041	20.003	1.027
ArAuO	Ar-Au	0.042	0.236	0.059	20.059	0.000	1.405
KrAuO	Kr-Au	0.042	0.232	0.058	20.057	0.001	1.381
XeAuO	Xe-Au	0.047	0.210	0.055	20.059	20.004	1.170
RnAuO	Rn-Au	0.046	0.186	0.050	20.054	20.004	1.087

Table S5. Different topological descriptors (au) at the bond critical points (BCP) in between Ng and M atoms in NgMY and Ng_2M_2Y (M = Cu, Ag; Y = NO_3, SO_4, CO_3) complexes at the MPW1B95/def2-TZVP level. [Reprinted from Ref. [77] with permission from Springer Nature. © 2016, Indian Academy of Sciences]

Systems	BCP	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$G(r_c)/\rho(r_c)$
$ArCuNO_3$	Ar-Cu	0.046	0.231	0.062	−0.067	−0.004	1.348
$KrCuNO_3$	Kr-Cu	0.05	0.209	0.059	−0.066	−0.007	1.180
$XeCuNO_3$	Xe-Cu	0.052	0.173	0.053	−0.062	−0.009	1.019
$RnCuNO_3$	Rn-Cu	0.05	0.150	0.046	−0.055	−0.009	0.920
$ArAgNO_3$	Ar-Ag	0.028	0.122	0.031	−0.031	0.000	1.107
$KrAgNO_3$	Kr-Ag	0.036	0.129	0.035	−0.038	−0.003	0.972
$XeAgNO_3$	Xe-Ag	0.043	0.128	0.038	−0.043	−0.006	0.884
$RnAgNO_3$	Rn-Ag	0.043	0.115	0.035	−0.042	−0.006	0.814
$ArCuSO_4$	Ar-Cu	0.045	0.227	0.061	−0.065	−0.004	1.356
$KrCuSO_4$	Kr-Cu	0.05	0.206	0.059	−0.066	−0.007	1.180
$XeCuSO_4$	Xe-Cu	0.053	0.171	0.052	−0.062	−0.009	0.981
$RnCuSO_4$	Rn-Cu	0.05	0.149	0.046	−0.055	−0.009	0.920
$ArAgSO_4$	Ar-Ag	0.028	0.121	0.03	−0.031	0.000	1.071
$KrAgSO_4$	Kr-Ag	0.036	0.129	0.035	−0.038	−0.003	0.972

$XeAgSO_4$	Xe-Ag	0.043	0.126	0.037	−0.043	−0.006	0.860
$RnAgSO_4$	Rn-Ag	0.043	0.113	0.035	−0.041	−0.007	0.814
$ArCuCO_3$	Ar-Cu	0.039	0.188	0.049	−0.051	−0.002	1.256
$KrCuCO_3$	Kr-Cu	0.043	0.17	0.047	−0.051	−0.005	1.093
$XeCuCO_3$	Xe-Cu	0.046	0.144	0.043	−0.049	−0.007	0.935
$RnCuCO_3$	Rn-Cu	0.044	0.125	0.038	−0.044	−0.007	0.864
$Ar_2Cu_2SO_4$	Ar-Cu	0.044	0.221	0.059	−0.062	−0.004	1.341
$Kr_2Cu_2SO_4$	Kr-Cu	0.049	0.205	0.058	−0.064	−0.007	1.184
$Xe_2Cu_2SO_4$	Xe-Cu	0.052	0.172	0.052	−0.061	−0.009	1.000
$Rn_2Cu_2SO_4$	Rn-Cu	0.049	0.149	0.046	−0.054	−0.008	0.939
$Ar_2Ag_2SO_4$	Ar-Ag	0.026	0.114	0.028	−0.028	0.000	1.077
$Kr_2Ag_2SO_4$	Kr-Ag	0.034	0.125	0.034	−0.037	−0.003	1.000
$Xe_2Ag_2SO_4$	Xe-Ag	0.042	0.126	0.037	−0.042	−0.005	0.881
$Rn_2Ag_2SO_4$	Rn-Ag	0.042	0.113	0.034	−0.041	−0.006	0.810
$Ar_2Au_2SO_4$	Ar-Au	0.058	0.242	0.069	−0.078	−0.009	1.190
$Kr_2Au_2SO_4$	Kr-Au	0.066	0.216	0.067	−0.080	−0.013	1.015
$Xe_2Au_2SO_4$	Xe-Au	0.071	0.166	0.06	−0.078	−0.018	0.845
$Rn_2Au_2SO_4$	Rn-Au	0.068	0.143	0.054	−0.072	−0.018	0.794
$Ar_2Ag_2CO_3$	Ar-Ag	0.026	0.111	0.028	−0.027	0.000	1.077
$Kr_2Ag_2CO_3$	Kr-Ag	0.034	0.124	0.033	−0.036	−0.003	0.971
$Xe_2Ag_2CO_3$	Xe-Ag	0.042	0.125	0.037	−0.042	−0.005	0.881
$Rn_2Ag_2CO_3$	Rn-Ag	0.041	0.112	0.034	−0.040	−0.006	0.829
$Ar_2Au_2CO_3$	Ar-Au	0.055	0.234	0.066	−0.073	−0.007	1.200
$Kr_2Au_2CO_3$	Kr-Au	0.063	0.212	0.065	−0.077	−0.012	1.032
$Xe_2Au_2CO_3$	Xe-Au	0.069	0.166	0.058	−0.075	−0.017	0.841
$Rn_2Au_2CO_3$	Rn-Au	0.066	0.143	0.053	−0.070	−0.017	0.803

Table S6. Topological descriptors (au) at the line critical point between Ng and M atoms in $[NgM\text{-}(bipy)]^+$ obtained from wave function generated at the MPW1B95/cc-pVTZ/WTBS//MPW1B95/cc-pVTZ level (All electron WTBS basis set is used only for Cu, Ag, Au, Kr, Xe and Rn). [Reprinted from Ref. [85] with permission from John Wiley and Sons. © 2016 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim]

Systems	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$G(r_c)/\rho(r_c)$
$[ArCu\text{-}(bipy)]^+$	0.042	0.211	0.060	−0.063	−0.003	1.417
$[KrCu\text{-}(bipy)]^+$	0.042	0.208	0.055	−0.059	−0.003	1.331
$[XeCu\text{-}(bipy)]^+$	0.044	0.177	0.050	−0.056	−0.006	1.146

[RnCu-(bipy)]$^+$	0.042	0.151	0.044	−0.050	−0.006	1.045
[ArAg-(bipy)]$^+$	0.029	0.143	0.035	−0.034	0.001	1.211
[KrAg-(bipy)]$^+$	0.036	0.15	0.039	−0.041	−0.002	1.097
[XeAg-(bipy)]$^+$	0.038	0.151	0.040	−0.043	−0.003	1.061
[RnAg-(bipy)]$^+$	0.038	0.136	0.037	−0.040	−0.003	0.984
[ArAu-(bipy)]$^+$	0.045	0.224	0.057	−0.059	−0.001	1.276
[KrAu-(bipy)]$^+$	0.048	0.246	0.063	−0.065	−0.002	1.312
[XeAu-(bipy)]$^+$	0.052	0.215	0.059	−0.065	−0.006	1.135
[RnAu-(bipy)]$^+$	0.051	0.186	0.053	−0.059	−0.006	1.044

Table S7. Energy decomposition analysis (EDA) results of the [NgM-(bipy)]$^+$ complexes taking Ng as one fragment and [M-(bipy)]+ as another, studied at the BLYP-D3(BJ)/QZ4P//MPW1B95/cc-pVTZ level. All the energy terms are in kcal/mol. The percentage values within the parentheses show the contribution towards the total attractive interaction, $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$. [Reprinted from Ref. [85] with permission from John Wiley and Sons. © 2016 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim]

Systems	ΔE_{int}	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}	ΔE_{disp}
[ArCu-(bipy)]$^+$	−8.5	−15.8 (48.1%)	−14.8 (45.1%)	24.3	−2.2 (6.8%)
[KrCu-(bipy)]$^+$	−11.1	−21.1 (50.1%)	−18.2 (43.2%)	30.9	−2.8 (6.7%)
[XeCu-(bipy)]$^+$	−17.1	−28.0 (49.9%)	−24.4 (43.5%)	38.9	−3.7 (6.7%)
[RnCu-(bipy)]$^+$	−18.7	−27.6 (49.0%)	−24.8 (43.9%)	37.7	−4.0 (7.1%)
[ArAg-(bipy)]$^+$	−5.7	−8.8 (45.7%)	−8.5 (43.9%)	13.6	−2.0 (10.5%)
[KrAg-(bipy)]$^+$	−8.5	−14.2 (48.7%)	−12.4 (42.6%)	20.6	−2.5 (8.7%)
[XeAg-(bipy)]$^+$	−13.0	−23.6 (51.8%)	−18.7 (40.9%)	32.6	−3.3 (7.3%)
[RnAg-(bipy)]$^+$	−15.0	−25.0 (51.5%)	−20.0 (41.2%)	33.5	−3.5 (7.3%)
[ArAu-(bipy)]$^+$	−8.0	−19.3 (50.1%)	−17.0 (44.0%)	30.5	−2.3 (5.8%)
[KrAu-(bipy)]$^+$	−13.2	−31.4 (52.1%)	−26.0 (43.2%)	47	−2.9 (4.8%)
[XeAu-(bipy)]$^+$	−20.3	−46.9 (54.4%)	−35.6 (41.3%)	65.9	−3.7 (4.3%)

[RnAu-(bipy)]$^+$	−22.9	−48.5 (54.4%)	−36.7 (41.2%)	66.3	−3.9 (4.4%)

Table S8. EDA results of MNgCCH and NgMCCH at the PBE-D3(BJ)/QZ4P//CCSD(T)/cc-pVTZ level. All energy values are in kcal/mol. The values in parentheses are percentage contribution toward the total attraction, $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$. [Reprinted from Ref. [86] with permission from American Chemical Society. © 2017, American Chemical Society]

Systems	**Fragments**	ΔE_{int}	ΔE_{elstat}	ΔE_{orb}	ΔE_{Pauli}	ΔE_{disp}
CuXeCCH	Cu + XeCCH	−33.3	−58.6 (52.9)	−51.3 (46.3)	77.5	−0.9 (0.8)
CuRnCCH	Cu + RnCCH	−38.1	−64.1 (54.9)	−51.8 (44.3)	78.7	−0.9 (0.7)
AgXeCCH	Ag + XeCCH	−25.8	−40.0 (50.5)	−38.2 (48.2)	53.3	−1.0 (1.3)
AgRnCCH	Ag + RnCCH	−31.1	−50.4 (54.0)	−41.9 (44.9)	62.2	−1.0 (1.1)
AuXeCCH	Au + XeCCH	−38.5	−75.9 (55.2)	−60.6 (44.0)	99.2	−1.1 (0.8)
AuRnCCH	Au + RnCCH	−45.1	−84.6 (57.4)	−61.8 (41.9)	102.4	−1.1 (0.7)
ArCuCCH	Ar + CuCCH	−8.9	−12.3 (45.5)	−14.0 (51.9)	18.1	−0.7 (2.6)
KrCuCCH	Kr + CuCCH	−11.2	−15.8 (47.1)	−17.0 (50.5)	22.4	−0.8 (2.4)
XeCuCCH	Xe + CuCCH	−14.9	−19.9 (47.4)	−21.1 (50.2)	27.2	−1.0 (2.4)
RnCuCCH	Rn + CuCCH	−15.7	−20.4 (47.3)	−21.7 (50.2)	27.5	−1.0 (2.4)
ArAgCCH	Ar + AgCCH	−5.3	−7.2 (47.6)	−7.2 (47.6)	9.9	−0.7 (4.8)
KrAgCCH	Kr + AgCCH	−7.5	−11.6 (50.7)	−10.4 (45.5)	15.5	−0.9 (3.8)
XeAgCCH	Xe + AgCCH	−10.9	−17.9 (53.0)	−14.8 (43.8)	22.9	−1.1 (3.1)
RnAgCCH	Rn + AgCCH	−12.1	−19.6 (53.6)	−15.8 (43.4)	24.5	−1.1 (3.0)
ArAuCCH	Ar + AuCCH	−7.6	−13.3 (47.6)	−13.8 (49.5)	20.3	−0.8 (2.9)
KrAuCCH	Kr + AuCCH	−10.6	−20.0 (50.3)	−18.8 (47.4)	29.1	−0.9 (2.3)

XeAuCCH	Xe + AuCCH	−15.4	−29.8 (52.5)	−25.9 (45.5)	41.5	−1.1 (2.0)
RnAuCCH	Rn + AuCCH	−16.9	−32.3 (53.2)	−27.3 (44.9)	43.9	−1.2 (1.9)

Table S9. Electron density descriptors (au) at the BCPs of M-Ng and Ng-C bonds in MNgCCH compounds obtained from the wave functions generated at the MP2/ccpVTZ/WTBS//CCSD(T)/cc-pVTZ level (WTBS for Cu, Ag, Au, Xe and Rn atoms). [Reprinted from Ref. [86] with permission from American Chemical Society. © 2017, American Chemical Society]

Systems	**BCP**	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$G(r_c)/\rho(r_c)$
CuXeCCH	Cu–•–Xe	0.048	0.155	0.047	−0.1	−0.008	0.979
CuRnCCH	Cu–•–Rn	0.047	0.134	0.042	−0.1	−0.009	0.894
AgXeCCH	Ag–•–Xe	0.038	0.123	0.034	0.0	−0.003	0.895
AgRnCCH	Ag–•–Rn	0.040	0.119	0.034	0.0	−0.005	0.850
AuXeCCH	Au–•–Xe	0.055	0.178	0.052	−0.1	−0.008	0.945
AuRnCCH	Au–•–Rn	0.054	0.153	0.047	−0.1	−0.009	0.870

Table S10. Electron density descriptors (in au) calculated at the MP2/cc-pVTZ/WTBS//CCSD(T)/VTZ level. [Reprinted from Ref. [87] with permission from American Chemical Society. © 2018, American Chemical Society]

Systems	**BCP**	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$	$G(r_c)/\rho(r_c)$
CuCCKrH	Kr–C	0.080	0.104	0.050	−0.073	−0.024	0.621
CuCCXeH	Xe–C	0.082	0.084	0.051	−0.081	−0.030	0.626
CuCCRnH	Rn–C	0.078	0.097	0.053	−0.081	−0.028	0.676
AgCCKrH	Kr–C	0.080	0.103	0.050	−0.073	−0.024	0.619
AgCCXeH	Xe–C	0.082	0.083	0.051	−0.081	−0.030	0.622
AgCCRnH	Rn–C	0.082	0.083	0.051	−0.081	−0.030	0.622
AuCCKrH	Kr–C	0.079	0.106	0.050	−0.073	−0.023	0.628
AuCCXeH	Xe–C	0.079	0.085	0.050	−0.078	−0.028	0.626
AuCCRnH	Rn–C	0.076	0.096	0.051	−0.078	−0.027	0.673
CuCCKrH	Kr–H	0.118	−0.040	0.060	−0.130	−0.070	0.118
CuCCXeH	Xe–H	0.110	0.021	0.067	−0.128	−0.062	0.110
CuCCRnH	Rn–H	0.100	0.079	0.070	−0.120	−0.050	0.100

AgCCKrH	Kr–H	0.116	−0.034	0.060	−0.128	−0.068	0.116
AgCCXeH	Xe–H	0.109	0.022	0.066	−0.127	−0.060	0.109
AgCCRnH	Rn–H	0.099	0.079	0.069	−0.119	−0.050	0.099
AuCCKrH	Kr–H	0.130	−0.075	0.067	−0.153	−0.086	0.130
AuCCXeH	Xe–H	0.115	0.020	0.072	−0.140	−0.067	0.115
AuCCRnH	Rn–H	0.104	0.085	0.075	−0.130	−0.054	0.104

Table S11. EDA Results of MCCNgH at the PBE-D3/QZ4P//CCSD(T)/VTZ Level. All energy values are in kcal/mol. The values in parentheses are the percentage contribution toward the total attraction, $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$. [Reprinted from Ref. [87] with permission from American Chemical Society. © 2018, American Chemical Society]

Systems	**Fragments**	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{orb}	ΔE_{disp}
CuCCKrH	CuCCKr + H	−27.1	94.6	−50.3 (41.3)	−71.3 (58.6)	−0.1 (0.1)
CuCCXeH	CuCCXe + H	−40.3	96.0	−56.3 (41.3)	−80.0 (58.7)	−0.1 (0.1)
CuCCRnH	CuCCRn + H	−44.3	86.3	−55.3 (42.3)	−75.2 (57.6)	−0.1 (0.1)
AgCCKrH	AgCCKr + H	−27.5	91.2	−49.0 (41.2)	−69.7 (58.7)	−0.1 (0.1)
AgCCXeH	AgCCXe + H	−39.9	95.4	−55.8 (41.2)	−79.4 (58.7)	−0.1 (0.1)
AgCCRnH	AgCCRn + H	−43.9	86.1	−55.0 (42.3)	−74.9 (57.6)	−0.1 (0.1)
AuCCKrH	AuCCKr + H	−29.5	104.5	−54.8 (40.9)	−79.0 (59.0)	−0.1 (0.1)
AuCCXeH	AuCCXe + H	−40.6	101.6	−58.6 (41.2)	−83.5 (58.7)	−0.1 (0.1)
AuCCRnH	AuCCRn + H	−44.6	90.4	−57.3 (42.4)	−77.7 (57.5)	−0.1 (0.1)
CuCCKrH	$CuCC^- + KrH^+$	−164.2	120.0	−175.7 (61.8)	−108.1 (38.0)	−0.5 (0.2)
CuCCXeH	$CuCC^- + XeH^+$	−162.4	144.2	−195.6 (63.8)	−110.4 (36.0)	−0.5 (0.2)
CuCCRnH	$CuCC^- + RnH^+$	−163.8	139.5	−201.1 (66.3)	−101.6 (33.5)	−0.6 (0.2)
AgCCKrH	$AgCC^- + KrH^+$	−165.4	114.0	−170.9 (61.2)	−108.0 (38.7)	−0.4 (0.1)
AgCCXeH	$AgCC^- + XeH^+$	−163.2	142.5	−192.7 (63.0)	−112.5 (36.8)	−0.5 (0.2)
AgCCRnH	$AgCC^- + RnH^+$	−164.6	137.6	−197.9 (65.5)	−103.7 (34.3)	−0.6 (0.2)
AuCCKrH	$AuCC^- + KrH^+$	−154.0	109.9	−166.2 (63.0)	−97.3 (36.9)	−0.5 (0.2)
AuCCXeH	$AuCC^- + XeH^+$	−153.8	132.8	−183.8 (64.2)	−102.1 (35.6)	−0.6 (0.2)
AuCCRnH	$AuCC^- + RnH^+$	−155.5	129.0	−189.2 (66.5)	−94.7 (33.3)	−0.7 (0.2)