

Electronic Supplementary Information

Prediction of Donor-Acceptor Type Novel Noble Gas Complexes in the Triplet Electronic State

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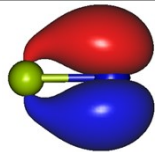
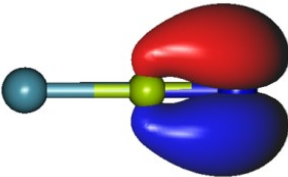
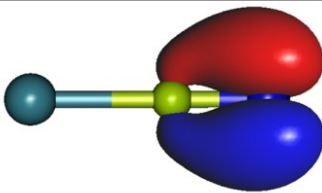
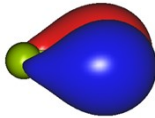
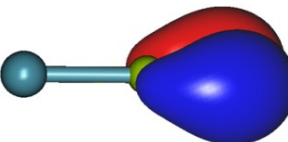
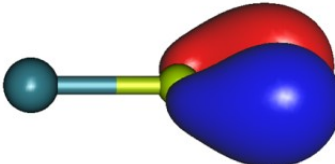
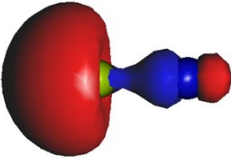
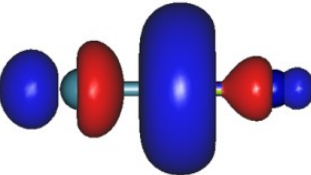
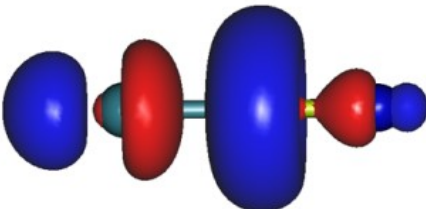
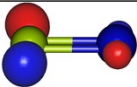
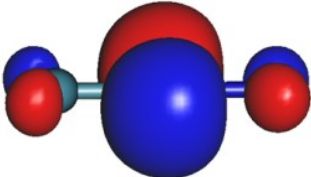
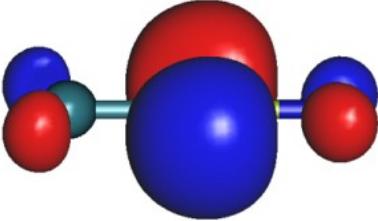
Energy Levels	BeN ⁺	KrBeN ⁺	XeBeN ⁺
HOMO-1			
HOMO			
LUMO			
LUMO+1			

Figure S1. Molecular orbital pictures of highest occupied and lowest unoccupied molecular orbitals of precursor BeN⁺ ion and NgBeN⁺ (Ng = Kr and Xe) complexes calculated using B3LYP method with DEF2 basis set. An isovalue of 0.02 has been used.

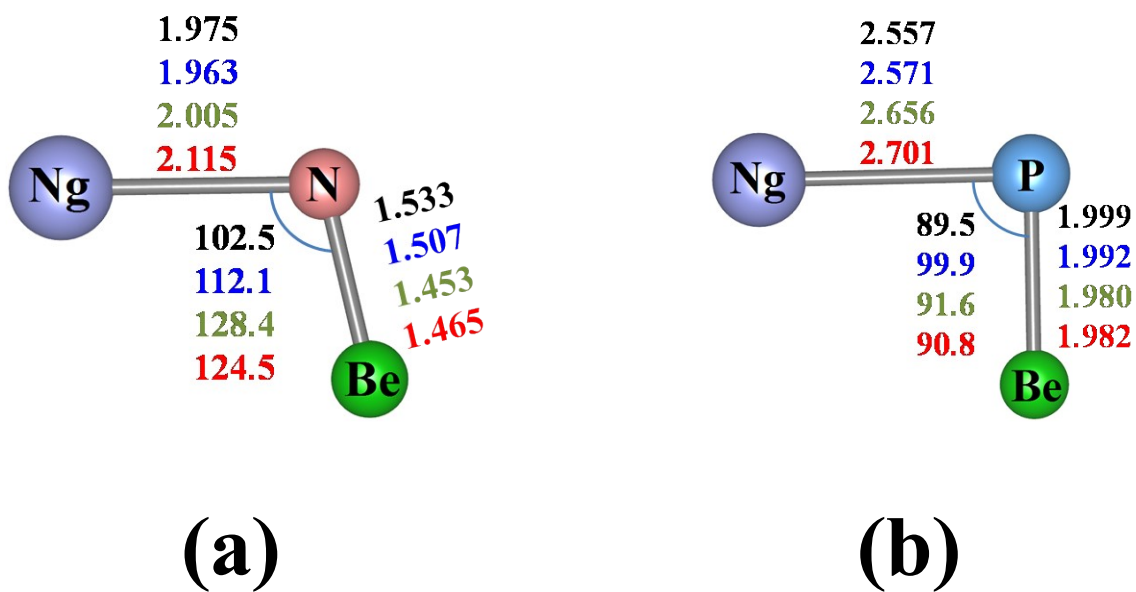


Figure S2. Optimized geometrical parameters of the minima state of (a) $^1\text{NgNBe}^+$ and (b) $^1\text{NgPBe}^+$ ($\text{Ng} = \text{Ar-Rn}$), respectively, where the bond lengths are in Å and bond angles are in degrees. The values in black, blue, green, and red are computed for Ar, Kr, Xe, and Rn containing complexes, respectively, at the CCSD(T)/AVTZ level of theory.

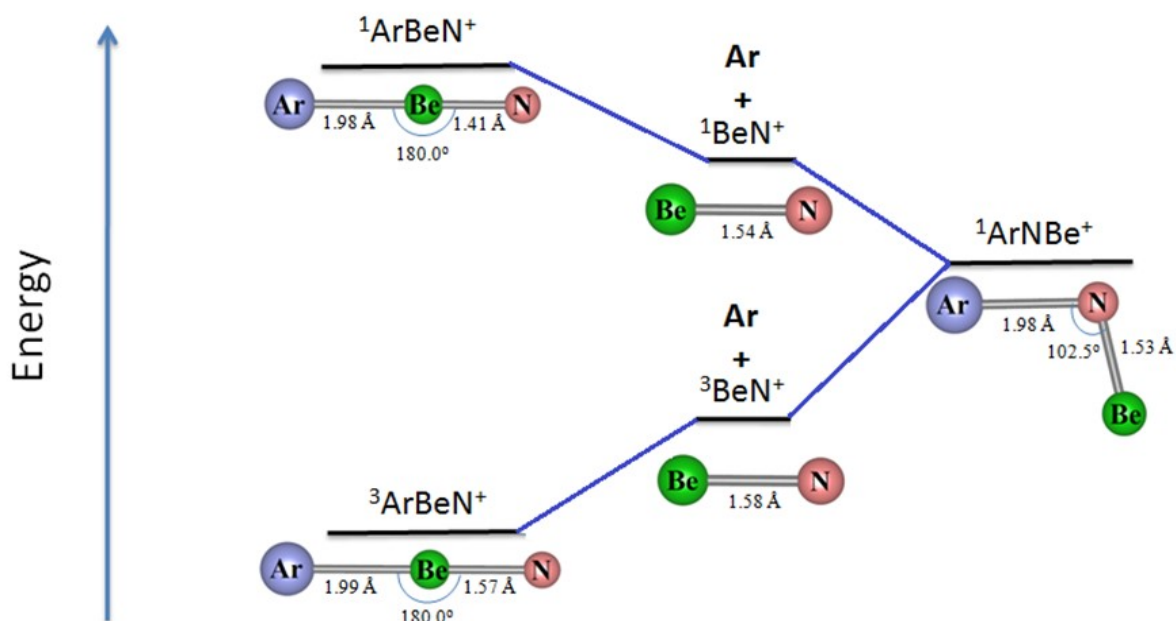


Figure S3. Graphical representation of the energy levels of bare BeN^+ ions and Ar bound BeN^+ complexes in their singlet and triplet potential energy surfaces. All geometries are optimized at CCSD(T)/AVTZ level.

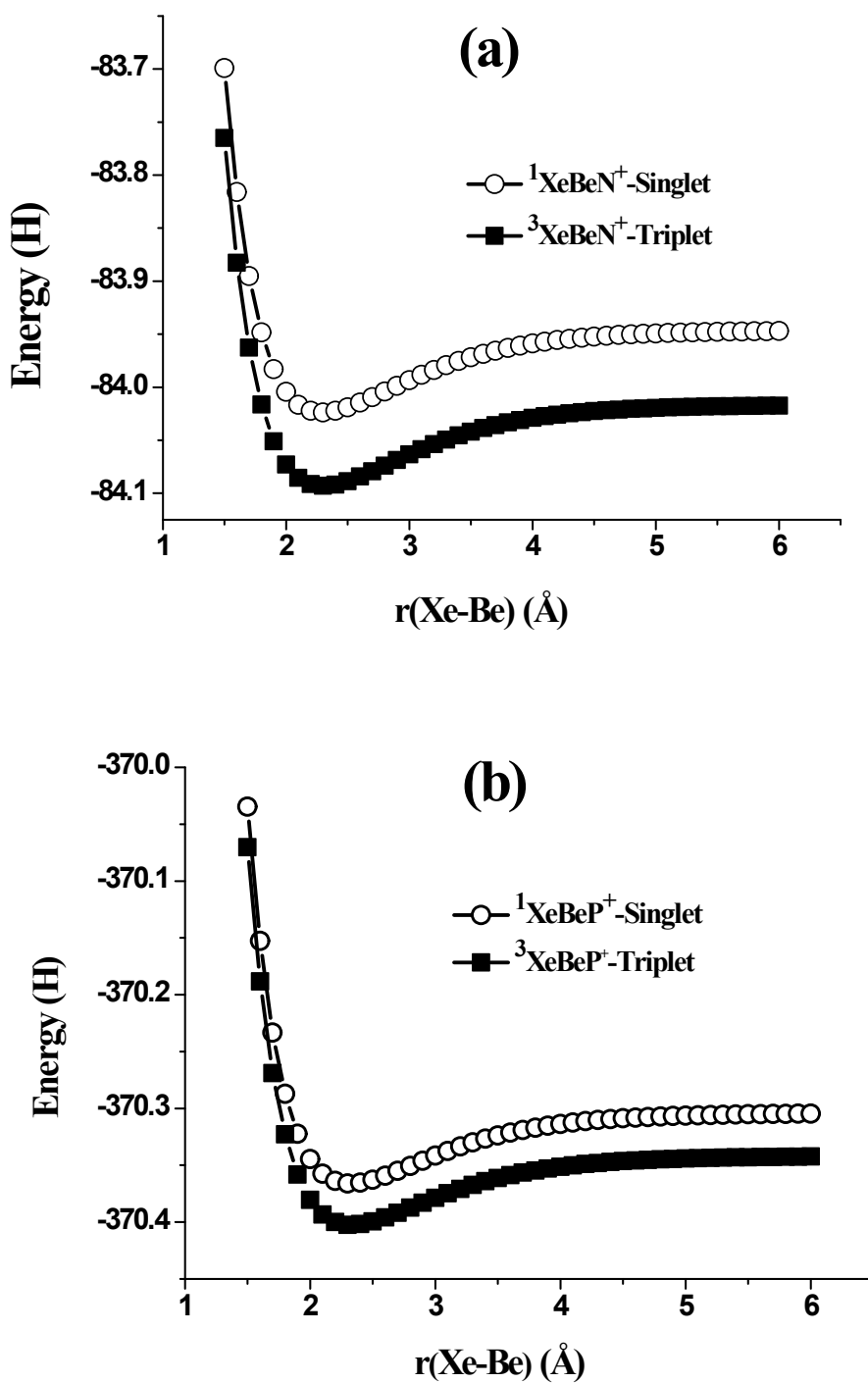
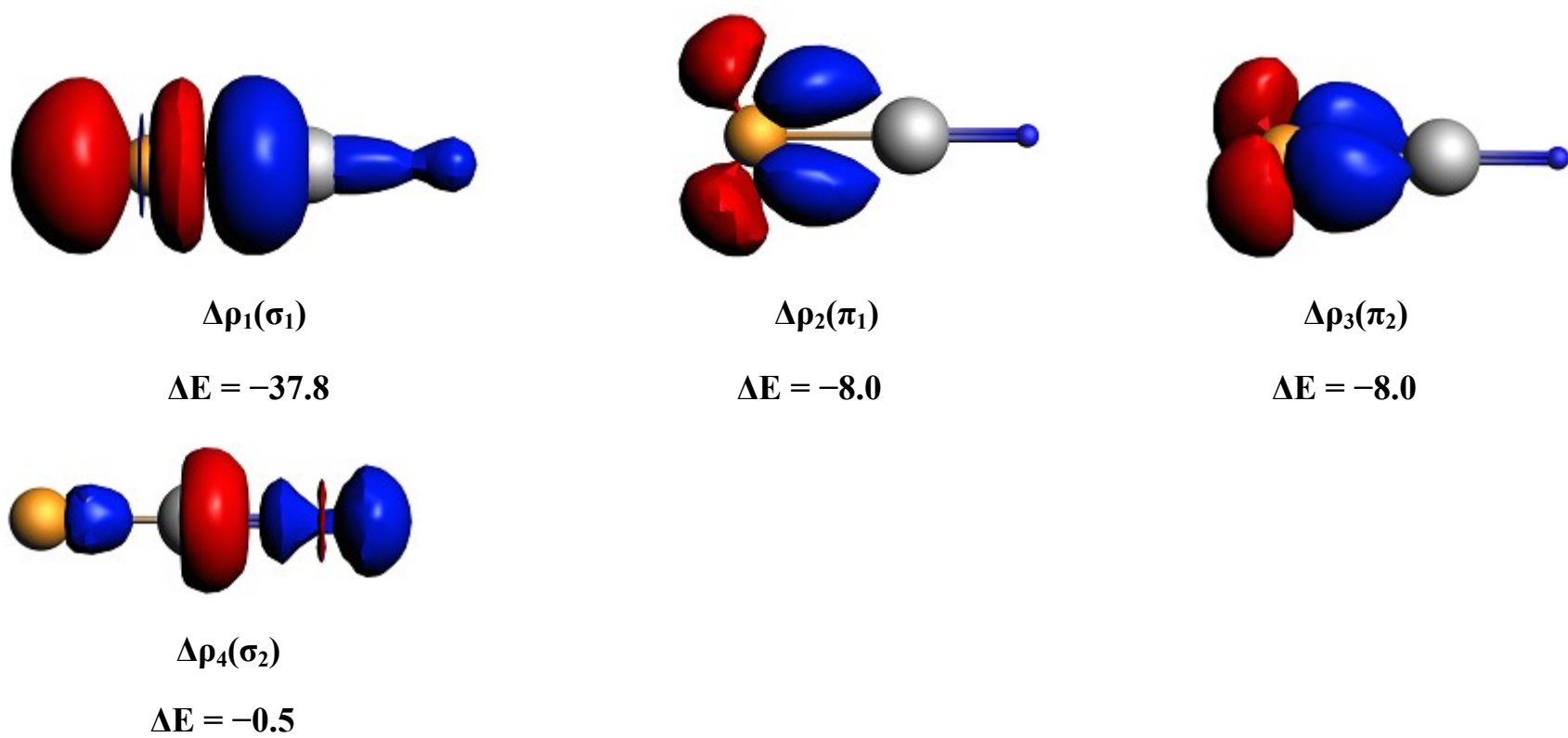


Figure S4. Potential energy profiles for both Singlet and Triplet (a) XeBeN^+ , (b) XeBeP^+ at the CCSD(T)/AVTZ level. The Be–Y bond distance has been fixed at 1.584 and 1.988 Å for calculations of XeBeN^+ and XeBeP^+ potential energy profiles, respectively.

KrBeN⁺ (Kr + BeN⁺)



XeBeN⁺ (Xe + BeN⁺)

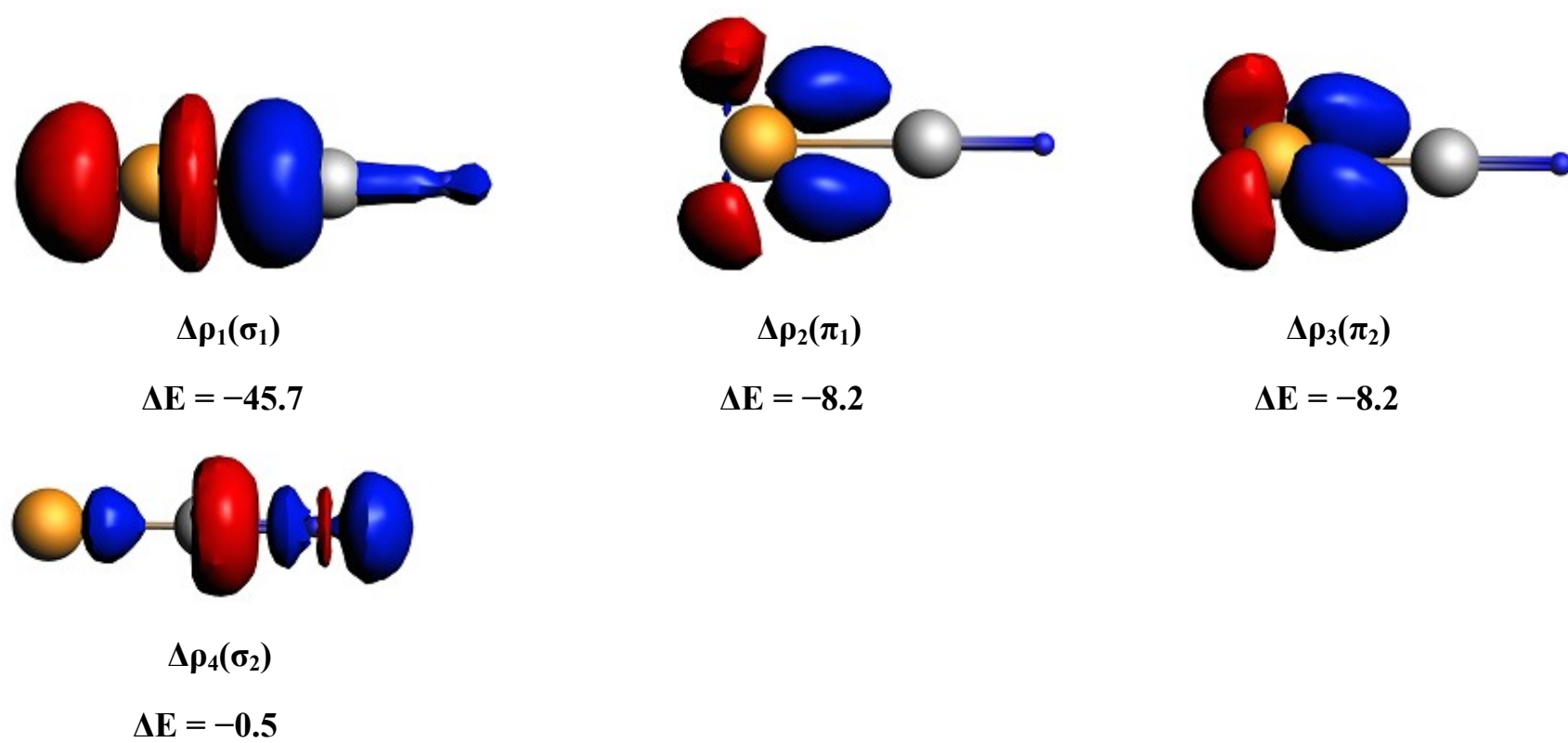
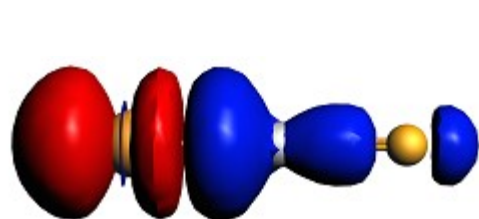


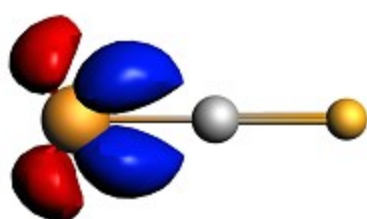
Figure S5. Plot of deformation densities $\Delta\rho(r)$, of the pair-wise orbital interactions in the predicted NgBeN⁺ (Ng = Kr and Xe) complexes at the B3LYP-D3/TZ2P level, where $\Delta\rho_1(r)$, $\Delta\rho_2(r)$, and $\Delta\rho_3(r)$, are the deformation density corresponding to Ng \rightarrow BeN⁺ (Ng = Kr and Xe) σ -, π -, and π -donations, respectively, while $\Delta\rho_4(r)$, corresponds to Ng \leftarrow BeN⁺ (Ng = Kr and Xe) σ -back donation. The associated orbital interaction energies are provided in kcal mol⁻¹. The direction of the charge flow is from red to blue region.

KrBeP⁺ (Kr + BeP⁺)



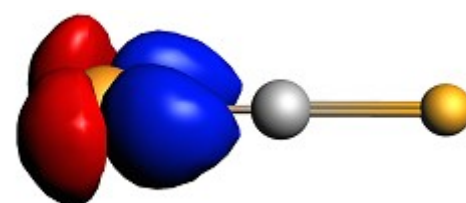
$$\Delta\rho_1(\sigma_1)$$

$$\Delta E = -33.2$$



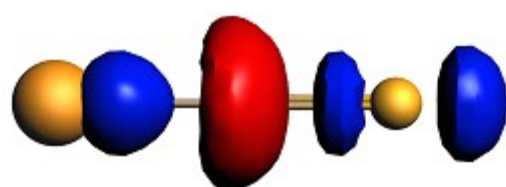
$$\Delta\rho_2(\pi_1)$$

$$\Delta E = -8.5$$



$$\Delta\rho_3(\pi_2)$$

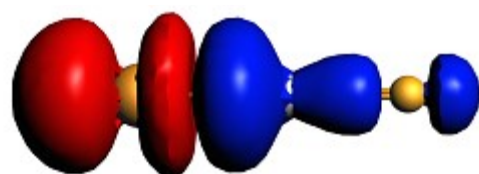
$$\Delta E = -8.5$$



$$\Delta\rho_4(\sigma_2)$$

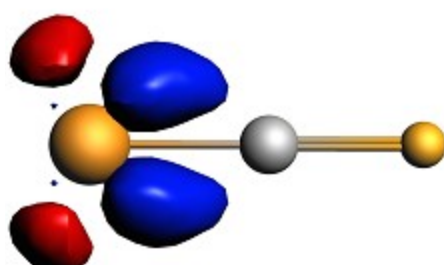
$$\Delta E = -1.3$$

XeBeP⁺ (Xe + BeP⁺)



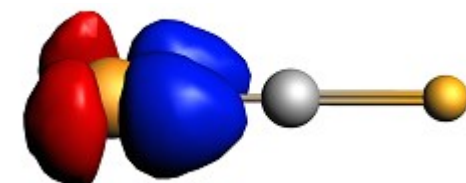
$$\Delta\rho_1(\sigma_1)$$

$$\Delta E = -40.0$$



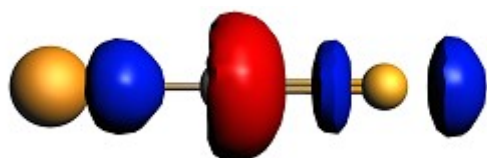
$$\Delta\rho_2(\pi_1)$$

$$\Delta E = -9.0$$



$$\Delta\rho_3(\pi_2)$$

$$\Delta E = -9.0$$



$$\Delta\rho_4(\sigma_2)$$

$$\Delta E = -1.3$$

Figure S6. Plot of deformation densities $\Delta\rho(r)$, of the pair-wise orbital interactions in the predicted NgBeP⁺ (Ng = Kr and Xe) complexes at the B3LYP-D3/TZ2P level, where $\Delta\rho_1(r)$, $\Delta\rho_2(r)$, and $\Delta\rho_3(r)$, are the deformation density corresponding to Ng \rightarrow BeP⁺ (Ng = Kr and Xe) σ -, π -, and π -donations, respectively, while $\Delta\rho_4(r)$, corresponds to Ng \leftarrow BeP⁺ (Ng = Kr and Xe) σ -back donation. 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–Be, Be–N Bond Lengths (R in Å) and Ng–Be–N Bond Angles (θ in Degrees) in the Predicted NgBeN⁺ (Ng = He–Rn) Complexes in their Triplet Electronic State as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set, CCSD(T) and MRCI method with AVTZ Basis Sets.

Complexes	Method	R (Ng–Be)	R (Be–N)	θ (Ng–Be–N)
HeBeN ⁺	B3LYP	1.517	1.564	180.0
	MP2	1.524	1.571	180.0
	CCSD(T)	1.518	1.581	180.0
	MRCI	1.518	1.582	180.0
NeBeN ⁺	B3LYP	1.720	1.568	180.0
	MP2	1.729	1.574	180.0
	CCSD(T)	1.684	1.583	180.0
	MRCI	1.657	1.568	180.0
ArBeN ⁺	B3LYP	1.989	1.568	180.0
	MP2	1.997	1.574	180.0
	CCSD(T)	1.980	1.583	180.0
	MRCI	1.961	1.574	180.0
KrBeN ⁺	B3LYP	2.135	1.569	180.0
	MP2	2.143	1.576	180.0
	CCSD(T)	2.118	1.584	180.0
	MRCI	2.115	1.584	180.0
XeBeN ⁺	B3LYP	2.321	1.570	180.0
	MP2	2.333	1.577	180.0
	CCSD(T)	2.304	1.584	180.0
	MRCI	2.291	1.589	180.0
RnBeN ⁺	B3LYP	2.405	1.571	180.0
	MP2	2.415	1.578	180.0
	CCSD(T)	2.388	1.585	180.0
	MRCI	2.368	1.583	180.0

Table S2. Calculated Values of Ng–Be, Be–P Bond Lengths (R in Å) and Ng–Be–P Bond Angles (θ in Degrees) in the Predicted NgBeP⁺ (Ng = He–Rn) Complexes in their Triplet Electronic State as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set and CCSD(T) and MRCI method with AVTZ Basis Sets.

Complexes	Method	R (Ng–Be)	R (Be–P)	θ (Ng–Be–P)
HeBeP ⁺	B3LYP	1.590	1.994	180.0
	MP2	1.613	2.008	180.0
	CCSD(T)	1.578	2.007	180.0
	MRCI	1.593	2.009	180.0
NeBeP ⁺	B3LYP	1.797	2.000	180.0
	MP2	1.807	2.013	180.0
	CCSD(T)	1.730	2.012	180.0
	MRCI	1.724	1.997	180.0
ArBeP ⁺	B3LYP	2.033	1.998	180.0
	MP2	2.037	2.010	180.0
	CCSD(T)	2.014	2.009	180.0
	MRCI	2.067	2.008	180.0
KrBeP ⁺	B3LYP	2.178	2.000	180.0
	MP2	2.181	2.011	180.0
	CCSD(T)	2.151	2.011	180.0
	MRCI	2.221	2.010	180.0
XeBeP ⁺	B3LYP	2.364	2.002	180.0
	MP2	2.370	2.014	180.0
	CCSD(T)	2.327	2.012	180.0
	MRCI	2.328	2.005	180.0
RnBeP ⁺	B3LYP	2.447	2.005	180.0
	MP2	2.449	2.016	180.0
	CCSD(T)	2.420	2.014	180.0
	MRCI	2.404	2.007	180.0

Table S3. Comparative Accounts of Be–Y Bond Lengths (R in Å), Be–Y Stretching Frequency (in cm⁻¹), and the Mulliken Charges on the Constituent Atoms in the Precursor BeY⁺ with the NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set.

Complexes	R (Be–N)		v (Be–N)		q(Be)		q(N)	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
BeN ⁺	1.580	1.585	984.1	993.5	0.697	0.809	0.303	0.191
HeBeN ⁺	1.564	1.571	1048.8	1053.8	0.617	0.773	0.227	0.117
NeBeN ⁺	1.568	1.574	1035.9	1043.7	0.624	0.773	0.235	0.122
ArBeN ⁺	1.568	1.574	1042.4	1047.2	0.389	0.555	0.170	0.026
KrBeN ⁺	1.569	1.576	1040.6	1045.3	0.321	0.475	0.173	0.073
XeBeN ⁺	1.570	1.577	1038.1	1043.2	0.238	0.383	0.164	0.070
RnBeN ⁺	1.571	1.578	1034.8	1040.2	0.251	0.381	0.155	0.060
Complexes	R (Be–P)		v (Be–P)		q(Be)		q(P)	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
BeP ⁺	2.022	2.036	650.0	647.1	0.504	0.630	0.496	0.370
HeBeP ⁺	1.994	2.008	719.7	718.6	0.419	0.608	0.456	0.312
NeBeP ⁺	2.000	2.013	704.8	707.7	0.450	0.627	0.448	0.296
ArBeP ⁺	1.998	2.010	714.5	715.9	0.247	0.449	0.373	0.213
KrBeP ⁺	2.000	2.011	712.5	714.7	0.166	0.353	0.391	0.231
XeBeP ⁺	2.002	2.014	709.4	712.4	0.065	0.236	0.401	0.245
RnBeP ⁺	2.005	2.016	706.0	709.8	0.070	0.228	0.393	0.235

Table S4. Calculated Values of Ng–Be Stretching Frequency, Be–Y Stretching Frequency and Ng–Be–Y Bending Frequency (in cm^{-1}) in the Predicted NgBeY^+ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set and the Corresponding IR Intensities (in km mol^{-1}) are Provided within the Parenthesis.

Complexes	Ng–Be Stretch		Be–N Stretch		Ng–Be–N Bend	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeN ⁺	642.4(7.1)	617.1(8.4)	1048.8(94.5)	1053.8(105.4)	157.5(88.1)	153.9(104.8)
NeBeN ⁺	444.9(27.4)	438.6(26.7)	1035.9(92.5)	1043.7(103.1)	133.6(136.1)	134.4(156.6)
ArBeN ⁺	515.6(30.6)	515.2(31.0)	1042.4(144.1)	1047.2(159.8)	149.6(104.9)	151.1(121.9)
KrBeN ⁺	487.6(35.0)	491.5(35.5)	1040.6(148.3)	1045.3(167.4)	148.1(96.8)	149.4(112.6)
XeBeN ⁺	469.0(34.0)	473.6(34.8)	1038.1(150.1)	1043.2(173.4)	147.2(81.8)	151.1(95.5)
RnBeN ⁺	455.0(33.8)	461.8(34.0)	1034.8(143.9)	1040.2(168.4)	146.1(74.7)	150.8(87.0)
Complexes	Ng–Be Stretch		Be–P Stretch		Ng–Be–P Bend	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeP ⁺	493.3(8.1)	446.5(14.1)	719.7(122.0)	718.6(137.0)	152.2(22.1)	143.6(30.4)
NeBeP ⁺	364.3(19.0)	348.0(20.3)	704.8(119.9)	707.7(129.6)	127.0(46.4)	115.1(57.2)
ArBeP ⁺	455.9(16.8)	461.0(16.9)	714.5(186.2)	715.9(204.9)	133.9(32.7)	133.9(41.3)
KrBeP ⁺	437.9(20.0)	447.9(19.8)	712.5(191.0)	714.7(213.1)	131.4(30.1)	131.3(38.0)
XeBeP ⁺	426.5(19.9)	437.2(19.9)	709.4(192.8)	712.4(218.9)	128.7(24.4)	130.5(31.0)
RnBeP ⁺	416.6(20.7)	429.9(20.2)	706.0(186.2)	709.8(211.4)	127.4(21.7)	129.8(27.4)

Table S5. Calculated Values of the Harmonic Vibrational Frequencies (in cm^{-1}) and Intrinsic Force Constants in the Parentheses (in N m^{-1}) Corresponding to Individual Internal Coordinates of NgBeY^+ ($\text{Ng} = \text{He, Ne, Ar, Kr, Xe, and Rn}$; $\text{Y} = \text{N and P}$) Complexes using B3LYP and MP2 Methods with DEF2 Basis Sets.

Complexes	Ng–Be Stretch		Be–N Stretch		Ng–Be–N Bend	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeN ⁺	529.3(67.4)	514.1(62.2)	1110.2(355.3)	1107.7(358.8)	157.5	153.9
NeBeN ⁺	311.2(72.5)	309.2(70.4)	1083.6(346.7)	1089.1(351.9)	133.6	134.4
ArBeN ⁺	335.2(115.2)	337.2 (115.0)	1113.6(351.0)	1117.3 (354.3)	149.6	151.1
KrBeN ⁺	300.2(114.0)	304.8(115.8)	1109.3(349.8)	1114.1(353.0)	148.1	149.4
XeBeN ⁺	282.2(109.3)	287.9(115.5)	1103.5(348.2)	1108.9(351.6)	147.2	151.1
RnBeN ⁺	270.2(105.6)	276.5(108.8)	1097.7(345.9)	1104.0(349.5)	146.1	150.8
Complexes	Ng–Be Stretch		Be–P Stretch		Ng–Be–P Bend	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeP ⁺	367.5(39.7)	338.3(32.6)	791.4(213.1)	775.4(212.4)	152.2	143.6
NeBeP ⁺	214.6(48.6)	206.5(44.3)	763.8(204.3)	761.2(206.0)	127.0	115.1
ArBeP ⁺	234.1(90.0)	237.5(92.1)	814.6(210.0)	817.7(210.8)	133.9	133.9
KrBeP ⁺	204.0(91.9)	208.9(96.2)	811.1(208.8)	817.2(210.1)	131.4	131.3
XeBeP ⁺	190.9(90.4)	196.0(95.0)	805.5(207.0)	812.5(208.7)	128.7	130.5
RnBeP ⁺	180.5(88.6)	186.7(94.3)	799.6(205.0)	808.6(207.2)	127.4	129.8

Table S6. Calculated Values of Ng–Be Binding Energies (BE) (in kJ mol⁻¹) in the Predicted NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set and CCSD(T) and MRCI Methods with AVTZ Basis Set.

Complexes	BE (Ng–Be)				BE (Ng–Be) ^a		
	B3LYP	MP2	CCSD(T)	MRCI	B3LYP	MP2	CCSD(T)
HeBeN ⁺	39.9	36.5	40.4	28.5	28.2	22.4	24.6
NeBeN ⁺	50.9	44.3	46.3	45.3	41.0	37.0	43.9
ArBeN ⁺	120.7	116.0	122.4	114.8	110.2	105.5	112.1
KrBeN ⁺	145.4	141.2	147.5	145.8	135.2	131.0	137.5
XeBeN ⁺	177.0	172.4	181.0	171.7	166.9	162.2	171.0
RnBeN ⁺	192.1	188.0	196.2	193.3	182.3	177.9	186.2
Complexes	BE (Ng–Be)				BE (Ng–Be) ^a		
	B3LYP	MP2	CCSD(T)	MRCI	B3LYP	MP2	CCSD(T)
HeBeP ⁺	22.3	26.5	24.3	27.1	13.6	8.1	10.4
NeBeP ⁺	31.3	35.2	35.7	36.4	23.9	21.2	27.3
ArBeP ⁺	85.5	85.1	91.5	83.1	77.7	77.2	83.5
KrBeP ⁺	105.6	106.6	112.5	103.7	97.9	98.9	104.7
XeBeP ⁺	131.0	132.9	140.4	136.7	123.5	125.3	132.7
RnBeP ⁺	143.7	146.5	153.4	149.8	136.3	138.9	145.9

^a Corresponds to the Zero Point Energy (ZPE) corrected Ng–Be binding energy.

Table S7. Calculated Values of Mulliken Atomic Spin Population on the Constituting Atoms in the bare BeY⁺ Ions and Predicted NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set.

Species	Y	Atomic Spin Population					
		Ng		Be		Y	
		B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
BeY ⁺	N	0.269	0.193	1.731	1.807
	P	0.294	0.214	1.706	1.786
HeBeY ⁺	N	0.004	0.005	0.296	0.211	1.700	1.784
	P	0.005	0.005	0.334	0.255	1.661	1.740
NeBeY ⁺	N	0.005	0.004	0.295	0.209	1.700	1.787
	P	0.005	0.004	0.317	0.238	1.678	1.758
ArBeY ⁺	N	0.006	0.003	0.274	0.193	1.721	1.803
	P	0.009	0.005	0.301	0.220	1.691	1.775
KrBeY ⁺	N	0.005	0.002	0.271	0.192	1.724	1.806
	P	0.008	0.005	0.296	0.217	1.696	1.778
XeBeY ⁺	N	0.005	0.001	0.263	0.187	1.732	1.812
	P	0.009	0.003	0.289	0.213	1.702	1.782
RnBeY ⁺	N	0.006	0.001	0.257	0.184	1.737	1.815
	P	0.009	0.004	0.281	0.210	1.709	1.785

Table S8. Calculated Values of Mulliken Charges on the Constituting Atoms in the Predicted NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP and MP2 Methods with the DEF2 Basis Set.

Complexes	<i>q</i> (Ng)		<i>q</i> (Be)		<i>q</i> (N)	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeN ⁺	0.156	0.109	0.617	0.773	0.227	0.117
NeBeN ⁺	0.140	0.104	0.624	0.773	0.235	0.122
ArBeN ⁺	0.442	0.379	0.389	0.555	0.170	0.066
KrBeN ⁺	0.506	0.452	0.321	0.475	0.173	0.073
XeBeN ⁺	0.597	0.548	0.238	0.383	0.164	0.070
RnBeN ⁺	0.594	0.559	0.251	0.381	0.155	0.060
Complexes	<i>q</i> (Ng)		<i>q</i> (Be)		<i>q</i> (P)	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeP ⁺	0.122	0.081	0.419	0.608	0.456	0.312
NeBeP ⁺	0.102	0.077	0.450	0.627	0.448	0.296
ArBeP ⁺	0.379	0.338	0.247	0.449	0.373	0.213
KrBeP ⁺	0.442	0.417	0.166	0.353	0.391	0.231
XeBeP ⁺	0.534	0.519	0.065	0.236	0.401	0.245
RnBeP ⁺	0.537	0.537	0.070	0.228	0.393	0.235

Table S9. Calculated Values of Natural Bonding Orbital (NBO) Charges on the Constituting Atoms in the Predicted NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP Method with the DEF2 Basis Set.

Complexes	<i>q</i>(Ng)	<i>q</i>(Be)	<i>q</i>(N)
HeBeN ⁺	0.057	1.567	−0.624
NeBeN ⁺	0.053	1.572	−0.625
ArBeN ⁺	0.143	1.493	−0.636
KrBeN ⁺	0.187	1.457	−0.643
XeBeN ⁺	0.249	1.406	−0.655
RnBeN ⁺	0.279	1.382	−0.661
Complexes	<i>q</i>(Ng)	<i>q</i>(Be)	<i>q</i>(P)
HeBeP ⁺	0.055	1.150	−0.205
NeBeP ⁺	0.049	1.162	−0.211
ArBeP ⁺	0.135	1.114	−0.250
KrBeP ⁺	0.176	1.086	−0.262
XeBeP ⁺	0.235	1.047	−0.281
RnBeP ⁺	0.262	1.028	−0.290

Table S10. Calculated Values of Atoms-in-Molecule (AIM) Charges on the Constituting Atoms in the Predicted NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP Method with the DEF2 Basis Set.

Complexes	<i>q</i>(Ng)	<i>q</i>(Be)	<i>q</i>(N)
HeBeN ⁺	0.014	1.722	−0.736
NeBeN ⁺	0.015	1.721	−0.736
ArBeN ⁺	0.053	1.697	−0.751
KrBeN ⁺	0.074	1.682	−0.756
XeBeN ⁺	0.099	1.663	−0.762
RnBeN ⁺	0.115	1.654	−0.769
Complexes	<i>q</i>(Ng)	<i>q</i>(Be)	<i>q</i>(P)
HeBeP ⁺	0.009	1.572	−0.581
NeBeP ⁺	0.010	1.571	−0.581
ArBeP ⁺	0.030	1.560	−0.590
KrBeP ⁺	0.042	1.558	−0.600
XeBeP ⁺	0.070	1.541	−0.611
RnBeP ⁺	0.086	1.529	−0.615

Table S11. Calculated Values of Ng–Y Bond Lengths (R in Å), Binding Energies (BE in kJ mol⁻¹), and Harmonic Vibrational Frequencies (ν in cm⁻¹) in the Singlet State of Bent NgYBe⁺ (Ng = Ar, Kr, Xe, and Rn; Y = N and P) Complexes as Obtained by Using CCSD(T) Method with AVTZ Basis Set.

Complexes	R (Ng–N)	ν (Ng–N)	^aBE (Ng–N)	^bBE (Ng–N)
ArNBe ⁺	1.975	339.1	92.0	–89.7
KrNBe ⁺	1.963	400.4	148.9	–32.8
XeNBe ⁺	2.005	468.0	237.5	55.8
RnNBe ⁺	2.115	436.6	265.2	83.6
Complexes	R (Ng–P)	ν (Ng–P)	^aBE (Ng–P)	^bBE (Ng–P)
ArPBe ⁺	2.557	166.2	43.8	–68.3
KrPBe ⁺	2.571	196.0	67.6	–44.5
XePBe ⁺	2.656	224.8	107.5	–4.6
RnPBe ⁺	2.712	211.2	138.1	16.2

^aBinding energy corresponding to the channel, NgYBe⁺ → Ng + ¹BeY⁺

^bBinding energy corresponding to the channel, NgYBe⁺ → Ng + ³BeY⁺

Table S12. Relative Energies (in kJ mol⁻¹) of the Predicted NgBeY⁺ (Ng = Ar, Kr, Xe, and Rn; Y = N and P) in the Singlet and Triplet Electronic States and the Singlet NgYBe⁺ Isomer Calculated by Using CCSD(T) Method with AVTZ Basis Set.

Ng	³NgBeN⁺	¹NgBeN⁺	¹NgNBe⁺
Ar	0.0	322.6	212.0
Kr	0.0	388.2	180.3
Xe	0.0	419.5	125.2
Rn	0.0	448.7	112.6
Ng	³NgBeP⁺	¹NgBeP⁺	¹NgPBe⁺
Ar	0.0	199.1	159.8
Kr	0.0	271.8	157.0
Xe	0.0	332.9	145.0
Rn	0.0	362.3	138.5

Table S13. Calculated Values of Ng–M 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 au), and Ratio of Local Electron Kinetic Energy Density and Electron Density (G/ρ in au) in the Predicted NgBeY⁺ (Ng = He–Rn; Y = N and P) Complexes in their Triplet Electronic State as Obtained by Using B3LYP 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
HeBeN ⁺	0.032	0.029	0.302	0.305	0.015	0.016	1.906	2.069
NeBeN ⁺	0.033	0.030	0.327	0.326	0.016	0.017	2.000	2.167
ArBeN ⁺	0.046	0.044	0.242	0.250	−0.001	−0.001	1.348	1.409
KrBeN ⁺	0.046	0.043	0.168	0.182	−0.007	−0.005	1.065	1.186
XeBeN ⁺	0.046	0.043	0.097	0.109	−0.013	−0.012	0.826	0.907
RnBeN ⁺	0.045	0.043	0.069	0.083	−0.015	−0.014	0.733	0.791
Complexes	ρ		$\nabla^2\rho$		E_d		G/ρ	
	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2	B3LYP	MP2
HeBeP ⁺	0.024	0.020	0.237	0.224	0.013	0.014	1.917	2.100
NeBeP ⁺	0.025	0.022	0.250	0.248	0.014	0.014	1.960	2.182
ArBeP ⁺	0.039	0.037	0.225	0.234	−0.002	−0.004	1.385	1.486
KrBeP ⁺	0.040	0.038	0.163	0.178	−0.004	−0.002	1.100	1.237
XeBeP ⁺	0.040	0.038	0.102	0.115	−0.009	−0.008	0.875	0.974
RnBeP ⁺	0.040	0.038	0.077	0.091	−0.011	−0.010	0.775	0.868