Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

OBCN isomerization, noble gas inserting compounds of identical valence electron number species: stability and bonding

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Electronic Supplementary Information

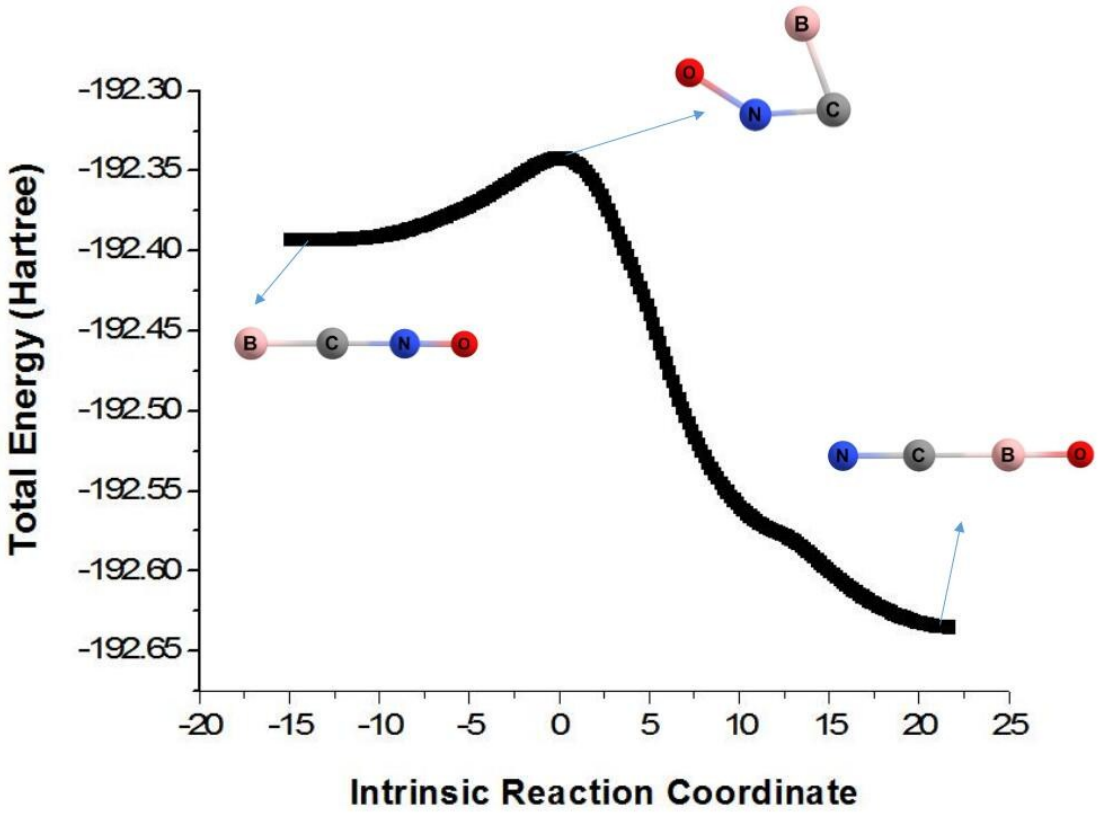


Fig. S1 IRC plot for the conversion of BCNO → OBCN calculated at the MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP level.

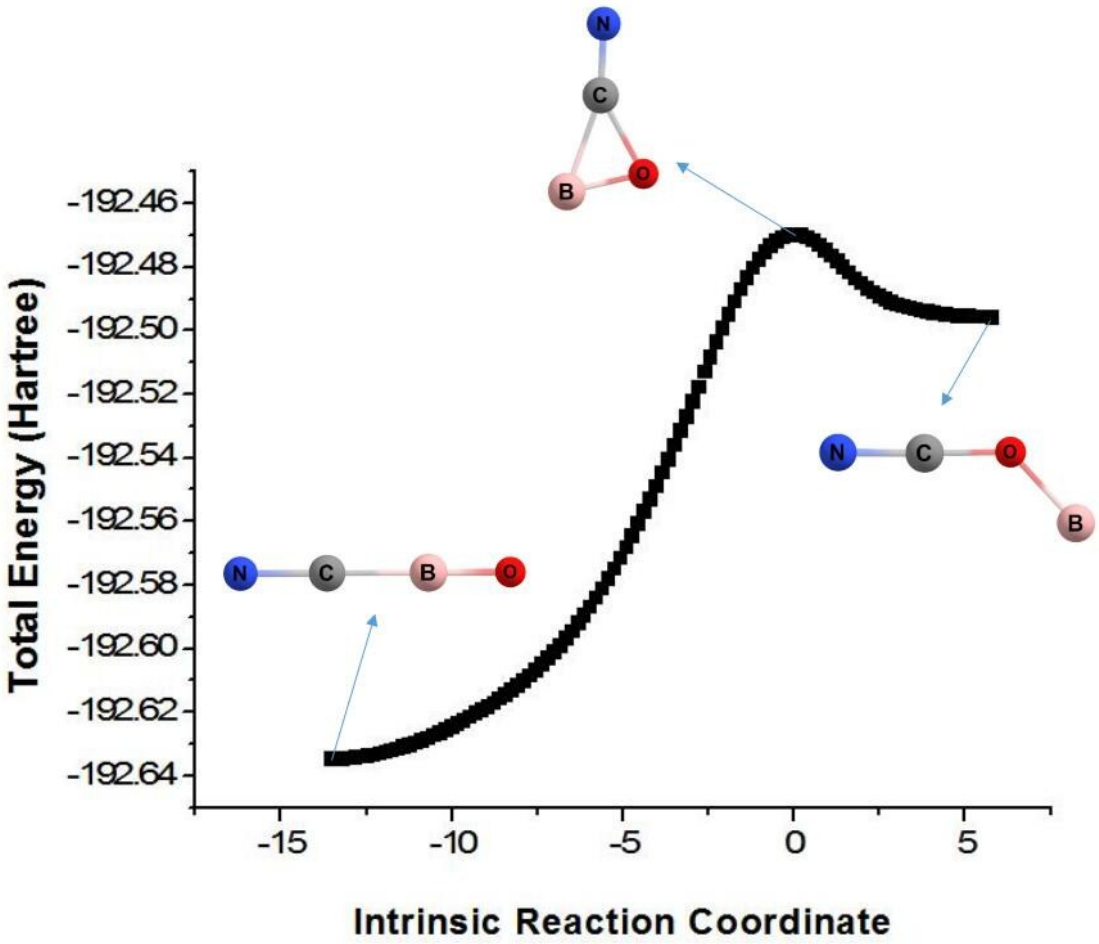


Fig. S2 IRC plot for the conversion of BOCN → OBCN calculated at the MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP level.

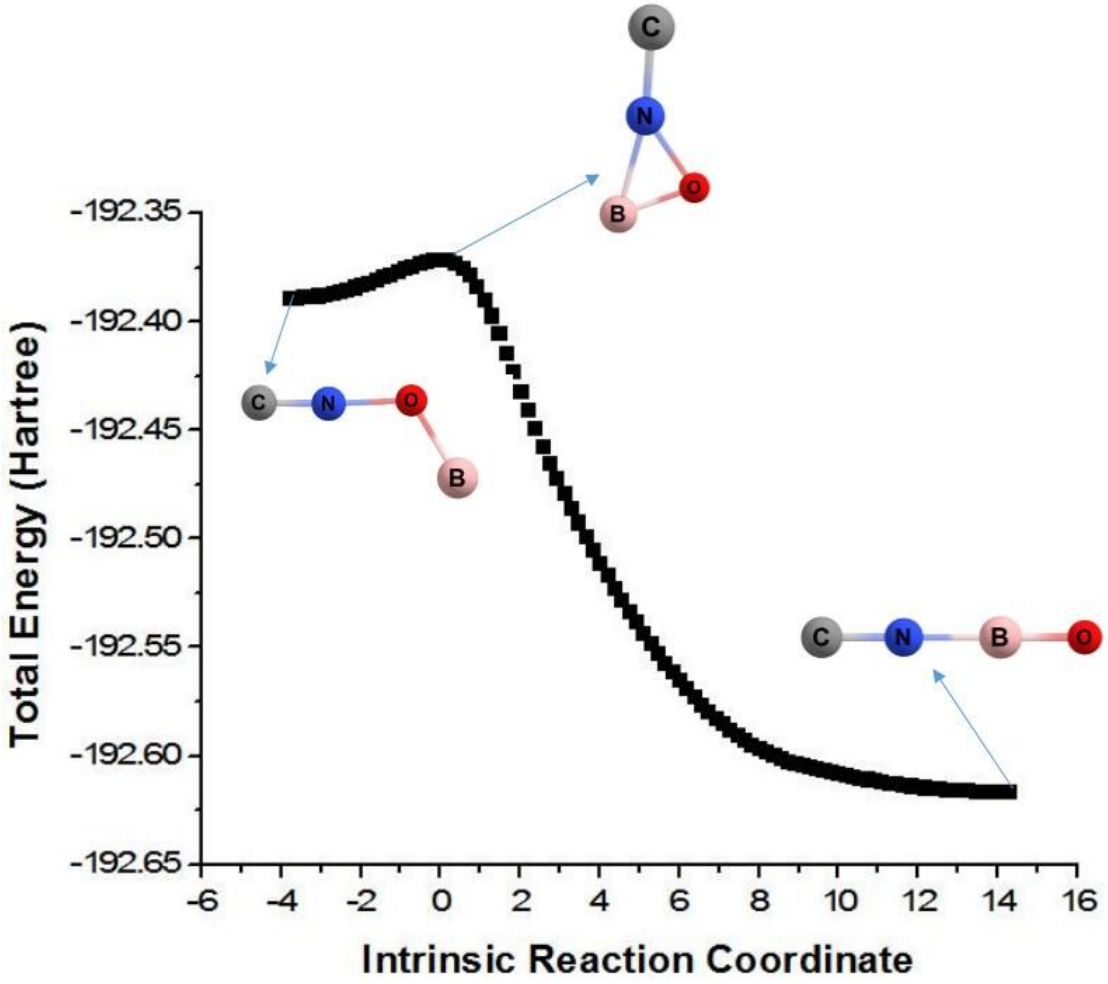


Fig. S3 IRC plot for the conversion of BONC → OBNC calculated at the MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP level.

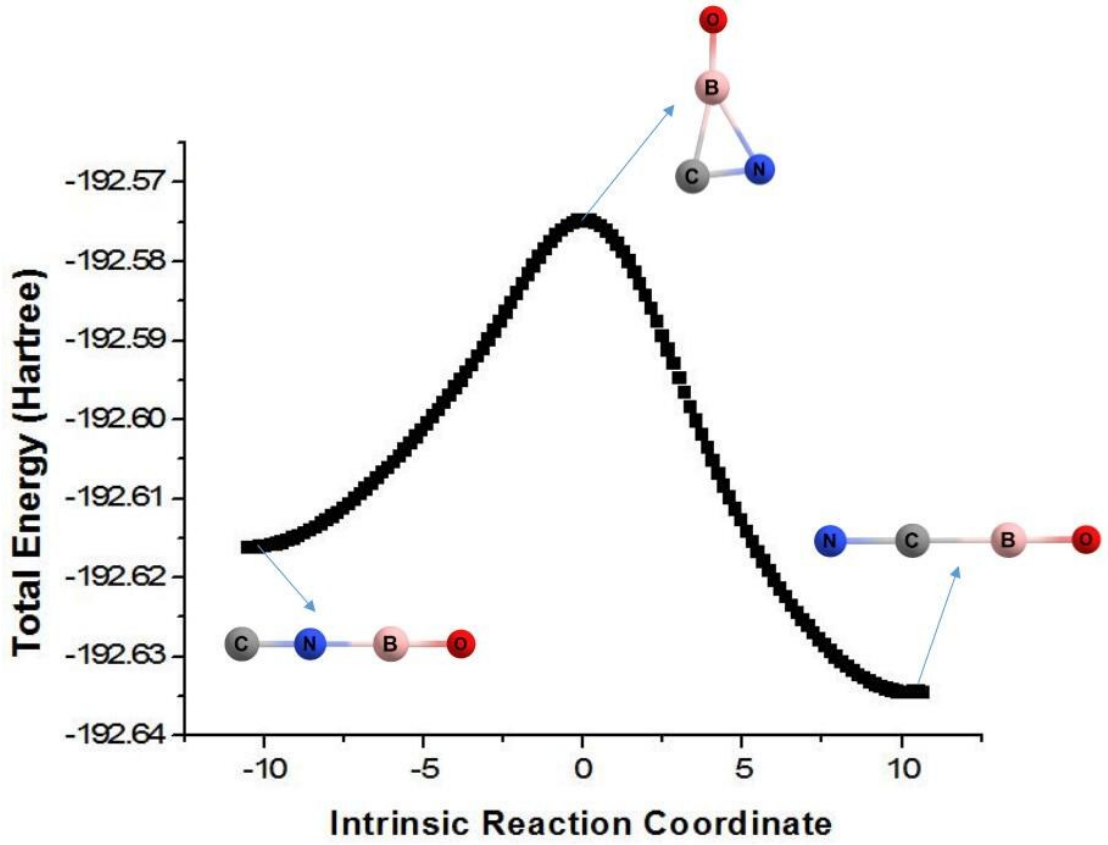


Fig. S4 IRC plots for the conversion of OBNC → OBCN calculated at the MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP level.

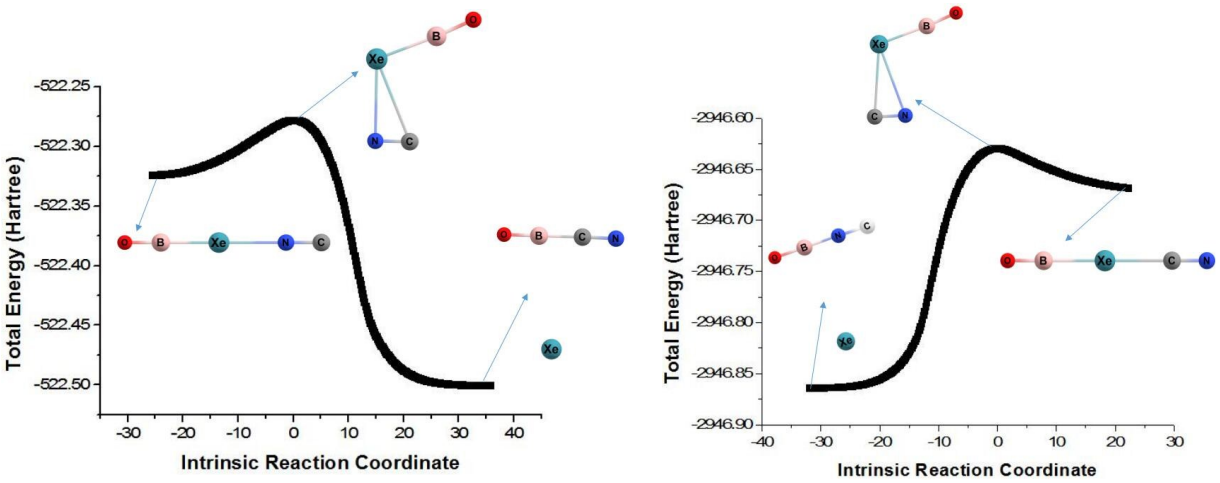


Fig. S5 IRC plots for the conversion of OBXeNC → OBCN + Xe and OBXeCN → OBNC + Xe calculated at the B3LYP-D3/aug-cc-pVTZ/aug-cc-pVTZ-PP level.

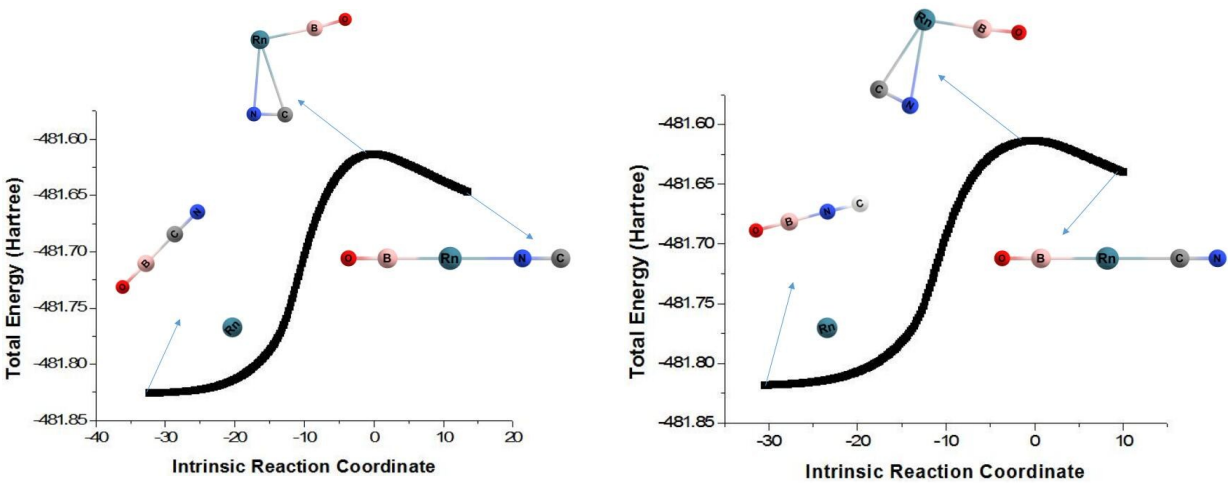
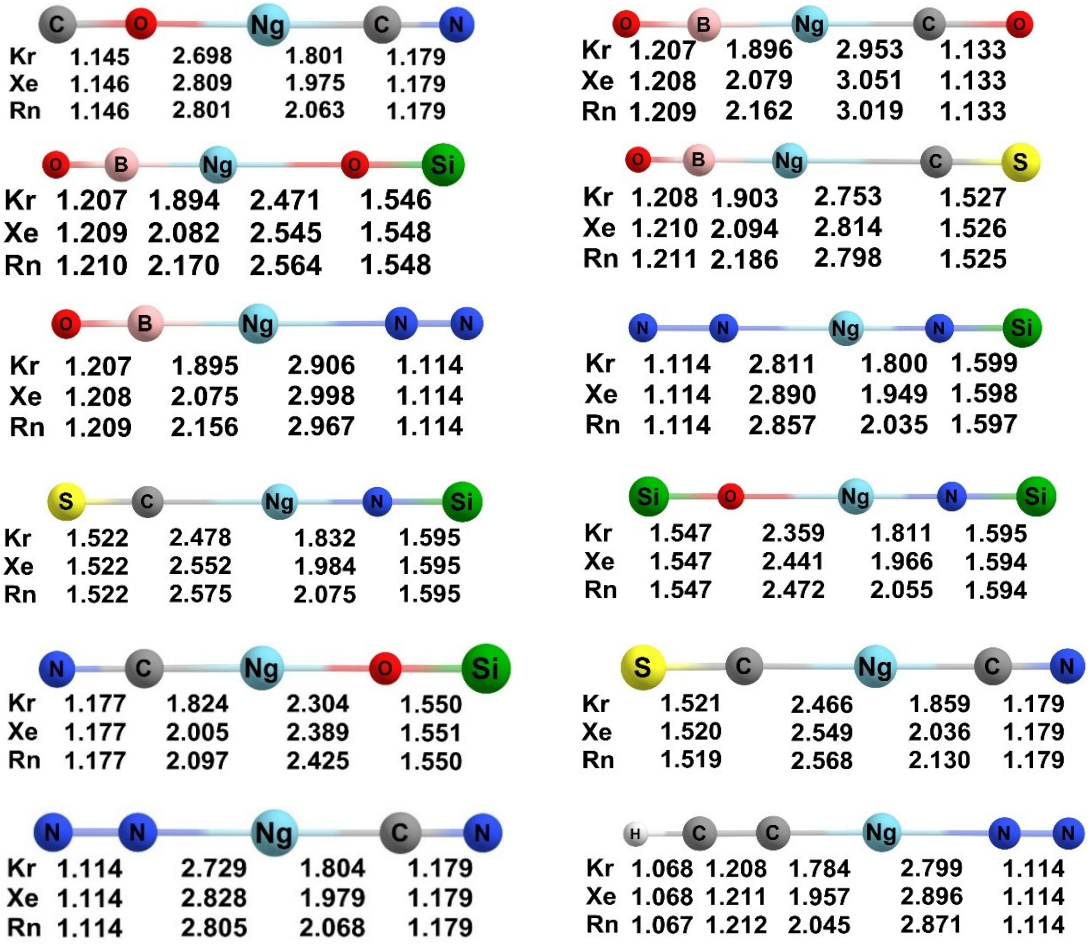


Fig. S6 IRC plots for the conversions of OBRnNC → OBCN + Rn and OBRnCN → OBNC + Rn calculated at the B3LYP-D3/aug-cc-pVTZ/aug-cc-pVTZ-PP level.



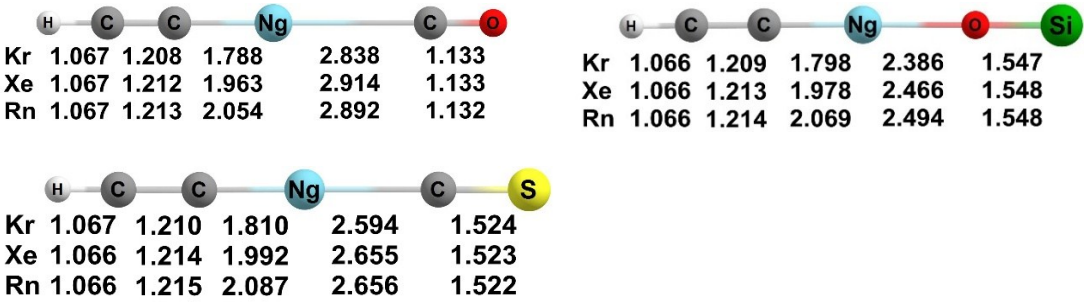


Fig. S7 The molecular geometry of monovalent cationic isoelectronic compounds $XNgY^+$(Ng= Kr, Xe, Rn), and the bond lengths (in units of Å) calculated by MP2/def2-TZVPPD.

Table S1 Energy changes Δ*E*, the enthalpy changes Δ*H* and Gibbs free energy changes Δ*G* calculated by MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP for different dissociation channels of OBNgCN (Ng = Kr, Xe, Rn). All these quantities are in units of kcal·mol^{-1}.

	Δ*E*			**Δ*H***			**Δ*G***		
Processes	Kr	Xe	Rn	Kr	Xe	Rn	Kr	Xe	Rn
OBNgCN → $OBNg^+ + CN^-$	217.65	241.98	256.74	215.77	240.09	254.84	195.83	220.26	236.34
OBNgCN → $OB^- + Ng + CN^+$	273.22	297.54	312.31	271.90	296.22	310.97	251.91	276.35	292.42
OBNgCN → OB + Ng + CN	45.18	69.51	84.27	43.94	68.26	83.01	23.16	47.59	63.67
OBNgCN → $OBNg^+ + CN^-$	131.12	138.87	144.84	130.44	138.12	144.06	118.18	125.88	133.10
OBNgCN → $OB^- + CNNg^+$	192.90	190.67	193.22	191.93	189.67	192.17	179.59	177.36	181.14
OBNgCN → OBCN + Ng	-128.69	-104.36	-89.60	-127.79	-103.47	-88.72	-137.49	-113.06	-96.98
OBNgCN → OBNC + Ng	-117.18	-92.85	-78.09	-116.19	-91.87	-77.12	-126.05	-101.62	-85.54

Table S2 Natural atom charges (a.u.), and WBIs calculated by MP2/aug-cc-pVTZ/ cc-pVTZ-PP level for the monovalent cationic compounds.

	q_{Ng}	q_{CO}	$q_{CN/OB}$	WBI_{C-O}	$WBI_{C-N/O-B}$	$WBI_{B-Ng/O-Ng}$	WBI_{C-Ng}	ΔE_{H-L}
$COKrCN^+$	0.946	0.006	0.048	1.963	2.961	0.013	1.036	14.313
$COXeCN^+$	1.122	0.009	-0.131	1.954	2.953	0.017	1.040	13.646
$CORnCN^+$	1.177	0.012	-0.189	1.940	2.958	0.021	1.018	13.120
$OBKrCO^+$	0.635	0.016	0.349	2.247	1.972	0.912	0.020	15.605
$OBXeCO^+$	0.768	0.023	0.208	2.252	1.946	1.007	0.030	15.138
$OBRnCO^+$	0.814	0.031	0.155	2.260	1.928	1.020	0.039	14.703
	q_{Ng}	q_{OB}	$q_{OSi/CS/NN}$	WBI_{O-B}	$WBI_{O-Si/C-S/N-N}$	WBI_{B-Ng}	$WBI_{O-Ng/C-Ng/N-Ng}$	ΔE_{H-L}
$OBKrOSi^+$	0.679	0.297	0.024	1.938	0.909	0.953	0.030	12.737
$OBXeOSi^+$	0.825	0.144	0.032	1.910	0.880	1.042	0.043	13.020
$OBRnOSi^+$	0.881	0.085	0.034	1.892	0.867	1.055	0.045	13.030
$OBKrCS^+$	0.650	0.322	0.029	1.954	2.790	0.912	0.040	12.880
$OBXeCS^+$	0.785	0.173	0.043	1.926	2.803	0.994	0.064	13.446
$OBRnCS^+$	0.837	0.112	0.052	1.906	2.812	1.000	0.078	13.655
$OBKrNN^+$	0.628	0.369	0.003	1.977	3.026	0.906	0.009	15.660
$OBXeNN^+$	0.759	0.236	0.005	1.951	3.025	1.006	0.012	15.104
$OBRnNN^+$	0.802	0.191	0.007	1.930	3.024	1.023	0.015	14.656
	q_{Ng}	q_{NSi}	$q_{NN/SC/SiO}$	WBI_{N-Si}	$WBI_{N-N/S-C/Si-O}$	WBI_{N-Ng}	$WBI_{N-Ng/C-Ng/O-Ng}$	ΔE_{H-L}
$NNKrNSi^+$	0.904	0.091	0.006	0.988	3.027	0.010	0.943	13.351
$NNXeNSi^+$	1.123	-0.132	0.009	0.986	3.026	0.017	0.932	12.421
$NNRnNSi^+$	1.168	-0.180	0.013	1.029	3.024	0.023	0.904	11.970
$SCKrNSi^+$	0.921	0.011	0.068	1.039	2.783	0.897	0.103	12.971
$SCXeNSi^+$	1.150	-0.238	0.088	1.049	2.800	0.846	0.166	12.277
$SCRnNSi^+$	1.208	-0.304	0.095	1.096	2.808	0.799	0.186	11.703
$SiOKrNSi^+$	0.970	-0.015	0.045	1.052	0.930	0.935	0.060	12.654

$SiOXeNSi^+$	1.192	-0.248	0.055	1.066	0.888	0.880	0.081	12.048
$SiORnNSi^+$	1.250	-0.307	0.058	1.111	0.873	0.838	0.084	11.480
	q_{Ng}	q_{CN}	$q_{SiO/SC/NN}$	WBI_{C-N}	$WBI_{Si-O/S-C/N-N}$	WBI_{C-Ng}	$WBI_{O-Ng/N-Ng/C-Ng}$	ΔE_{H-L}
$NCKrOSi^+$	0.974	-0.036	0.062	2.957	0.843	1.007	0.077	13.113
$NCXeOSi^+$	1.153	-0.225	0.072	2.952	0.810	0.979	0.098	13.129
$NCRnOSi^+$	1.217	-0.290	0.073	2.956	0.800	0.944	0.100	13.064
$NCXeCS^+$	0.912	-0.025	0.112	2.970	2.823	0.936	0.147	13.341
$NCRnCS^+$	1.089	-0.218	0.129	2.963	2.834	0.909	0.202	13.628
$NCKrCS^+$	1.156	-0.291	0.134	2.966	2.839	0.867	0.222	13.054
$NCKrNN^+$	0.941	0.047	0.012	2.962	3.017	1.027	0.023	14.628
$NCXeNN^+$	1.115	-0.133	0.018	2.955	3.015	1.028	0.033	13.676
$NCRnNN^+$	1.169	-0.194	0.025	2.960	3.011	1.002	0.043	13.191
	q_{Ng}	q_{CCH}	$q_{NN/CO/OSi/CS}$	WBI_{C-C}	$WBI_{N-N/C-O/O-Si/C-S}$	WBI_{C-Ng}	$WBI_{N-Ng/C-Ng/O-Ng}$	ΔE_{H-L}
$HCCKrNN^+$	0.920	0.073	0.008	2.867	3.021	1.034	0.016	14.244
$HCCXeNN^+$	1.091	-0.103	0.012	2.871	3.019	1.041	0.024	13.220
$HCCRnNN^+$	1.140	-0.157	0.017	2.887	3.016	1.023	0.032	12.758
$HCCKrCO^+$	0.910	0.064	0.026	2.870	2.247	1.020	0.036	14.266
$HCCXeCO^+$	1.077	-0.116	0.039	2.875	2.255	1.017	0.058	13.264
$HCCRnCO^+$	1.123	-0.174	0.051	2.892	2.265	0.990	0.076	12.814
$HCCKrOSi^+$	0.950	0.010	0.040	2.884	0.901	1.027	0.053	13.029
$HCCXeOSi^+$	1.127	-0.178	0.051	2.890	0.867	1.010	0.071	12.414
$HCCRnOSi^+$	1.186	-0.239	0.054	2.905	0.853	0.982	0.074	11.874
$HCCKrCS^+$	0.913	0.030	0.057	2.885	2.792	0.992	0.089	13.772
$HCCXeCS^+$	1.084	-0.161	0.078	2.893	2.805	0.970	0.138	12.768
$HCCRnCS^+$	1.142	-0.230	0.088	2.909	2.813	0.933	0.161	12.134

Table S3 Electron density ρ, Laplacian $\nabla^2\rho$, electron local energy density *H*, the ratio of local kinetic energy density *G*(***r***) and electron density ρ(***r***) and electron localization function (ELF) at the bond critical points (BCPs) of the B/C/N–Ng bonds in the Ng inserted compounds calculated by the MP2/aug-cc-pVTZ/cc-pVTZ-PP method.

	O/B-Ng					Ng-C				
	ρ(r)	**$\nabla^2\rho$(r)**	**H(r)**	**G(r)/ρ(r)**	**ELF**	**ρ(r)**	**$\nabla^2\rho$(r)**	**H(r)**	**G(r)/ρ(r)**	**ELF**
$COKrCN^+$	0.019	0.091	0.003	0.994	0.032	0.195	-0.305	-0.157	0.414	0.905
$COXeCN^+$	0.020	0.083	0.003	0.917	0.038	0.162	-0.127	-0.111	0.488	0.787
$CORnCN^+$	0.021	0.091	0.002	0.945	0.039	0.145	-0.012	-0.086	0.573	0.685
$OBKrCO^+$	0.121	0.036	-0.112	0.997	0.342	0.018	0.057	0.001	0.734	0.057
$OBXeCO^+$	0.120	-0.196	-0.114	0.540	0.611	0.019	0.053	0.001	0.669	0.072
$OBRnCO^+$	0.117	-0.239	-0.090	0.258	0.848	0.021	0.060	0.000	0.687	0.080
	B-Ng					**O-Ng/C- Ng/N-Ng**				
	ρ(r)	**$\nabla^2\rho$(r)**	**H(r)**	**G(r)/ρ(r)**	**ELF**	**ρ(r)**	**$\nabla^2\rho$(r)**	**H(r)**	**G(r)/ρ(r)**	**ELF**
$OBKrOSi^+$	0.127	-0.026	-0.121	0.902	0.404	0.038	0.149	0.000	0.979	0.081
$OBXeOSi^+$	0.125	-0.264	-0.115	0.396	0.740	0.040	0.136	-0.002	0.898	0.102
$OBRnOSi^+$	0.118	-0.197	-0.081	0.265	0.935	0.041	0.144	-0.003	0.938	0.097
$OBKrCS^+$	0.125	-0.030	-0.118	0.888	0.388	0.029	0.074	-0.001	0.683	0.113
$OBXeCS^+$	0.123	-0.267	-0.111	0.363	0.723	0.032	0.069	-0.003	0.622	0.189
$OBRnCS^+$	0.116	-0.180	-0.076	0.268	0.938	0.035	0.076	-0.004	0.650	0.190
$OBKrNN^+$	0.120	0.053	-0.110	1.024	0.331	0.015	0.063	0.003	0.864	0.033
$OBXeNN^+$	0.120	-0.178	-0.114	0.579	0.588	0.016	0.060	0.002	0.792	0.042
$OBRnNN^+$	0.117	-0.253	-0.096	0.283	0.803	0.019	0.069	0.002	0.814	0.047
	B/C/N-Ng					**Ng-C**				
	ρ(r)	**$\nabla^2\rho$(r)**	**H(r)**	**G(r)/ρ(r)**	**ELF**	**ρ(r)**	**$\nabla^2\rho$(r)**	**H(r)**	**G(r)/ρ(r)**	**ELF**
$NNKrNSi^+$	0.018	0.074	0.002	0.875	0.038	0.192	-0.065	-0.126	0.571	0.810

$NNXeNSi^+$	0.020	0.072	0.002	0.814	0.048	0.161	0.003	-0.109	0.679	0.685
$NNRnNSi^+$	0.023	0.083	0.001	0.840	0.054	0.145	0.110	-0.083	0.764	0.587
$SCKrNSi^+$	0.051	0.096	-0.008	0.640	0.208	0.182	-0.030	-0.115	0.587	0.813
$SCXeNSi^+$	0.053	0.083	-0.011	0.609	0.243	0.151	0.034	-0.098	0.704	0.641
$SCRnNSi^+$	0.053	0.094	-0.012	0.662	0.218	0.134	0.135	-0.073	0.795	0.529
$SiOKrNSi^+$	0.048	0.171	-0.003	0.953	0.105	0.190	-0.061	-0.124	0.574	0.822
$SiOXeNSi^+$	0.049	0.150	-0.006	0.891	0.123	0.156	0.022	-0.104	0.700	0.633
$SiORnNSi^+$	0.049	0.163	-0.006	0.952	0.110	0.140	0.126	-0.078	0.785	0.531
	C-Ng					**O-Ng/N-Ng/C-Ng**				
	ρ(r)	**$\nabla^2\rho(r)$**	**H(r)**	**G(r)/ρ(r)**	**ELF**	**ρ(r)**	**$\nabla^2\rho(r)$**	**H(r)**	**G(r)/ρ(r)**	**ELF**
$NCKrOSi^+$	0.191	-0.241	-0.141	0.422	0.904	0.055	0.186	-0.006	0.950	0.132
$NCXeOSi^+$	0.154	-0.082	-0.101	0.524	0.726	0.055	0.161	-0.009	0.893	0.148
$NCRnOSi^+$	0.136	0.028	-0.076	0.612	0.615	0.055	0.177	-0.008	0.967	0.126
$SCKrCN^+$	0.178	-0.177	-0.121	0.430	0.899	0.053	0.093	-0.009	0.619	0.248
$SCXeCN^+$	0.145	-0.064	-0.091	0.514	0.745	0.054	0.079	-0.012	0.591	0.276
$SCRnCN^+$	0.128	0.038	-0.068	0.605	0.621	0.055	0.092	-0.013	0.650	0.242
$NNKrCN^+$	0.194	-0.298	-0.155	0.413	0.905	0.022	0.087	0.002	0.875	0.050
$NNXeCN^+$	0.161	-0.122	-0.109	0.491	0.786	0.023	0.080	0.001	0.810	0.059
$NNRnCN^+$	0.143	-0.006	-0.084	0.578	0.682	0.026	0.090	0.001	0.844	0.063
	C-Ng					**N-Ng/C-Ng/O-Ng**				
	ρ(r)	**$\nabla^2\rho(r)$**	**H(r)**	**G(r)/ρ(r)**	**ELF**	**ρ(r)**	**$\nabla^2\rho(r)$**	**H(r)**	**G(r)/ρ(r)**	**ELF**
$HCCKrNN^+$	0.200	-0.341	-0.171	0.432	0.879	0.019	0.077	0.002	0.886	0.039
$HCCXeNN^+$	0.167	-0.144	-0.117	0.486	0.817	0.020	0.072	0.002	0.818	0.048
$HCCRnNN^+$	0.149	-0.023	-0.091	0.572	0.722	0.022	0.081	0.001	0.846	0.053
$HCCKrCO^+$	0.199	-0.329	-0.167	0.428	0.884	0.022	0.067	0.001	0.736	0.071
$HCCXeCO^+$	0.165	-0.135	-0.115	0.493	0.811	0.024	0.064	0.000	0.681	0.091
$HCCRnCO^+$	0.147	-0.012	-0.088	0.579	0.712	0.027	0.072	-0.001	0.706	0.097
$HCCKrOSi^+$	0.198	-0.298	-0.158	0.423	0.901	0.045	0.168	-0.002	0.973	0.098
$HCCXeOSi^+$	0.161	-0.110	-0.110	0.513	0.772	0.047	0.149	-0.005	0.903	0.117
$HCCRnOSi^+$	0.143	0.009	-0.084	0.600	0.667	0.047	0.161	-0.005	0.960	0.106
$HCCKrCS^+$	0.194	-0.272	-0.150	0.424	0.897	0.040	0.088	-0.004	0.667	0.159
$HCCXeCS^+$	0.157	-0.099	-0.105	0.512	0.787	0.043	0.079	-0.007	0.620	0.201
$HCCRnCS^+$	0.139	0.018	-0.079	0.602	0.675	0.046	0.088	-0.008	0.665	0.190

Table S4 EDA results with the ETS-NOCV scheme at the level PBE-D3/TZ2P// CCSD(T)/cc-pVTZ/ cc-pVTZ-PP. All energy terms are in units of kcal·mol^{-1}. The percentages within the parentheses show the contributions towards the total attractive energy ΔE_{elstat} +ΔE_{orb} + ΔE_{dis}, and those within the square brackets for ΔE(σ1) show the contributions towards the total orbital interaction energy ΔE_{orb}.

	Fragments	**ΔE_{pauli}**	**ΔE_{elstat}**	**ΔE_{orb}**	**ΔE_{dis}**	**ΔE_{int}**	**$\Delta E(\sigma 1)$**	**$\Delta E(\sigma 2)$**	**$\Delta E(\pi 1)$**	**$\Delta E(\pi 2)$**
OBKrCN	OB+KrCN	214.41	-70.14(26.60)	-192.70(73.08)	-0.83(0.31)	-49.27	-126.17(65.48)	-4.38	-26.92	-19.84
OBXeCN	OB+XeCN	223.04	-71.71(25.51)	-208.44(74.15)	-0.97(0.35)	-58.09	-145.94(70.02)	-3.96	-25.76	-19.77
OBRnCN	OB+RnCN	224.30	-73.59(25.64)	-212.38(74.01)	-0.99(0.34)	-62.66	-152.31(71.72)	-3.96	-24.15	-20.04
OBKrCN	OBKr+CN	107.21	-33.05(18.38)	-146.02(81.19)	-0.79(0.44)	-72.65	-109.92(75.28)	-1.02	-11.41	-5.10
OBXeCN	OBXe+CN	134.56	-42.13(19.63)	-171.49(79.92)	-0.95(0.44)	-80.01	-128.14(74.72)	-1.20	-15.43	-5.31
OBRnCN	OBRn+CN	153.86	-48.28 (20.54)	-184.66(78.55)	-2.15(0.91)	-81.23	-138.09(74.78)	-1.46	-16.12	-6.80
OBKrNSi	OB+KrNSi	189.84	-64.26(26.89)	-172.83(72.33)	-1.87(0.78)	-49.11	-116.92(67.65)	-3.41	-15.57	-23.99
OBXeNSi	OB+XeNSi	200.29	-65.91(25.29)	-192.54(73.88)	-2.15(0.83)	-60.30	-139.44(72.42)	-3.29	-15.40	-23.29
OBRnNSi	OB+RnNSi	197.29	-65.87(25.24)	-192.94(73.94)	-2.12(0.81)	-63.63	-141.76(73.47)	-3.24	-15.27	-22.25
OBKrNSi	OBKr+NSi	147.51	-65.30(30.00)	-149.90(68.87)	-2.45(1.13)	-70.14	-65.42(43.64)	-2.25	-69.12	-5.07

OBXeNSi	OBXe+NSi	191.93	-87.48(32.25)	-180.87(66.67)	-2.94(1.08)	-79.36	-67.22(37.17)	-2.53	-93.34	3.33
OBRnNSi	OBRn+NSi	199.24	-93.36(33.03)	-186.31(65.92)	-2.95(1.04)	-83.37	-66.14(35.50)	-2.55	-99.42	4.16
OBKrOB	OBKr+OB	112.27	-34.55(22.07)	-120.32(76.84)	-1.71(1.09)	-44.32	-85.55(71.10)	-1.27	-16.70	-7.80
OBXeOB	OBXe+OB	149.01	-46.66(23.00)	-154.20(76.00)	-2.04(1.01)	-53.89	-112.93(73.24)	-1.57	-20.76	-9.56
OBRnOB	OBRn+OB	166.40	-53.68(23.86)	-169.28(75.23)	-2.05(0.91)	-58.61	-125.70(74.24)	-1.85	-21.17	-10.58
NCKrCN	NCKr+CN	169.89	-51.27(22.48)	-174.88(76.69)	-1.89(0.83)	-58.15	-119.25(68.19)	-3.15	-11.48	-18.50
NCXeCN	NCXe+CN	197.51	-59.43(22.11)	-207.10(77.05)	-2.24(0.83)	-71.26	-146.47(70.73)	-3.40	-11.94	-20.63
NCRnCN	NCRn+CN	204.35	-62.94(22.46)	-215.00(76.73)	-2.25(0.80)	-75.84	-153.72(71.50)	-3.60	-14.25	-19.99
SiNKrNSi	SiNKr+NSi	184.64	-78.80(32.22)	-163.30(66.76)	-2.50(1.02)	-59.96	-78.22(47.90)	1.66	-67.52	-3.39
SiNXeNSi	SiNXe+NSi	237.02	-98.96(32.29)	-204.50(66.72)	-3.04(0.99)	-69.48	-57.70(28.22)	-2.73	-49.64	-40.08
SiNRnNSi	SiNRn+NSi	255.05	-116.63(34.78)	-215.65(64.31)	-3.04(0.91)	-80.27	-71.34(33.08)	-1.23	-115.81	-9.46
OBKrCCH	OB+KrCCH	171.64	-55.43(24.75)	-166.69(74.44)	-1.82(0.81)	-52.29	-117.79(70.67)	-2.77	-20.83	-12.71
OBXeCCH	OB+XeCCH	184.32	-58.88(23.92)	-185.18(75.23)	-2.10(0.85)	-61.83	-137.83(74.43)	-2.57	-22.44	-12.40
OBRnCCH	OB+RnCCH	187.50	-61.14(24.17)	-189.73(75.01)	-2.08(0.82)	-65.44	-143.16(75.46)	-1.16	-21.62	-12.42
OBKrCCH	OBKr+CCH	278.01	-124.53(32.33)	-259.01(67.25)	-1.63(0.42)	-	-97.43(37.62)	-2.61	-10.67	-79.05
OBXeCCH	OBXe+CCH	288.56	-136.31(33.59)	-267.46(65.90)	-2.09(0.51)	-	-105.35(39.39)	-2.23	-11.23	-76.67
OBRnCCH	OBRn+CCH	294.67	-143.73(34.05)	-276.32(65.46)	-2.05(0.49)	-	-105.68(38.25)	-2.35	-12.78	-74.56
NCKrCCH	NC+KrCCH	157.25	-48.50(21.38)	-176.48(77.80)	-1.87(0.82)	-69.60	-128.55(72.84)	-5.21	-2.19	-18.29
NCXeCCH	NC+XeCCH	181.82	-56.41(21.45)	-204.37(77.71)	-2.20(0.84)	-81.16	-153.20(74.96)	-6.72	-2.30	-21.07
NCRnCCH	NC+RnCCH	190.54	-60.32(21.94)	-212.36(77.25)	-2.21(0.80)	-84.36	-159.38(75.05)	-8.19	-2.52	-20.77
NCKrCCH	NCKr+CCH	255.46	-113.23(34.48)	-213.16(64.92)	-1.97(0.60)	-72.90	-87.20(40.91)	-5.47	-17.08	-87.30
NCXeCCH	NCXe+CCH	292.18	-131.78(35.08)	-241.57(64.30)	-2.35(0.63)	-83.51	-87.96(36.41)	-2.08	-33.86	-86.18
NCRnCCH	NCRn+CCH	295.71	-136.50(35.35)	-247.24(64.04)	-2.35(0.61)	-90.38	-126.30(51.08)	-1.92	-19.35	-77.59
SiNKrCCH	SiN+KrCCH	195.64	-83.80(31.32)	-181.25(67.74)	-2.53(0.95)	-71.95	-85.79(47.33)	-0.17	-1.20	-79.07
SiNXeCCH	SiN+XeCCH	231.30	-103.09(32.74)	-208.83(66.31)	-3.00(0.95)	-83.61	-111.39(53.34)	-5.11	-2.85	-76.83
SiNRnCCH	SiN+RnCCH	230.70	-106.24(33.46)	-208.30(65.60)	-2.99(0.94)	-86.83	-112.91(54.20)	-4.79	-3.05	-74.42
SiNKrCCH	SiNKr+CCH	239.27	-104.30(32.33)	-216.32(67.06)	-1.98(0.61)	-83.34	-90.62(41.89)	-5.54	-5.49	-77.74
SiNXeCCH	SiNXe+CCH	263.53	-117.01(33.11)	-234.03(66.23)	-2.34(0.66)	-89.85	-125.28(53.53)	-1.79	-16.13	-72.78
SiNRnCCH	SiNRn+CCH	256.28	-116.67(33.39)	-230.41(65.94)	-2.32(0.66)	-93.12	-125.40(54.53)	-1.26	-16.53	-69.17

Table S5 EDA results with the ETS-NOCV scheme at the level PBE-D3/TZ2P// CCSD(T)/cc-pVTZ/ cc-pVTZ-PP. All energy terms are in units of *k*cal·mol^{-1}. The percentages within the parentheses show the contributions towards the total attractive energy $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{dis}$, and those within the square brackets for $\Delta E(\sigma 1)$ show the contributions towards the total orbital interaction energy ΔE_{orb}.

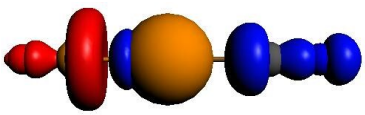
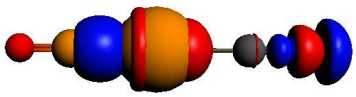
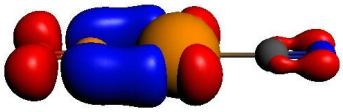
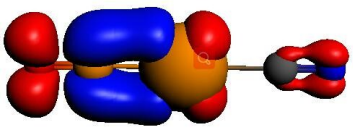
	Fragments	ΔE_{paul}	ΔE_{elstat}	ΔE_{orb}	ΔE_{dis}	ΔE_{int}	$\Delta E(\sigma 1)$	$\Delta E(\sigma$	$\Delta E(\pi$	$\Delta E(\pi$
$COKrCN^+$	$COKr^+$+CN	357.2	-	-	-	-	-	-	-	-
$COXeCN^+$	$COXe^+$+CN	342.8	-	-	-	-	-	-	-	-
CORnCN	$CORn^+$+CN	307.4	-	-	-	-	-	-	-	-
$OBKrCO^+$	OB+$KrCO^+$	312.3	-	-	-	-	-	-	-	-
OBXeCO	OB+$XeCO^+$	291.7	-	-	-	-	-	-8.61	-	-
OBRnCO	OB+$RnCO^+$	292.1	-	-	-	-	-	-	-8.53	-8.53
OBKrOSi	OB+$KrOSi^+$	326.2	-	-	-	-	-	-9.79	-	-
OBXeOSi	OB+$XeOSi^+$	302.0	-	-	-	-	-	-8.11	-	-
OBRnOSi	OB+$RnOSi^+$	299.3	-	-	-	-	-	-8.00	-	-
$OBKrCS^+$	OB+$KrCS^+$	315.9	-	-	-	-	-	-9.70	-	-
$OBXeCS^+$	OB+$XeCS^+$	291.1	-	-	-	-	-	-7.73	-	-
$OBRnCS^+$	OB+$RnCS^+$	286.8	-	-	-	-	-	-7.49	-	-
$OBKrNN^+$	OB+$KrNN^+$	322.6	-	-	-	-	-	-	-	-
OBXeNN	OB+$XeNN^+$	307.7	-	-	-	-	-	-9.32	-	-
OBRnNN	OB+$RnNN^+$	294.7	-	-	-	-	-	-	-	-
NNKrNSi	$NNKr^+$+NSi	343.6	-	-	-	-	-	-	-	-
NNXeNSi	$NNXe^+$+NSi	350.5	-	-	-	-	-	-3.39	-	-

NNRnNSi	NNRn$^+$+NSi	336.7	-	-	-	-	-	-8.60	-	-
SCKrNSi$^+$	SCKr$^+$+NSi	306.6	-	-	-	-	-	-	-2.96	-5.03
SCXeNSi$^+$	SCXe$^+$+NSi	321.7	-	-	-	-	-	-7.15	-	-
SCRnNSi$^+$	SCRn$^+$+NSi	303.7	-	-	-	-	-	-	-	-
SiOKrNSi	SiOKr$^+$+NSi	333.9	-	-	-	-	-	-9.42	-	-
SiOXeNSi	SiOXe$^+$+NSi	334.3	-	-	-	-	-	-	-	-
SiORnNS	SiORn$^+$+NS	314.7	-	-	-	-	-	-	-	-
NCKrOSi$^+$	NC+KrOSi$^+$	348.9	-	-	-	-	-	-	-	-
NCXeOSi	NC+XeOSi$^+$	310.7	-	-	-	-	-	-	-	-
NCRnOSi	NC+RnOSi$^+$	297.2	-	-	-	-	-	-	-	-
SCKrCN$^+$	SCKr$^+$+CN	311.7	-	-	-	-	-	-	-	-
SCXeCN$^+$	SCXe$^+$+CN	283.8	-	-	-	-	-	-9.55	-	-
SCRnCN$^+$	SCRn$^+$+CN	272.0	-	-	-	-	-	-9.13	-	-
NNKrCN$^+$	NNKr$^+$+CN	349.4	-	-	-	-	-	-	-	-
NNXeCN	NNXe$^+$+CN	312.6	-	-	-	-	-	-	-	-
NNRnCN	NNRn$^+$+CN	300.6	-	-	-	-	-	-	-	-
HCCKrN	HCC+KrNN	473.2	-	-	-	-	-	-8.89	-	-
HCCXeN	HCC+XeNN	431.9	-	-	-	-	-	-	-6.37	-2.53
HCCRnN	HCC++RnN	316.2	-	-	-	-	-	-	-	-
HCCKrC	HCC++KrC	470.1	-	-	-	-	-	-	-5.45	-8.30
HCCXeC	HCC++XeC	428.7	-	-	-	-	-	-1.62	-	-
HCCRnC	HCC++RnC	414.5	-	-	-	-	-	-0.90	-	-
HCCKrOS	HCC+KrOSi	472.5	-	-	-	-	-	-	-	-
HCCXeO	HCC+XeOSi	427.2	-	-	-	-	-	-5.86	-	-
HCCRnO	HCC+RnOS	412.5	-	-	-	-	-	-2.63	-	-
HCCKrCS	HCC+KrCS$^+$	453.8	-	-	-	-	-	-9.70	-	-
HCCXeCS	HCC+XeCS$^+$	409.6	-	-	-	-	-	-1.35	-	-
HCCRnC	HCC+RnCS$^+$	393.0	-	-	-	-	-	-0.77	-	-

Table S6 EDA results with the ETS-NOCV scheme at the level PBE-D3/TZ2P// CCSD(T)/cc-pVTZ/cc-pVTZ-PP. All energy terms are in units of *k*cal·mol^{-1}. The percentages within the parentheses show the contributions towards the total attractive energy ΔE_{elstat} +ΔE_{orb} + ΔE_{dis}, and those within the square brackets for ΔE(σ1) show the contributions towards the total orbital interaction energy ΔE_{orb}.

	Fragments	**ΔE_{pau}**	**ΔE_{elstat}**	**ΔE_{orb}**	**ΔE_{dis}**	**ΔE_{int}**	***ΔE*(σ1)**	***ΔE*(σ**	***ΔE*(π**	***ΔE*(π**
COKrCN$^+$	CO+KrCN$^+$	7.73	-	-	-	-5.10	-	—	-1.20	-1.20
COXeCN$^+$	CO+XeCN$^+$	9.52	-	-	-	-4.65	-	—	-1.20	-1.20
CORnCN$^+$	CO+RnCN$^+$	13.3	-	-	-	-3.82	-	—	-1.42	-1.42
OBKrCO$^+$	OBKr$^+$+CO	8.01	-	-	-	-9.33	-	—	-0.67	-0.67
OBXeCO$^+$	OBXe$^+$+CO	10.3	-	-	-	-7.75	-	_	-0.68	-0.68
OBRnCO$^+$	OBRn$^+$+CO	15.1	-	-	-	-6.90	-	_	-0.81	-0.81
OBKrOSi$^+$	OBKr$^+$+OSi	23.6	-	-	-	-	-	-0.57	-2.91	-2.91
OBXeOSi$^+$	OBXe$^+$+OSi	31.4	-	-	-	-	-	-0.77	-2.87	-2.87
OBRnOSi	OBRn$^+$+OS	38.9	-	-	-	-	-	-0.99	-3.27	-3.27
OBKrCS$^+$	OBKr$^+$+CS	18.7	-	-	-	-	-	_	-1.81	-1.81
OBXeCS$^+$	OBXe$^+$+CS	25.9	-	-	-	-	-	_	-2.05	-2.05
OBRnCS$^+$	OBRn$^+$+CS	35.3	-	-	-	-	-	-0.67	-2.42	-2.42
OBKrNN$^+$	OBKr$^+$+NN	4.19	-	-	-	-5.93	-	_	-0.73	-0.73
OBXeNN$^+$	OBXe$^+$+NN	5.08	-	-	-	-5.35	-	_	-0.73	-0.73
OBRnNN$^+$	OBRn$^+$+NN	7.48	-	-	-	-4.96	-	_	-0.83	-0.83
NNKrNSi$^+$	NN+KrNSi$^+$	4.66	-	-	-	-4.93	-	_	_	_
NNXeNSi	NN+XeNSi	6.27	-	-	-	-4.87	-	_	-0.62	-0.62
NNRnNSi	NN+RnNSi	8.98	-	-	-	-4.61	-	_	-0.75	-0.75

$SCKrNSi^+$	$SC+KrNSi^+$	30.4	-	-	-	-	-	-0.57	-1.75	-1.75
$SCXeNSi^+$	$SC+XeNSi^+$	42.7	-	-	-	-	-	-1.00	-2.50	-2.50
$SCRnNSi^+$	$SC+RnNSi^+$	51.3	-	-	-	-	-	-1.32	-2.98	-2.98
$SiOKrNSi^+$	$SiO+KrNSi^+$	30.2	-	-	-	-	-	-0.59	-2.29	-2.29
SiOXeNSi	SiO+XeNSi	39.6	-	-	-	-	-	-0.93	-2.72	-2.72
SiORnNSi	SiO+RnNSi	45.7	-	-	-	-	-	-1.16	-3.11	-3.11
$NCKrOSi^+$	$NCKr^+$+OSi	40.2	-	-	-	-	-	-0.78	-4.26	-4.26
$NCXeOSi^+$	$NCXe^+$+OSi	50.2	-	-	-	-	-	-1.05	-4.40	-4.40
$NCRnOSi^+$	$NCRn^+$+OS	57.9	-	-	-	-	-	-1.28	-4.91	-4.91
$SCKrCN^+$	$SC+KrCN^+$	44.8	-	-	-	-	-	-0.70	-3.17	-3.17
$SCXeCN^+$	$SC+XeCN^+$	56.1	-	-	-	-	-	-1.11	-3.78	-3.78
$SCRnCN^+$	$SC+RnCN^+$	67.7	-	-	-	-	-	-1.58	-4.41	-4.41
$NNKrCN^+$	$NN+KrCN^+$	9.72	-	-	-	-7.73	-	_	-1.21	-1.21
$NNXeCN^+$	$NN+XeCN^+$	12.3	-	-	-	-6.58	-	_	-1.30	-1.30
$NNRnCN^+$	$NN+RnCN^+$	17.8	-	-	-	-5.50	-	_	-1.58	-1.58
HCCKrNN	$HCCKr^+$+N	7.49	-	-	-	-6.27	-	_	-0.92	-0.92
HCCXeN	$HCCXe^+$+N	9.70	-	-	-	-5.53	-	_	-1.02	-1.02
HCCRnN	$HCCRn^+$+N	14.3	-	-	-	-4.55	-	_	-1.24	-1.24
HCCKrCO	$HCCKr^+$+C	11.1	-	-	-	-9.34	-	_	-0.72	-0.72
HCCXeCO	$HCCXe^+$+C	15.0	-	-	-	-8.96	-	_	-0.86	-0.86
HCCRnC	$HCCRn^+$+C	21.2	-	-	-	-8.00	-	_	-1.08	-1.08
HCCKrOSi	$HCCKr^+$+O	30.0	-	-	-	-	-	-0.60	-3.09	-3.09
HCCXeOS	$HCCXe^+$+O	39.0	-	-	-	-	-	-0.84	-3.29	-3.29
HCCRnOS	$HCCRn^+$+O	46.5	-	-	-	-	-	-1.04	-3.72	-3.72
$HCCKrCS^+$	$HCCKr^+$+CS	29.4	-	-	-	-	-	_	-2.14	-2.14
HCCXeCS	$HCCXe^+$+C	40.3	-	-	-	-	-	-0.68	-2.73	-2.73
HCCRnCS	$HCCRn^+$+C	51.8	-	-	-	-	-	-1.05	-3.29	-3.29

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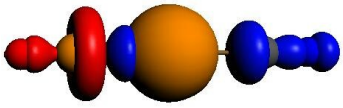
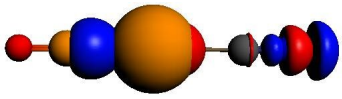
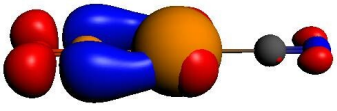
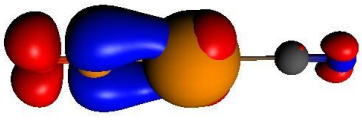

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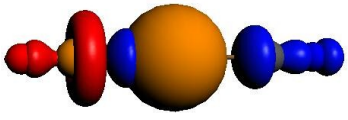
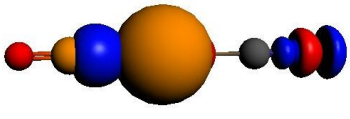
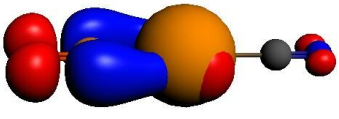
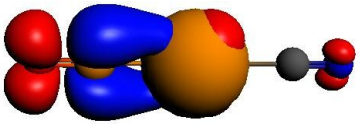
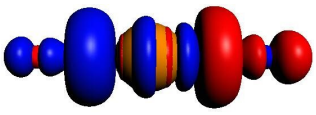
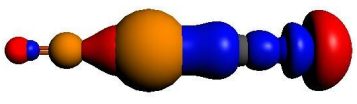
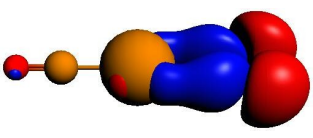
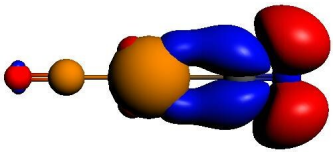





$\Delta E(\sigma 1)$ = -141.85 $\Delta E(\sigma 2)$ = -5.65 $\Delta E(\pi 1)$ = -4.51 $\Delta E(\pi 2)$ =-4.51

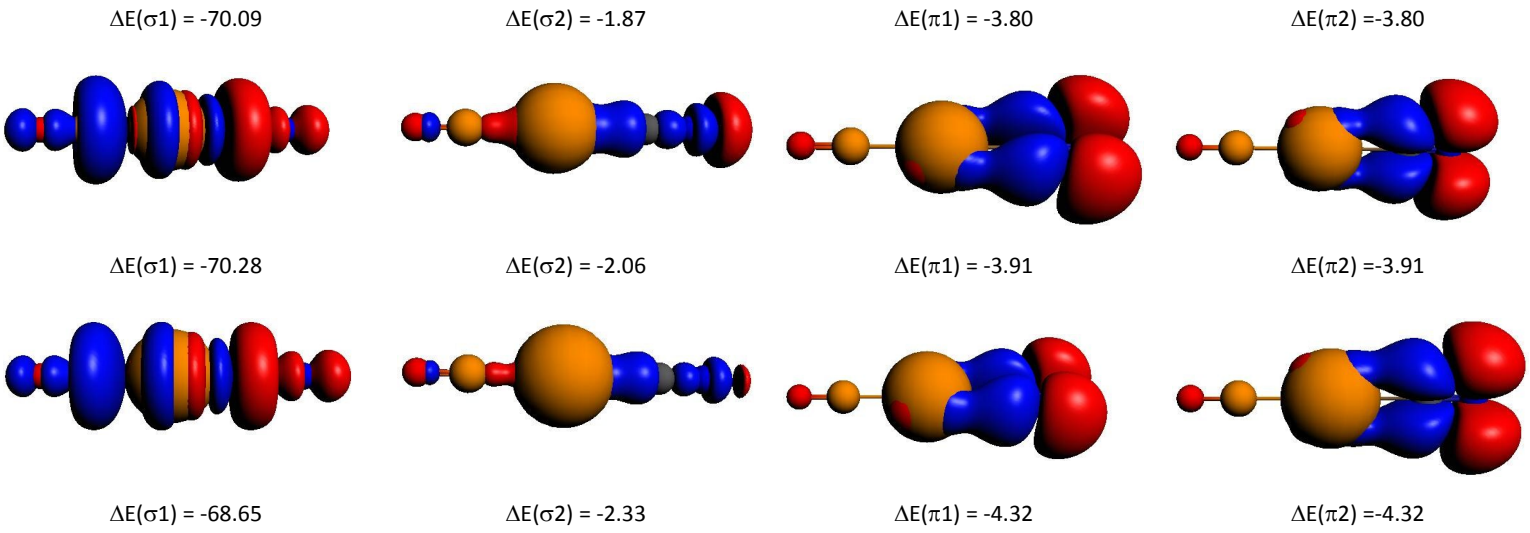


Fig. S8 Plots of deformation densities Δρ(***r***) of the pair-wise orbital interactions between the two fragments OB^- + $NgCN^+$ (The first three rows) and $OBNg^+$ + CN^- (The last three rows) for OBNgCN compound at the revPBE-D3/TZ2P//MP2/ aug-cc-pVTZ/ cc-pVTZ-PP level. From top to bottom, Ng = Kr, Xe, Rn, respectively. Red and blue denote negative or positive Δρ(***r***), respectively.

Table S7 Frequencies (cm^{-1}) and infrared intensity (in parentheses) of some vibrational modes for monovalent cationic compounds of calculated at the level of theory MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP.

	ν_1	ν_2	$\nu_{3(O\text{-}Ng)}$	$\nu_{4(C\text{-}Ng)}$	-	$\nu_{5(C\text{-}N/C\text{-}O)}$
$COKrCN^+$	40.9(2)	99.4(1)	124.9(13)	536.2(6)	-	2066.9(107)
$COXeCN^+$	41.7(2)	102.9(0)	126.2(12)	502.1(1)	-	2063.0(140)
$CORnCN^+$	43.3(1)	107.6(9)	124.9(13)	472.6(0)	-	2062.3(213)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(B\text{-}Ng)}$	$\nu_{5(O\text{-}B)}$	$\nu_{6(C\text{-}O)}$
$OBKrCO^+$	37.3(2)	297.9(35)	122.6(9)	470.4(8)	1966.5(41)	2148.7(7)
$OBXeCO^+$	37.6(1)	291.2(26)	122.4(9)	429.6(3)	1951.8(33)	2149.7(6)
$OBRnCO^+$	38.4(1)	291.6(22)	132.9(8)	401.6(2)	1947.9(29)	2152.9(5)
	ν_1	ν_2	$\nu_{3(O\text{-}Ng)}$	$\nu_{4(B\text{-}Ng)}$	$\nu_{5(O\text{-}B)}$	$\nu_{6(O\text{-}Si)}$
$OBKrOSi^+$	65.0(13)	319.4(28)	170.2(29)	474.9(0)	1971.6(49)	1168.6(259)
$OBXeOSi^+$	46.0(0)	313.6(19)	167.5(32)	429.0(0)	1953.4(40)	1164.4(318)
$OBRnOSi^+$	44.4(0)	310.1(18)	169.5(26)	399.6(0)	1947.6(36)	1166.9(333)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(B\text{-}Ng)}$	$\nu_{5(O\text{-}B)}$	$\nu_{6(C\text{-}S)}$
$OBKrCS^+$	44.4(0)	316.0(28)	135.3(22)	459.4(0)	1963.7(29)	1353.9(0)
$OBXeCS^+$	43.4(0)	310.9(19)	135.9(24)	414.9(1)	1945.2(21)	1358.3(0)
$OBRnCS^+$	41.8(0)	306.8(15)	141.0(21)	384.6(1)	1938.6(17)	1364.0(0)
	ν_1	ν_2	$\nu_{3(N\text{-}Ng)}$	$\nu_{4(B\text{-}Ng)}$	$\nu_{5(O\text{-}B)}$	$\nu_{6(N\text{-}N)}$
$OBKrNN^+$	31.5(2)	291.2(35)	108.75(7.99)	472.58(11.82)	1968.5(45)	2188.0(11)
$OBXeNN^+$	32.4(1)	285.8(26)	113.5(7)	432.8(6)	1953.2(37)	2186.0(14)
$OBRnNN^+$	33.9(1)	285.3(22)	125.2(0)	405.2(4)	1949.0(34)	2186.1(17)

	ν_1	ν_2	$\nu_{3(N\text{-}Ng)}$	$\nu_{4(Ng\text{-}N)}$	$\nu_{5(N\text{-}Si)}$	$\nu_{6(N\text{-}N)}$
$NNKrNSi^+$	33.9(1)	153.6(28)	108.6(13)	397.6(20)	1251.2(55)	2187.2(15)
$NNXeNSi^+$	36.0(1)	170.2(24)	116.2(14)	382.9(4)	1263.2(129)	2184.3(19)
$NNRnNSi^+$	36.6(1)	183.7(22)	128.9(14)	359.0(3)	1261.4(127)	2185.7(25)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(Ng\text{-}N)}$	$\nu_{5(N\text{-}Si)}$	$\nu_{6(S\text{-}C)}$
$SCKrNSi^+$	46.1(6)	251.4(25)	146.8(84)	366.9(22)	1243.3(319)	1374.0(4)
$SCXeNSi^+$	43.1(5)	255.3(24)	151.4(59)	356.3(24)	1253.9(378)	1374.1(2)
$SCRnNSi^+$	41.3(5)	250.1(21)	159.3(44)	336.4(14)	1252.2(329)	1377.9(1)
	ν_1	ν_2	$\nu_{3(O\text{-}Ng)}$	$\nu_{4(Ng\text{-}N)}$	$\nu_{5(Si\text{-}O)}$	$\nu_{6(N\text{-}Si)}$
$SiOKrNSi^+$	44.6(11)	204.9(40)	175.0(68)	393.7(4)	1261.8(126)	1164.2(460)
$SiOXeNSi^+$	43.8(10)	210.4(36)	175.9(62)	374.3(9)	1268.2(187)	1165.6(508)
$SiORnNSi^+$	41.4(9)	206.1(34)	179.9(52)	350.7(4)	1264.7(164)	1169.8(510)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(O\text{-}Ng)}$	$\nu_{5(O\text{-}Si)}$	$\nu_{6(N\text{-}C)}$
$NCKrOSi^+$	58.7(1)	138.5(23)	506.8(23)	205.7(55)	1161.5(435)	2075.5(86)
$NCXeOSi^+$	57.1(1)	145.0(20)	476.1(27)	200(49)	1160.3(473)	2073.3(91)
$NCRnOSi^+$	54.3(1)	146.4(18)	451.4(21)	200.3(38)	1165.9(466)	2074.9(92)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(Ng\text{-}C)}$	$\nu_{5(C\text{-}S)}$	$\nu_{6(N\text{-}C)}$
$NCKrCS^+$	59.6(0)	179.9(9)	169.4(69)	443.3(60)	1380.8(13)	2046.9(196)
$NCXeCS^+$	55.0(0)	178.0(8.0)	167.9(48)	436.1(49)	1381.4(11)	2054.0(169)
$NCRnCS^+$	53.5(0)	182.3(6)	171.4(35)	419.0(37)	1385.9(7)	2056.9(161)
	ν_1	ν_2	$\nu_{3(N\text{-}Ng)}$	$\nu_{4(C\text{-}Ng)}$	$\nu_{5(N\text{-}N)}$	$\nu_{6(N\text{-}C)}$
$NCKrNN^+$	46.6(2)	135.0(1)	133.5(14)	532.1(4)	2187.2(22)	2066.0(36)
$NCXeNN^+$	46.9(2)	137.8(0)	133.3(14)	497.4(0)	2184.2(26)	2062.4(56)
$NCRnNN^+$	48.8(1)	150.2(0)	143.1(13)	468.6(0)	2184.5(30)	2063.6(66)
	ν_1	ν_2	$\nu_{3(N\text{-}Ng)}$	$\nu_{4(C\text{-}Ng)}$	$\nu_{5(C\text{-}C)}$	$\nu_{6(N\text{-}N)}$
$HCCKrNN^+$	41.7(0)	206.5(9)	120.8(10)	596.3(0)	2115.9(21)	2188.6(14)
$HCCXeNN^+$	42.7(0)	207.8(10)	123.1(10)	547.5(1)	2089.4(31)	2187.1(17)
$HCCRnNN^+$	44.1(1)	202.6(9)	132.9(9)	512.6(2)	2081.6(29)	2186.3(21)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(Ng\text{-}C)}$	$\nu_{5(C\text{-}C)}$	$\nu_{6(C\text{-}O)}$
$HCCKrCO^+$	48.9(1)	219.2(6)	130.4(13)	588.6(0)	2113.6(25)	2153.4(6)
$HCCXeCO^+$	49.4(1)	219.2(6)	133.0(13)	539.4(5)	2086.3(37)	2154.9(4)
$HCCRnCO^+$	49.2(1)	218.7(4)	142.5(12)	503.2(6)	2076.9(35)	2157.9(3)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(O\text{-}Ng)}$	$\nu_{5(O\text{-}Si)}$	$\nu_{6(C\text{-}C)}$
$HCCKrOSi^+$	55.2(8)	250.5(13)	573.1(16)	183.4(41)	1168.7(309)	2108.2(29)
$HCCXeOSi^+$	53.4(8)	246.4(16)	523.8(27)	179.6(41)	1167.9(362)	2079.6(37)
$HCCRnOS^+$	51.5(7)	239.4(16)	491.6(24)	181.0(33)	1171.3(367)	2070.7(32)
	ν_1	ν_2	$\nu_{3(C\text{-}Ng)}$	$\nu_{4(Ng\text{-}C)}$	$\nu_{5(C\text{-}S)}$	$\nu_{6(C\text{-}C)}$
$HCCKrCS^+$	53.7(4)	260.8(12)	149(39)	547.8(34)	1368.8(1)	2099.0(54)
$HCCXeCS^+$	51.2(4)	263.8(14)	149.2(36)	502.3(46)	1371.0(2)	2069.9(63)
$HCCRnCS^+$	49.1(4)	254.9(13)	154.7(28)	470.7(42)	1376.7(1)	2059.7(56)

CCSD(T)/ aug-cc-pVTZ/ cc-pVTZ-PP coordinates:

OBKrCN

0 1

O	0.000000	0.000000	3.344581
B	0.000000	0.000000	2.133941
C	0.000000	0.000000	-2.289141
N	0.000000	0.000000	-3.461504
Kr	0.000000	0.000000	0.014973

OBXeCN

0 1

O	0.000000	0.000000	3.471106
B	0.000000	0.000000	2.259209
C	0.000000	0.000000	-2.382170
N	0.000000	0.000000	-3.553903
Xe	0.000000	0.000000	0.001953

OBRnCN

0 1

O	0.000000	0.000000	-3.551914
B	0.000000	0.000000	-2.339190
C	0.000000	0.000000	2.434855
N	0.000000	0.000000	3.606035
Rn	0.000000	0.000000	0.003022

OBKrNC

0 1

O	0.000000	0.000000	3.196839
B	0.000000	0.000000	1.989446
C	0.000000	0.000000	-3.429685
N	0.000000	0.000000	-2.243787
Kr	0.000000	0.000000	0.021186

OBXeNC

0 1

O	0.000000	0.000000	-3.372508
B	0.000000	0.000000	-2.162432
C	0.000000	0.000000	3.511971
N	0.000000	0.000000	2.326299
Xe	0.000000	0.000000	0.008080

OBRnNC

0 1

O	0.000000	0.000000	-3.465074
B	0.000000	0.000000	-2.254422
C	0.000000	0.000000	3.555602
N	0.000000	0.000000	2.370390
Rn	0.000000	0.000000	0.012400