Electronic Supplementary Information

Theoretical Prediction of Donor-Acceptor type Novel Complexes with Strong Noble Gas−Boron Covalent Bond

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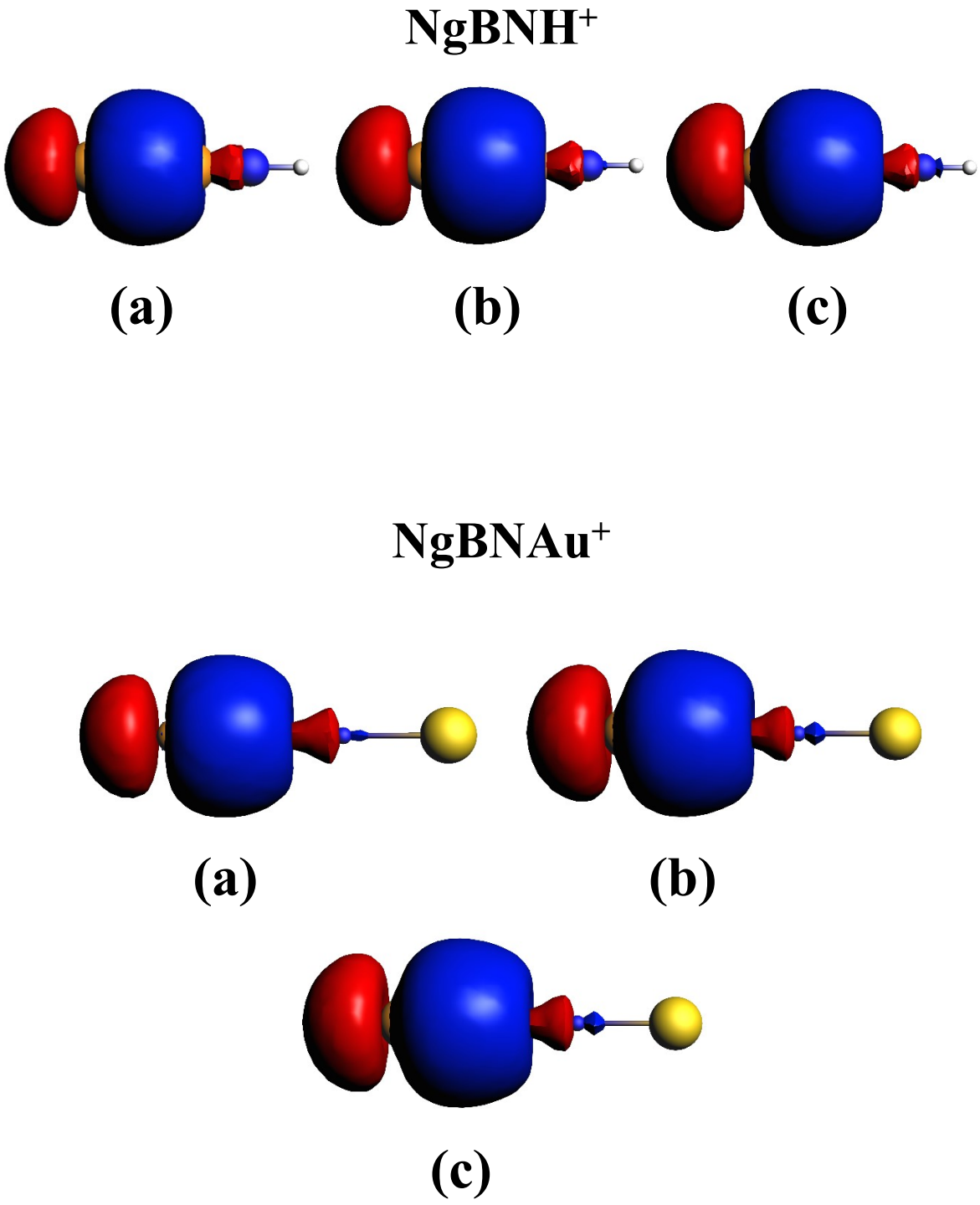
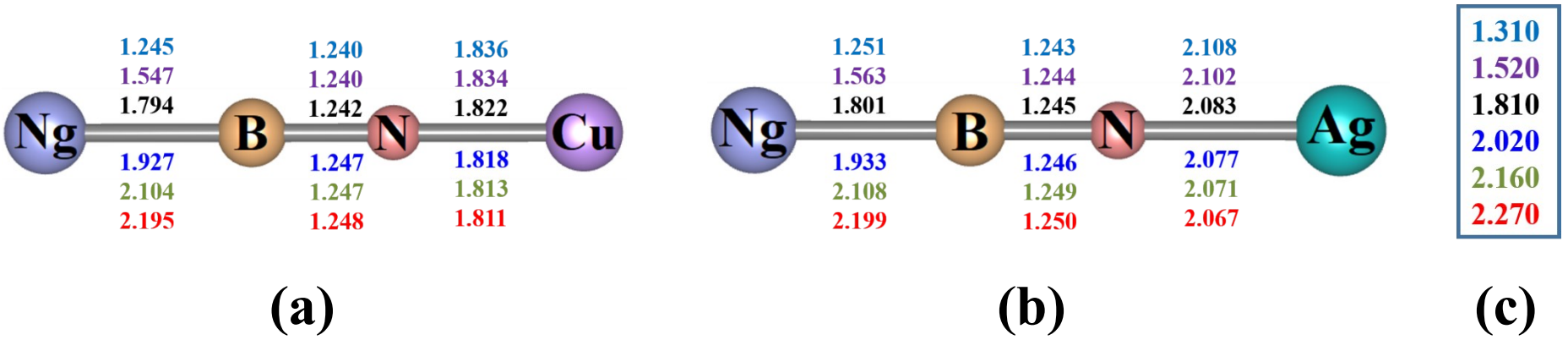


Figure S1. The plot of natural bonding orbitals (NBO) of Ng−B bonds in $NgBNH^+$ and $NgBNAu^+$ (Ng = (a) Kr, (b) Xe, and (c) Rn) ions calculated at B3LYP-D3/TZ2P level.



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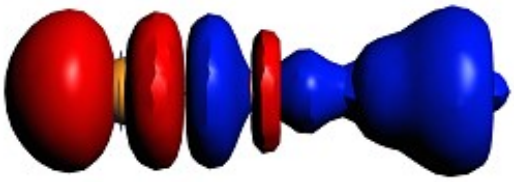
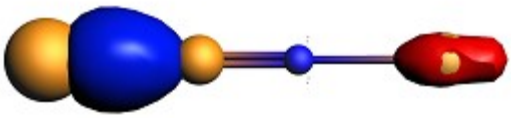
$KrBNCu^+$ ($Kr + BNCu^+$)



$\Delta\rho_1(\sigma_1)$

$\Delta E = -77.3$



$\Delta\rho_2(\sigma_2)$

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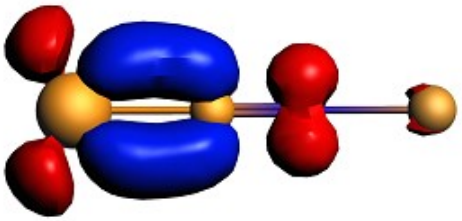

$\Delta\rho_3(\pi_1)$

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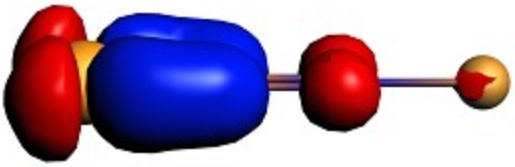
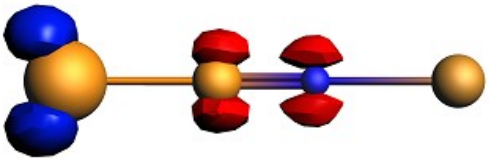


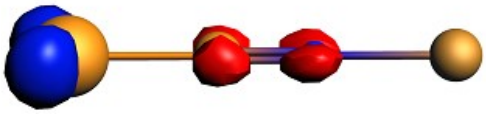
$\Delta\rho_4(\pi_2)$

$\Delta E = -10.1$



$\Delta\rho_5(\pi_3)$

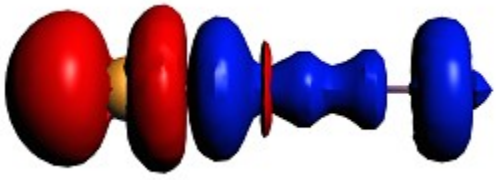
$\Delta E = -0.1$



$\Delta\rho_6(\pi_4)$

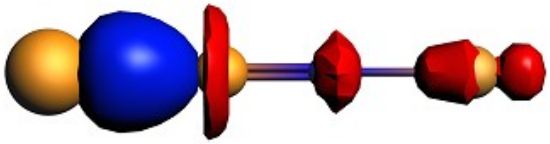
$\Delta E = -0.1$

$XeBNCu^+$ ($Xe + BNCu^+$)



$\Delta\rho_1(\sigma_1)$

$\Delta E = -91.8$



$\Delta\rho_2(\sigma_2)$

$\Delta E = -9.9$

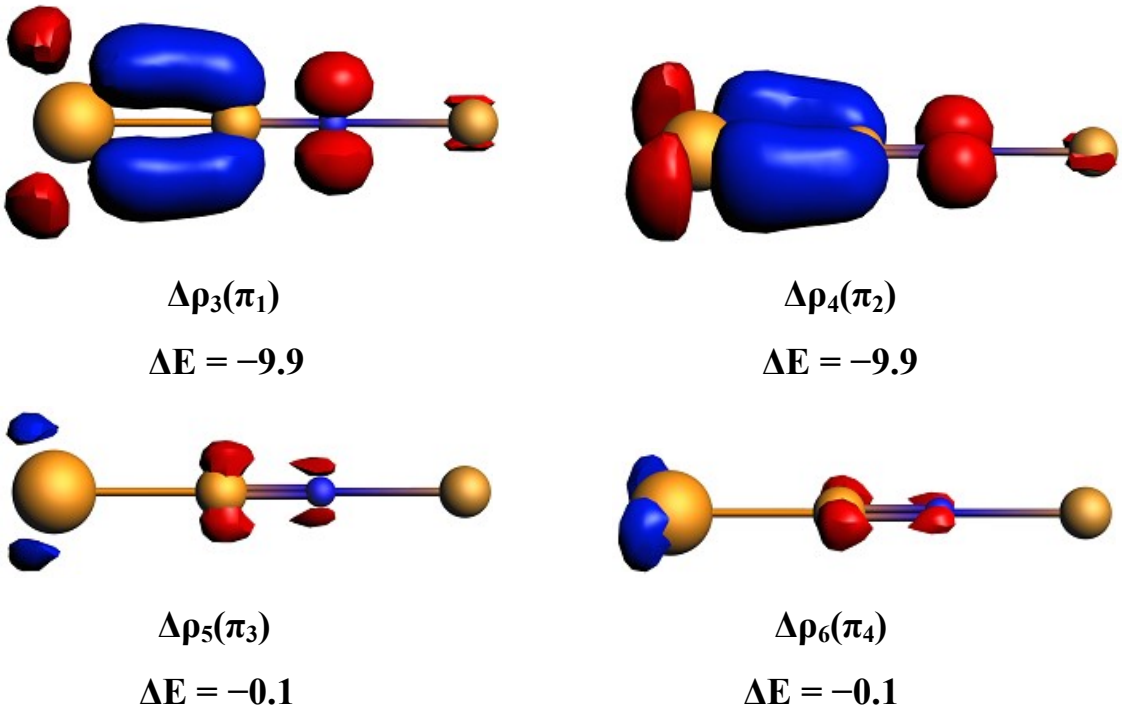
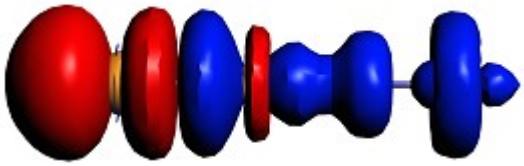


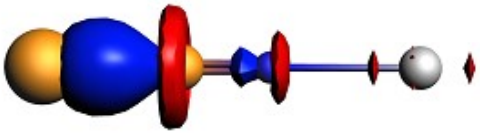
Figure S3. Plot of deformation densities Δρ(r), of the pair-wise orbital interactions in the predicted $NgBNCu^+$ (Ng = Kr and Xe) complexes at the B3LYP-D3/TZ2P level, where $\Delta\rho_1(r)$, $\Delta\rho_3(r)$, and $\Delta\rho_4(r)$ are the deformation densities corresponding to Ng → $BNCu^+$ (Ng = Kr and Xe) σ-, π-, and π-donations, respectively, while $\Delta\rho_2(r)$, $\Delta\rho_5(r)$, and $\Delta\rho_6(r)$ correspond to Ng ← $BNCu^+$ (Ng = Kr and Xe) σ-, π-, and π-back donations, respectively. The associated orbital interaction energies are provided in kcal mol^{-1}. The direction of the charge flow is from red to blue region.

$KrBNAg^+$ ($Kr + BNAg^+$)



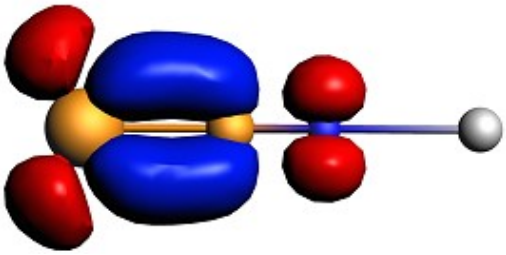
$\Delta\rho_1(\sigma_1)$

$\Delta E = -76.6$



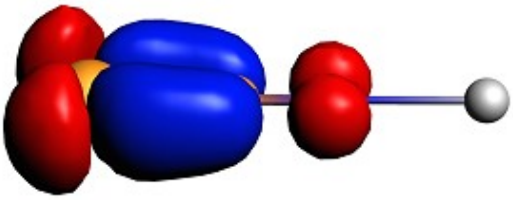
$\Delta\rho_2(\sigma_2)$

$\Delta E = -8.4$



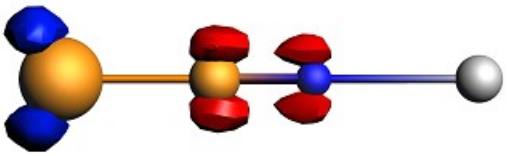
$\Delta\rho_3(\pi_1)$

$\Delta E = -9.4$



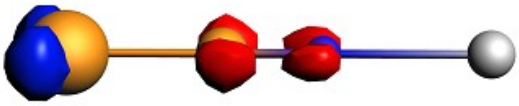
$\Delta\rho_4(\pi_2)$

$\Delta E = -9.4$



$\Delta\rho_5(\pi_3)$

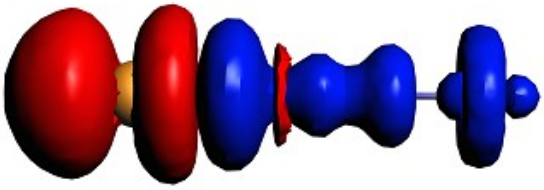
$\Delta E = -0.1$



$\Delta\rho_6(\pi_4)$

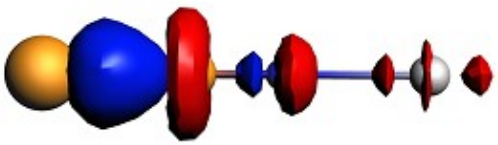
$\Delta E = -0.1$

$XeBNAg^+$ ($Xe + BNAg^+$)



$\Delta\rho_1(\sigma_1)$

$\Delta E = -90.4$



$\Delta\rho_2(\sigma_2)$

$\Delta E = -7.2$

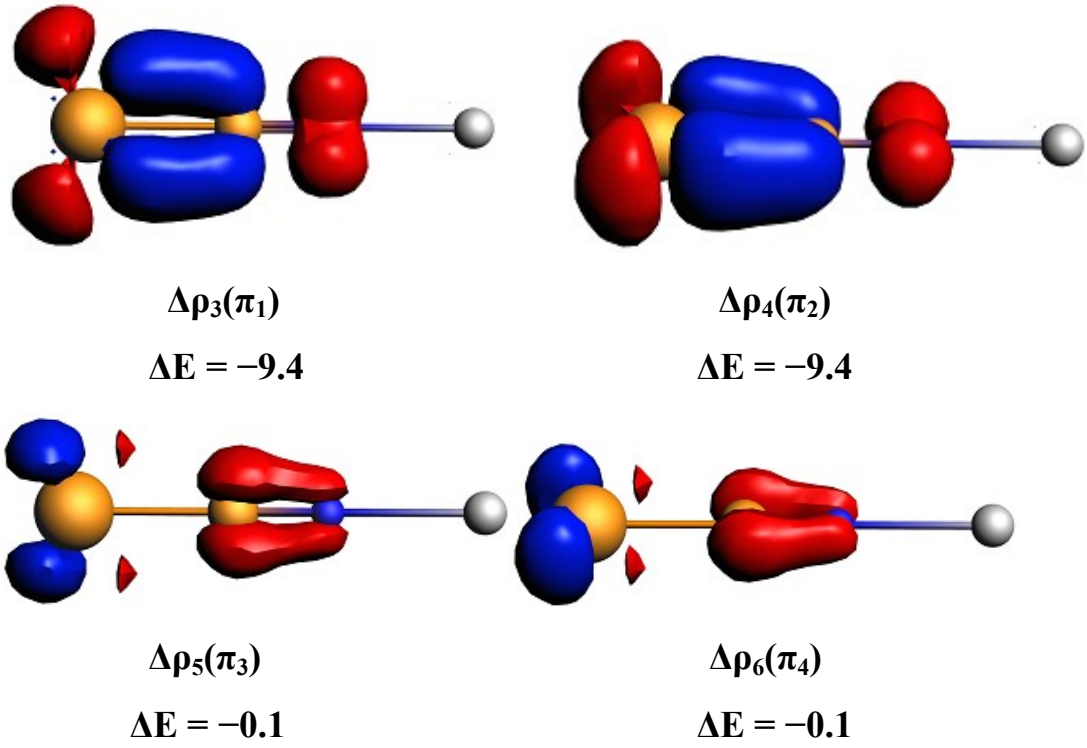


Figure S4. Plot of deformation densities Δρ(r), of the pair-wise orbital interactions in the predicted $NgBNAg^+$ (Ng = Kr and Xe) complexes at the B3LYP-D3/TZ2P level, where $\Delta\rho_1(r)$, $\Delta\rho_3(r)$, and $\Delta\rho_4(r)$ are the deformation densities corresponding to Ng → $BNAg^+$ (Ng = Kr and Xe) σ-, π-, and π-donations, respectively, while $\Delta\rho_2(r)$, $\Delta\rho_5(r)$, and $\Delta\rho_6(r)$ correspond to Ng ← $BNAg^+$ (Ng = Kr and Xe) σ-, π-, and π-back donations, respectively. The associated orbital interaction energies are provided in kcal mol^{-1}. The direction of the charge flow is from red to blue region.

Table S1. Calculated Values of Ng−B, B−N and N−H Bond Lengths (in Å) in the Predicted $NgBNH^+$ (Ng = He, Ne, Ar, Kr, Xe, and Rn) Ions as Obtained by Using B3LYP and MP2 Methods with DEF2 Basis Set and CCSD(T) Method with AVTZ Basis Set.

Ions	Method	R (Ng−B)	R (B−N)	R (N−H)
BNH^+	**B3LYP**	…	1.200	1.010
	MP2	…	1.218	1.009
	CCSD(T)	…	1.215	1.009
$HeBNH^+$	**B3LYP**	1.232	1.202	1.007
	MP2	1.227	1.219	1.006
	CCSD(T)	1.230	1.217	1.006
$NeBNH^+$	**B3LYP**	1.505	1.202	1.005
	MP2	1.502	1.217	1.004
	CCSD(T)	1.501	1.215	1.005
$ArBNH^+$	**B3LYP**	1.769	1.209	1.002
	MP2	1.762	1.223	1.002
	CCSD(T)	1.772	1.221	1.002
$KrBNH^+$	**B3LYP**	1.915	1.212	1.001
	MP2	1.904	1.226	1.002
	CCSD(T)	1.909	1.224	1.002
$XeBNH^+$	**B3LYP**	2.095	1.215	1.000
	MP2	2.080	1.230	1.001
	CCSD(T)	2.092	1.228	1.001
$RnBNH^+$	**B3LYP**	2.188	1.216	1.000
	MP2	2.173	1.231	1.000
	CCSD(T)	2.184	1.229	1.000

Table S2. Calculated Values of Ng−B, B−N and N−Au Bond Lengths (in Å) in the Predicted $NgBNAu^+$ (Ng = He, Ne, Ar, Kr, Xe, and Rn) Ions as Obtained by Using B3LYP and MP2 Methods with DEF2 Basis Set and CCSD(T) Method with AVTZ Basis Set.

Ions	Method	R (Ng−B)	R (B−N)	R (N−Au)
$BNAu^+$	**B3LYP**	…	1.238	1.950
	MP2	…	1.296	1.955
	CCSD(T)	…	1.264	1.952
$HeBNAu^+$	**B3LYP**	1.237	1.219	1.968
	MP2	1.235	1.242	1.948
	CCSD(T)	1.239	1.235	1.977
$NeBNAu^+$	**B3LYP**	1.541	1.220	1.969
	MP2	1.539	1.242	1.948
	CCSD(T)	1.537	1.234	1.976
$ArBNAu^+$	**B3LYP**	1.783	1.223	1.957
	MP2	1.776	1.244	1.934
	CCSD(T)	1.788	1.237	1.962
$KrBNAu^+$	**B3LYP**	1.927	1.225	1.954
	MP2	1.915	1.246	1.930
	CCSD(T)	1.921	1.239	1.958
$XeBNAu^+$	**B3LYP**	2.102	1.228	1.949
	MP2	2.086	1.249	1.924
	CCSD(T)	2.099	1.242	1.953
$RnBNAu^+$	**B3LYP**	2.195	1.229	1.947
	MP2	2.178	1.250	1.922
	CCSD(T)	2.190	1.243	1.950

Table S3. Comparison of Ng−B Bond Length (R in Å) and Ng−B Binding Energies (BE in kJ mol^{-1}) (Ng = He and Xe) in the Various Donor−Acceptor Type Chemical Systems Containing Ng−B Bonding Motif at MP2/DEF2 Level of Theory.

Ions	R (Ng−B)		BE(Ng−B)	
	He	Xe	He	Xe
[a]**NgBNH$^+$**	1.227	2.080	135.5	398.3
[a]**NgBNAu$^+$**	1.235	2.086	75.1	299.8
[b]**NgBO$^+$**	1.243	2.084	120.9	426.5
[b]**NgBS$^+$**	1.268	2.102	76.7	331.6
[c]**Ng$_3$B$_3^+$**	1.510	2.240	4.1	119.4
[c]**Ng$_4$B$_4^{2+}$**	1.379	2.298	39.2	234.5
[c]**Ng$_5$B$_5^{3+}$**	1.372	2.257	53.2	278.4
[c]**Ng$_6$B$_6^{4+}$**	1.374	2.245	66.1	370.3
[d]**NgBH$_3$BF^{2+}**	1.232	2.091	152.4	554.0
[d]**NgBH$_3$BH^{2+}**	1.241	2.095	144.4	551.6
[d]**NgBH$_3$BCH$_3^{2+}$**	1.242	2.098	129.8	495.2

[a]Presently reported systems; [b]Ref. 62; [c]Ref. 58; [d]Ref. 11

Table S4. Calculated Values of the Harmonic Vibrational Frequencies (in cm^{-1}) and Intrinsic Force Constants (in N m^{-1}) in the Parentheses Corresponding to Individual Internal Coordinates of $NgBNM^+$ (Ng = He, Ne, Ar, Kr, Xe, and Rn; M = H and Au) Ions using B3LYP and MP2 Methods with DEF2 Basis Set.

Ions	M	Ng−B Stretch		B−N Stretch		N−M Stretch		Ng−B−N Bend		B−N−M Bend	
		B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
$HeBNM^+$	H	1123.6 (277.8)	1131.4 (286.9)	2148.4 (1640.6)	2049.2 (1470.6)	3698.6 (744.1)	3714.9 (751.8)	276.5	255.7	689.8	665.2
	Au	1083.7 (251.8)	1084.6 (255.8)	2116.3 (1469.9)	1983.2 (1252.2)	380.8 (226.7)	390.5 (257.7)	231.1	182.1	165.5	172.8
$NeBNM^+$	H	574.8 (229.2)	635.5 (245.9)	2123.5 (1646.2)	2038.7 (1503.1)	3717.5 (752.1)	3736.8 (760.8)	236.3	236.9	655.2	635.5
	Au	600.6 (183.3)	628.9 (202.1)	2079.2 (1458.5)	1960.0 (1264.9)	268.2 (232.1)	272.1 (265.7)	100.2	188.8	215.3	118.6
$ArBNM^+$	H	530.9 (264.0)	550.0 (296.2)	2089.1 (1579.6)	2017.4 (1454.6)	3748.5 (766.0)	3761.4 (771.8)	257.4	248.2	643.8	635.8
	Au	642.1 (246.8)	672.5 (278.5)	2073.3 (1436.6)	1973.6 (1266.5)	231.9 (248.9)	238.1 (284.0)	261.7	234.4	104.1	107.3
$KrBNM^+$	H	457.5 (244.7)	477.8 (278.9)	2072.3 (1559.3)	1999.8 (1435.3)	3758.1 (770.3)	3767.4 (774.5)	252.0	244.2	635.5	629.1
	Au	612.6 (233.8)	645.0 (268.7)	2061.2 (1422.9)	1961.6 (1254.1)	178.9 (254.1)	184.5 (289.5)	260.9	236.2	97.0	99.9
$XeBNM^+$	H	417.7 (220.0)	438.7 (253.1)	2047.6 (1528.6)	1974.6 (1406.9)	3769.4 (775.4)	3775.1 (778.0)	242.3	238.0	626.0	623.9
	Au	599.6 (215.1)	632.6 (249.8)	2042.1 (1400.3)	1942.8 (1233.9)	153.7 (260.5)	159.4 (296.6)	256.8	236.8	91.1	94.0
$RnBNM^+$	H	387.7 (202.9)	407.0 (233.0)	2037.5 (1518.1)	1964.1 (1397.8)	3775.3 (778.1)	3780.1 (780.3)	235.3	230.9	618.5	615.8
	Au	586.8 (199.5)	618.9 (231.7)	2033.6 (1391.6)	1934.4 (1227.0)	131.3 (263.7)	136.2 (300.3)	249.7	229.6	87.8	90.5

Table S5. Calculated Values of Mulliken Charges on the Constituent Atoms in the Predicted NgBNM$^+$ (Ng = He−Rn; M = H and Au) Ions as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set.

Ions	*q*(Ng)		*q*(B)		*q*(N)		*q*(H)	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBNH$^+$	0.088	0.063	−0.027	0.061	0.648	0.583	0.291	0.293
NeBNH$^+$	0.211	0.207	−0.277	−0.182	0.778	0.675	0.288	0.301
ArBNH$^+$	0.400	0.387	−0.111	0.064	0.440	0.272	0.270	0.277
KrBNH$^+$	0.376	0.338	0.032	0.186	0.338	0.207	0.255	0.268
XeBNH$^+$	0.661	0.660	−0.226	−0.037	0.324	0.128	0.240	0.249
RnBNH$^+$	0.639	0.647	−0.166	0.014	0.292	0.096	0.235	0.243
Ions	***q*(Ng)**		***q*(B)**		***q*(N)**		***q*(Au)**	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBNAu$^+$	0.078	0.055	−0.393	−0.222	1.047	0.799	0.268	0.368
NeBNAu$^+$	0.193	0.191	−0.620	−0.430	1.168	0.881	0.259	0.358
ArBNAu$^+$	0.366	0.359	−0.353	−0.094	0.804	0.449	0.183	0.286
KrBNAu$^+$	0.315	0.282	−0.254	−0.067	0.787	0.536	0.153	0.249
XeBNAu$^+$	0.578	0.574	−0.395	−0.120	0.694	0.326	0.124	0.220
RnBNAu$^+$	0.564	0.569	−0.397	−0.124	0.723	0.349	0.110	0.206

Table S6. Calculated Values of Atoms-in-Molecule (AIM) Charges[a] on the Constituent Atoms in the Predicted $NgBNM^+$ (Ng = He−Rn; M = H and Au) Ions as Obtained by Using B3LYP Method with the DEF2 Basis Set.

Ions	*q*(Ng)	*q*(B)	*q*(N)	*q*(H)
$HeBNH^+$	–0.001	1.999	–1.588	0.590
$NeBNH^+$	0.044	2.014	–1.643	0.585
$ArBNH^+$	0.105	1.987	–1.664	0.572
$KrBNH^+$	0.189	1.917	–1.671	0.565

[a]Since we have used the pseudo-potentials for Xe, Au, and Rn atoms, thereby, we have restricted our calculations for $NgBNH^+$ (Ng = He-Kr) only.

Table S7. Calculated Values of the NBO Occupancy, Contribution from the Atoms Constructing that NBO, Atomic Contributions Towards that NBO and the Wiberg Bond Index (WBI) of Ng−B Bonds in $NgBNM^+$ (Ng = He−Rn; M = H and Au) Ions Calculated at B3LYP-D3/TZ2P Level.

Ions	Bonds	NBO Occupancy	WBI	Atomic Contribution (%)	Atomic Orbitals Contribution to NBO (%)	
$HeBNH^+$	He−B	1.995	0.51	He (85.3)	s (99.9)	p (0.1)
				B (14.7)	s (43.2)	p (56.4)
$NeBNH^+$	Ne−B	1.997	0.45	Ne (89.4)	s (29.7)	p (70.1)
				B (10.6)	s (42.4)	p (57.1)
$ArBNH^+$	Ar−B	1.997	0.87	Ar (77.0)	s (20.7)	p (78.8)
				B (23.0)	s (44.8)	p (54.9)
$KrBNH^+$	Kr−B	1.997	0.96	Kr (72.8)	s (15.9)	p (83.5)
				B (27.2)	s (45.6)	p (54.1)
$XeBNH^+$	Xe−B	1.997	1.07	Xe (67.0)	s (13.5)	p (86.0)
				B (33.0)	s (47.0)	p (52.7)
$RnBNH^+$	Rn−B	1.997	1.09	Rn (65.2)	s (9.5)	p (90.2)
				B (34.8)	s (47.8)	p (51.9)
Ions	**Bonds**	**NBO Occupancy**	**WBI**	**Atomic Contribution (%)**	**Atomic Orbitals Contribution to NBO (%)**	
$HeBNAu^+$	He−B	1.995	0.51	He (85.6)	s (99.9)	p (0.1)
				B (14.5)	s (42.7)	p (56.8)
$NeBNAu^+$	Ne−B	1.996	0.41	Ne (90.1)	s (29.7)	p (70.2)
				B (9.9)	s (40.9)	p (58.6)
$ArBNAu^+$	Ar−B	1.996	0.83	Ar (78.0)	s (21.4)	p (78.1)
				B (22.0)	s (44.4)	p (55.3)
$KrBNAu^+$	Kr−B	1.996	0.93	Kr (74.1)	s (16.8)	p (82.8)
				B (25.9)	s (45.2)	p (54.5)
$XeBNAu^+$	Xe−B	1.996	1.03	Xe (68.2)	s (14.7)	p (85.8)
				B (32.8)	s (46.5)	p (53.1)
$RnBNAu^+$	Rn−B	1.996	1.06	Rn (66.8)	s (10.2)	p (89.4)
				B (33.2)	s (47.3)	p (52.4)

Table S8. Calculated Values of Ng−B, B−N and N−Cu Bond Lengths (in Å) in the Predicted $NgBNCu^+$ (Ng = He, Ne, Ar, Kr, Xe, and Rn) Ions as Obtained by Using B3LYP and MP2 Methods with DEF2 Basis Set and CCSD(T) Method with AVTZ Basis Set.

Ions	Method	R (Ng−B)	R (B−N)	R (N−Cu)
$HeBNCu^+$	**B3LYP**	1.241	1.223	1.848
	MP2	1.241	1.248	1.831
	CCSD(T)	1.245	1.240	1.836
$NeBNCu^+$	**B3LYP**	1.551	1.225	1.845
	MP2	1.550	1.249	1.828
	CCSD(T)	1.547	1.240	1.834
$ArBNCu^+$	**B3LYP**	1.789	1.228	1.835
	MP2	1.783	1.250	1.816
	CCSD(T)	1.794	1.242	1.822
$KrBNCu^+$	**B3LYP**	1.933	1.230	1.832
	MP2	1.922	1.252	1.812
	CCSD(T)	1.927	1.244	1.818
$XeBNCu^+$	**B3LYP**	2.108	1.232	1.827
	MP2	2.092	1.254	1.806
	CCSD(T)	2.104	1.247	1.813
$RnBNCu^+$	**B3LYP**	2.200	1.234	1.825
	MP2	2.185	1.256	1.804
	CCSD(T)	2.195	1.248	1.811

Table S9. Calculated Values of Ng−B, B−N and N−Ag Bond Lengths (in Å) in the Predicted $NgBNAg^+$ (Ng = He, Ne, Ar, Kr, Xe, and Rn) Ions as Obtained by Using B3LYP and MP2 Methods with DEF2 Basis Set and CCSD(T) Method with AVTZ Basis Set.

Ions	Method	R (Ng−B)	R (B−N)	R (N−Ag)
$HeBNAg^+$	**B3LYP**	1.244	1.224	2.089
	MP2	1.246	1.252	2.086
	CCSD(T)	1.251	1.243	2.108
$NeBNAg^+$	**B3LYP**	1.558	1.226	2.082
	MP2	1.563	1.253	2.079
	CCSD(T)	1.563	1.244	2.102
$ArBNAg^+$	**B3LYP**	1.793	1.228	2.068
	MP2	1.788	1.252	2.061
	CCSD(T)	1.801	1.245	2.083
$KrBNAg^+$	**B3LYP**	1.936	1.230	2.062
	MP2	1.927	1.254	2.055
	CCSD(T)	1.933	1.246	2.077
$XeBNAg^+$	**B3LYP**	2.111	1.232	2.056
	MP2	2.096	1.257	2.048
	CCSD(T)	2.108	1.249	2.071
$RnBNAg^+$	**B3LYP**	2.203	1.233	2.052
	MP2	2.188	1.258	2.045
	CCSD(T)	2.199	1.250	2.067

Table S10. Calculated Values of Ng–B, B–N, N–M Stretch and Ng–B–N, N−B−M Bending Frequencies (in cm^{-1}) along with their Corresponding IR Intensities (in km mol^{-1}) are Provided within the Parenthesis in the Predicted $NgBNM^+$ (Ng = He−Rn; M = Cu and Ag) Ions as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set.

Ions	Ng–B Stretch		B–N Stretch		N–Cu Stretch		Ng–B–N Bend		B–N–Cu Bend	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
$HeBNCu^+$	1182.9 (0.1)	1185.0 (1.3)	1991.3 (3.5)	1827.5 (0.1)	540.5 (0.1)	544.5 (0.8)	212.0 (7.4)	200.3 (0.2)	197.6 (51.0)	169.1 (55.3)
$NeBNCu^+$	639.4 (28.6)	672.1 (19.9)	1976.4 (39.2)	1828.3 (16.4)	545.7 (12.2)	552.9 (12.0)	159.2 (6.7)	178.0 (17.8)	184.6 (28.4)	149.1 (12.2)
$ArBNCu^+$	685.9 (1.3)	727.0 (1.2)	1966.3 (60.9)	1836.6 (24.2)	567.1 (4.5)	574.2 (6.1)	220.2 (22.6)	207.7 (15.8)	189.6 (12.3)	169.0 (16.8)
$KrBNCu^+$	630.3 (0.1)	674.5 (0.1)	1957.5 (66.8)	1828.5 (22.1)	573.1 (5.4)	580.3 (6.6)	217.8 (20.5)	205.1 (15.5)	189.7 (10.4)	170.9 (12.0)
$XeBNCu^+$	593.8 (2.2)	638.7 (3.7)	1943.3 (66.3)	1815.5 (16.2)	580.5 (4.2)	587.6 (5.2)	210.9 (17.4)	201.4 (15.3)	188.5 (12.6)	170.6 (14.3)
$RnBNCu^+$	563.2 (3.3)	606.1 (5.9)	1937.0 (75.7)	1810.0 (19.0)	584.1 (5.0)	591.5 (5.8)	203.2 (17.6)	194.6 (13.7)	185.3 (13.0)	166.9 (14.8)
Ions	**Ng–B Stretch**		**B–N Stretch**		**N–Ag Stretch**		**Ng–B–N Bend**		**B–N–Ag Bend**	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
$HeBNAg^+$	1165.0 (0.2)	1157.0 (1.7)	1990.5 (6.5)	1806.2 (7.8)	440.7 (1.0)	451.5 (3.1)	238.8 (1.1)	208.1 (3.4)	160.2 (53.7)	124.3 (49.3)
$NeBNAg^+$	629.5 (24.8)	648.0 (19.0)	1973.2 (40.2)	1800.2 (11.3)	446.9 (7.4)	459.1 (11.1)	186.3 (23.2)	181.6 (10.9)	147.9 (9.8)	100.5 (15.2)
$ArBNAg^+$	679.1 (0.5)	718.3 (0.4)	1966.5 (64.1)	1819.3 (20.3)	468.2 (3.7)	480.6 (5.8)	230.6 (17.1)	209.9 (10.7)	150.6 (12.8)	124.8 (14.9)
$KrBNAg^+$	625.5 (0.1)	668.7 (0.5)	1958.2 (69.3)	1812.5 (17.9)	474.2 (4.1)	486.6 (5.8)	227.5 (16.3)	208.7 (10.7)	149.0 (10.5)	125.8 (12.5)
$XeBNAg^+$	590.6 (3.9)	634.7 (6.7)	1945.0 (68.3)	1801.1 (12.1)	481.2 (3.5)	493.7 (4.9)	218.1 (13.5)	203.1 (8.8)	147.9 (10.9)	127.0 (12.8)
$RnBNAg^+$	560.5 (5.3)	603.1 (9.2)	1938.8 (76.2)	1795.8 (13.5)	484.9 (4.1)	497.7 (5.3)	210.7 (11.8)	197.2 (7.6)	145.0 (11.0)	124.4 (13.1)

Table S11. Calculated Values of Ng−B Binding Energies (BE) (in kJ mol^{-1}) in the Predicted NgBNCu$^+$ and NgBNAg$^+$ (Ng = He−Rn) Ions as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set and CCSD(T) Method with AVTZ Basis Set.

Ions	BE (Ng−B)			BE (Ng−B)[a]		
	B3LYP	MP2	CCSD(T)	B3LYP	MP2	CCSD(T)
HeBNCu$^+$	76.9	79.1	63.2	50.8	54.4	39.0
NeBNCu$^+$	61.5	68.5	53.3	40.1	47.9	33.5
ArBNCu$^+$	183.5	199.1	179.3	161.4	177.8	157.9
KrBNCu$^+$	219.4	238.8	220.2	197.8	217.6	199.4
XeBNCu$^+$	267.8	291.4	274.8	246.6	271.0	254.0
RnBNCu$^+$	284.7	308.8	293.4	263.9	288.7	272.8
Ions	**BE (Ng−B)**			**BE (Ng−B)[a]**		
	B3LYP	**MP2**	**CCSD(T)**	**B3LYP**	**MP2**	**CCSD(T)**
HeBNAg$^+$	81.5	66.4	61.5	56.3	43.0	38.6
NeBNAg$^+$	65.8	55.3	51.2	45.3	36.1	33.0
ArBNAg$^+$	184.0	181.0	171.7	162.9	161.0	153.2
KrBNAg$^+$	218.9	219.6	211.1	198.3	199.5	191.5
XeBNAg$^+$	266.0	270.8	263.9	245.8	251.6	244.5
RnBNAg$^+$	282.4	287.5	281.7	262.6	268.6	262.5

[a]Corresponds to the zero point energy (ZPE) corrected Ng−B binding energy.

Table S12. Calculated Values of NBO Charges on the Constituent Atoms in the Predicted $NgBNM^+$ (Ng = He−Rn; M = Cu and Ag) Ions as Obtained by Using B3LYP and MP2 Methods with the AVTZ Basis Set Using MOLPRO Program.

Ions	*q*(Ng)		*q*(B)		*q*(N)		*q*(Cu)	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
$HeBNCu^+$	0.287	0.274	0.836	0.821	−1.067	−1.053	0.944	0.959
$NeBNCu^+$	0.226	0.223	1.013	0.984	−1.179	−1.162	0.940	0.955
$ArBNCu^+$	0.504	0.509	0.685	0.644	−1.108	−1.093	0.919	0.940
$KrBNCu^+$	0.590	0.598	0.614	0.564	−1.118	−1.099	0.914	0.937
$XeBNCu^+$	0.713	0.732	0.505	0.437	−1.125	−1.101	0.908	0.932
$RnBNCu^+$	0.742	0.763	0.504	0.433	−1.149	−1.125	0.904	0.929
Ions	***q*(Ng)**		***q*(B)**		***q*(N)**		***q*(Ag)**	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
$HeBNAg^+$	0.285	0.271	0.812	0.786	−1.053	−1.027	0.957	0.970
$NeBNAg^+$	0.222	0.217	0.990	0.952	−1.168	−1.137	0.955	0.969
$ArBNAg^+$	0.498	0.500	0.664	0.614	−1.098	−1.069	0.936	0.955
$KrBNAg^+$	0.582	0.588	0.594	0.534	−1.108	−1.074	0.932	0.952
$XeBNAg^+$	0.703	0.720	0.487	0.408	−1.115	−1.076	0.926	0.947
$RnBNAg^+$	0.731	0.750	0.486	0.405	−1.139	−1.100	0.922	0.945

Table S13. Calculated Values of Ng−B Bond Critical Point (BCP) Electron Density (ρ in e a_0^{-3}), Laplacian of Electron Density ($\nabla^2\rho$ in e a_0^{-5}), the Local Electron Energy Density (E_d in a.u.), and Ratio of Local Electron Kinetic Energy Density and Electron Density (G/ρ in a.u.) in the Predicted $NgBNM^+$ (Ng = He−Rn; M = Cu and Ag) Complexes as Obtained by UsingB3LYP and MP2 Methods with the DEF2 Basis Set.

Complexes	ρ		$\nabla^2\rho$		E_d		G/ρ	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
$HeBNCu^+$	0.095	0.091	0.859	0.955	−0.026	−0.017	2.537	2.802
$NeBNCu^+$	0.073	0.069	0.625	0.702	−0.021	−0.013	2.425	2.725
$ArBNCu^+$	0.105	0.104	0.299	0.385	−0.079	−0.075	1.457	1.654
$KrBNCu^+$	0.104	0.104	0.079	0.169	−0.090	−0.089	1.058	1.260
$XeBNCu^+$	0.105	0.107	−0.134	−0.072	−0.094	−0.103	0.571	0.794
$RnBNCu^+$	0.100	0.102	−0.162	−0.174	−0.074	−0.092	0.333	0.471
Complexes	**ρ**		**$\nabla^2\rho$**		**E_d**		**G/ρ**	
	B3LYP	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**	**B3LYP**	**MP2**
$HeBNAg^+$	0.093	0.089	0.854	0.946	−0.025	−0.015	2.532	2.831
$NeBNAg^+$	0.071	0.066	0.616	0.676	−0.019	−0.011	2.437	2.727
$ArBNAg^+$	0.104	0.102	0.302	0.388	−0.077	−0.073	1.462	1.667
$KrBNAg^+$	0.103	0.102	0.085	0.177	−0.088	−0.086	1.058	1.284
$XeBNAg^+$	0.104	0.105	−0.126	−0.060	−0.092	−0.100	0.587	0.810
$RnBNAg^+$	0.100	0.101	−0.159	−0.163	−0.074	−0.096	0.340	0.495

Table S14: EDA-NOCV Results of NgBNM$^+$ (Ng = He−Rn; M = Cu and Ag) Ions Considering Ng as One Fragment and BNM$^+$ as Another Fragment at the B3LYP-D3/TZ2P Level of Theory. All Energy Terms are Expressed in kcal mol^{-1}.

Ions	ΔE^{Pauli}	ΔE^{elstat}	ΔE_T^{orb}	ΔE_1^{orb}	ΔE_2^{orb}	ΔE_3^{orb}	ΔE_4^{orb}	ΔE_5^{orb}	ΔE_6^{orb}	ΔE_7^{orb}	ΔE^{disp}	ΔE^{int}
HeBNCu$^+$	62.2	−13.1	−65.9	−38.1	−21.9	−2.4	−2.4	−0.5	…[a]	…[a]	−0.1	−16.9
NeBNCu$^+$	64.4	−24.8	−53.1	−32.4	−9.6	−4.1	−4.1	−1.0	−1.0	−0.3	−0.2	−13.7
ArBNCu$^+$	91.2	−32.8	−102.4	−66.7	−13.9	−9.9	−9.9	−0.2	−0.2	−0.5	−0.6	−44.5
KrBNCu$^+$	91.0	−32.5	−111.8	−77.3	−11.7	−10.1	−10.1	−0.1	−0.1	…[a]	−0.7	−53.9
XeBNCu$^+$	88.8	−30.6	−123.1	−91.8	−9.9	−9.9	−9.9	−0.1	−0.1	−0.4	−0.8	−65.8
RnBNCu$^+$	83.3	−28.8	−123.8	−96.7	−8.3	−8.9	−8.9	−0.1	−0.1	…[a]	−1.0	−70.2
Ions	ΔE^{Pauli}	ΔE^{elstat}	ΔE_T^{orb}	ΔE_1^{orb}	ΔE_2^{orb}	ΔE_3^{orb}	ΔE_4^{orb}	ΔE_5^{orb}	ΔE_6^{orb}	ΔE_7^{orb}	ΔE^{disp}	ΔE^{int}
HeBNAg$^+$	52.8	−10.6	−59.6	−37.6	−17.7	−2.0	−2.0	…[a]	…[a]	…[a]	−0.0	−17.3
NeBNAg$^+$	53.8	−19.8	−48.0	−31.5	−6.9	−4.2	−4.2	−0.4	−0.4	…[a]	−0.1	−14.1
ArBNAg$^+$	80.2	−26.9	−96.2	−66.3	−10.0	−9.3	−9.3	−0.2	−0.2	…[a]	−0.4	−43.3
KrBNAg$^+$	80.6	−26.7	−105.7	−76.6	−8.4	−9.4	−9.4	−0.1	−0.1	…[a]	−0.6	−52.4
XeBNAg$^+$	79.4	−25.3	−117.1	−90.4	−7.2	−9.3	−9.3	−0.1	−0.1	−0.4	−0.7	−63.7
RnBNAg$^+$	74.8	−23.8	−118.1	−95.0	−5.9	−8.3	−8.3	−0.1	−0.1	…[a]	−0.9	−67.9

[a]The corresponding value is below the cut-off value of ADF to be listed in the EDA-NOCV results.