Supporting Information for

Exploring the structure bonding and stability of noble gas compound promoted by superhalogens. A case study on $HNgMX_3$ (Ng=Ar-Rn, M=Be-Ca, X=F-Br) via combined high-level ab initio and DFT calculations

Lin-Yu Wu,‡[a] Jin-Feng Li,‡ [b] Ru-Fang Zhao,[c] Lan Luo,[c] Yong-Cheng Wang,*[a] and Bing Yin*[c]

CONTENTS

1. Superhalogen MX_3 1

Fig. S1 The optimized structures and selected bond lengths (in Å) of the MX_3^- and MX_3 (M=Be, Mg, Ca; X=F, Cl, Br) level (The bond lengths at ωB97XD /Def2-TZVP level are shown in the parentheses) 1

Table S1. The comparison of VDE values of superhalogen MX_3 (M=Be, Mg, Ca； X=F, Cl, Br) at various theoretical levels (eV) 1

Fig. S2 Comparison of VDE values (eV) at different theoretical levels at MP2/def2-TZVP, ωB97XD/def2-TZVP and CCSD(T)/def2-TZVP//MP2/def2-TZVP level of theory 1

Fig. S3 The optimized structures and selected bond lengths (in Å) of the HNgY at MP2/def2-TZVP level (The bond lengths at ωB97XD /def2-TZVP level are shown in the parentheses). 2

2.The dissociation process of HMX_3 3

Fig. S4 The optimized structures and selected bond lengths (in Å) of the HMX_3 (M=Be, Mg, Ca; X=F, Cl, Br) at MP2/def2-TZVP level (The bond lengths at ωB97XD /def2-TZVP level are shown in the parentheses) 3

Table S2. The ZPE-uncorrected dissociation energy (ΔE, kcal/mol), the ZPE corrected dissociation energy (ΔE_0, kcal/mol) and dissociation free energy change (ΔG, kcal/mol) at 298.15 K for dissociation process 4

Fig. S5 Comparison of dissociation energy of $HMX_3 \rightarrow HX+MX_2$ 5

Fig. S6 Comparison of dissociation energy of $HMX_3 \rightarrow H^+ + MX_3^-$ 5

Fig. S7 Comparison of dissociation energy of $HMX_3 \rightarrow H+MX_3$ 5

3.Geometrical parameters of stable structures 6

Table S3. Comparison of bond length (Å) in $HNgMX_3$ at various theoretical levels 6

Fig. S8 Comparison of M-X bond length in HNgY with MX_3^- and MX_3 at various theoretical levels. 6

Fig. S9 Comparison of H-Ng-X2 bond angel in HNgY with MX_3^- and MX_3 at various theoretical levels 7

Fig. S10 The changed trend of H···Ng, H···X2 and M···X3 distances along Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca 7

Fig. S11 The optimized structures and selected bond lengths (in Å) of the HNg^+ (Ng=Ar-Rn) at MP2/def2-TZVP level (The bond lengths at ωB97XD /def2-TZVP level are shown in the parentheses) 8

Table S4. Comparison of H-Ng bond length (in Å) in HNgY with HNg^+ at various theoretical levels 8

4.Charge distribution analysis of HngY 9

Table S5. Calculated natural charges of each atom (|e|) of $HNgMX_3$ at CCSD/def2-TZVP//MP2/def2-TZVP level. 9

Fig. S12 The natural charges trend of Ng, H atoms and H+Ng in HNgY along Ar-Kr-Xe-Rn, Be-Mg-Ca as well as F-Cl-Br 10

Table S6. Wiberg bond indices (WBI) values, atom-atom overlap-weighted NAO bond order and MO bond order of HNgY bonds at CCSD/def2-TZVP // MP2/def2-TZVP level 11

Fig. S13 Comparison of Wiberg bond indices (WBI) values for M-X3, Ng-X3 and Ng-H along Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca 14

Table S7 MO bond order (Occupancy) Bond orbital 15

Table S8 Analysis of charge density descriptors (a.u.) at the bond critical point (BCPs) of the part of $HNgMX_3$ molecules by AIM at CCSD/def2-TZVP // MP2/def2-TZVP level. 16
Fig. S14 Variation of relative energy (ΔE, kcal/mol) and hardness (η, eV), of HNgBeF3 and HXeMgCl3 with reaction coordinates corresponding to trace the the IRC path. The most stable structure has been taken as the reference for calculating the rotational barrier. 16
Table S9 The LUMO and HOMO energy of $HNgMX_3$ as well as the energy gap and chemical hardness at CCSD/def2-TZVP // MP2/def2-TZVP level. 17
Fig. S15 Comparison of chemical hardness (η) values for HNgMX3 along VDE, Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca. 18
5.Thermodynamic and kinetic stability of HNgY 19
Table S10. The fragment energies of $HNgMX_3$ (Ng=Ar-Rn; M=Be, Mg, Ca; X=F, Cl, Br) along six pathways (kcal/mol) 19
Fig. S16 The optimized geometries of transition state in $HNgMX_3$ (Ng=Ar-Rn) are performed at the MP2/def2-TZVP level (the corresponding value from ωB97XD/def2-TZVP level in parentheses). 28
Table S11. The energy barriers of $HNgMX_3$ along channel 5 at various levels (in kcal/mol). 29
Fig. S17 The comparison of the change in X2-Ng and X3-Ng bond length from stable configuration to transition state (Å) 30
Table S12. Comparison of bond length (Å) in HNgY with stable and transition state at various theoretical levels 31
Fig. S18 Comparison of the difference of H-Ng bond length and H-Ng-X2 Angle from stable configuration to transition state along Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca 31
Table S13. The natural charges of the transition state at CCSD/def2-TZVP //MP2/def2-TZVP level (|e|) 32
Fig. S19 The natural charges trend of X2 , X3 atoms in transition state along Ar-Kr-Xe-Rn, Be-Mg-Ca, as well as the F-Cl-Br 33
Fig. S20 The natural charges trend of Ng, H atoms and Ng+H in transition state along Ar-Kr-Xe-Rn, Be-Mg-Ca, as well as the F-Cl-Br 33
Fig. S21 The relative energy barriers obtained from CCSD(T) calculation and chemical hardness 34
Fig. S22 The relative energy barriers obtained from CCSD(T) calculation and chemical hardness 34
6.Geometry and stability of HNgX 35
Fig. S23 The optimized geometries of transition state in $HNgMX_3$ (Ng=Ar-Rn) are performed at the MP2/def2-TZVP level (the corresponding value from ωB97XD/def2-TZVP level in parentheses). 35
Fig. S24 Comparison of the change of H-Ng and X-Ng bond length from stable configuration to transition state along F-Cl-Br and Ar-Kr-Xe-Rn 35
Table S14. The fragment energies of HNgX (Ng=Ar-Rn; X=F, Cl, Br) (kcal/mol) 36
Fig. S25 Comparison of dissociation energy of HNgX→HX+Ng along F-Cl-Br and Ar-Kr-Xe-Rn 36
Table S15. The activation energies of HNgX (Ng=Ar-Rn; X=F, Cl, Br) (kcal/mol) 37
Fig. S26 Comparison of energy barrier of HNgX→HX+Ng along F-Cl-Br and Ar-Kr-Xe-Rn 37
Cartesian coordinates 38

1. Superhalogen MX_3

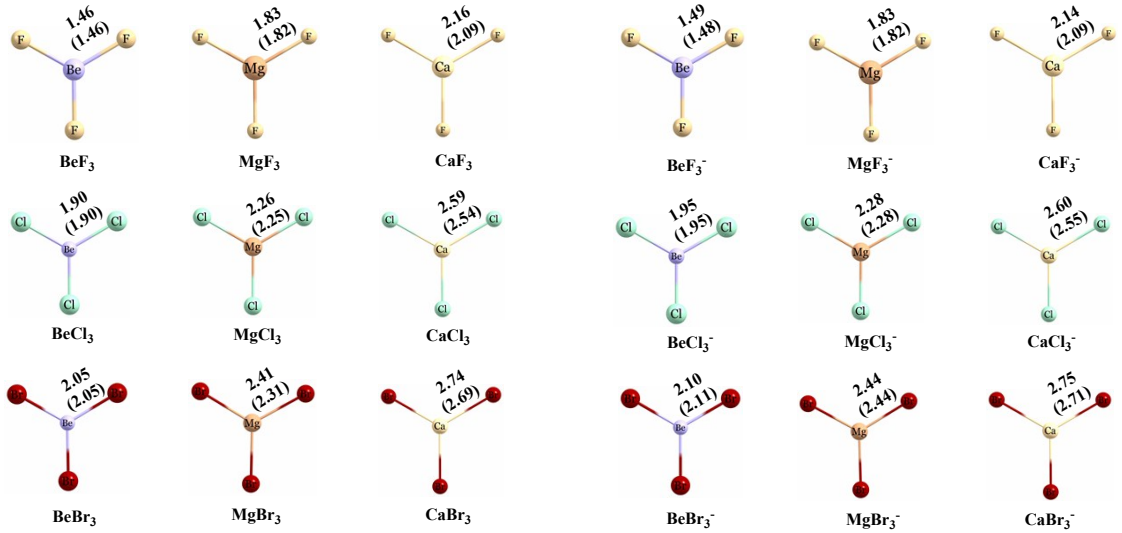

Fig. S1 The optimized structures and selected bond lengths (in Å) of the MX_3^- and MX_3 (M=Be, Mg, Ca; X=F, Cl, Br) level (The bond lengths at ωB97XD /Def2-TZVP level are shown in the parentheses)

Table S1. The comparison of VDE values of superhalogen MX_3 (M=Be, Mg, Ca； X=F, Cl, Br) at various theoretical levels (eV)

Ligand	MP2	ωB97XD	CCSD(T)-SP
		def2-TZVP	
BeF_3	7.51	6.76	7.41
$BeCl_3$	6.03	5.76	5.94
$BeBr_3$	5.61	5.36	5.52
MgF_3	7.77	6.82	7.63
$MgCl_3$	6.52	6.18	6.43
$MgBr_3$	6.09	5.77	6.00
CaF_3	7.43	6.73	7.27
$CaCl_3$	6.58	6.23	6.51
$CaBr_3$	6.21	5.86	6.14

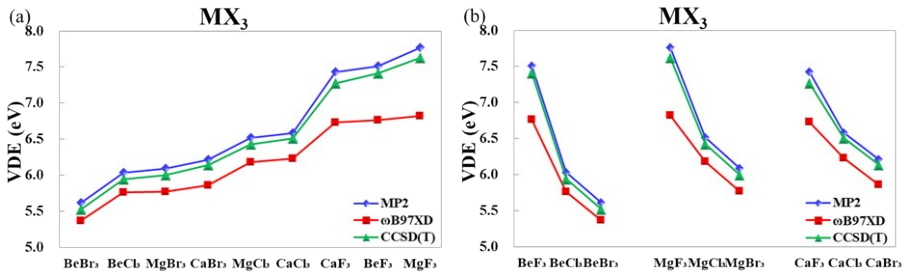

Fig. S2 Comparison of VDE values (eV) at different theoretical levels at MP2/def2-TZVP, ωB97XD/def2-TZVP and CCSD(T)/def2-TZVP//MP2/def2-TZVP level of theory

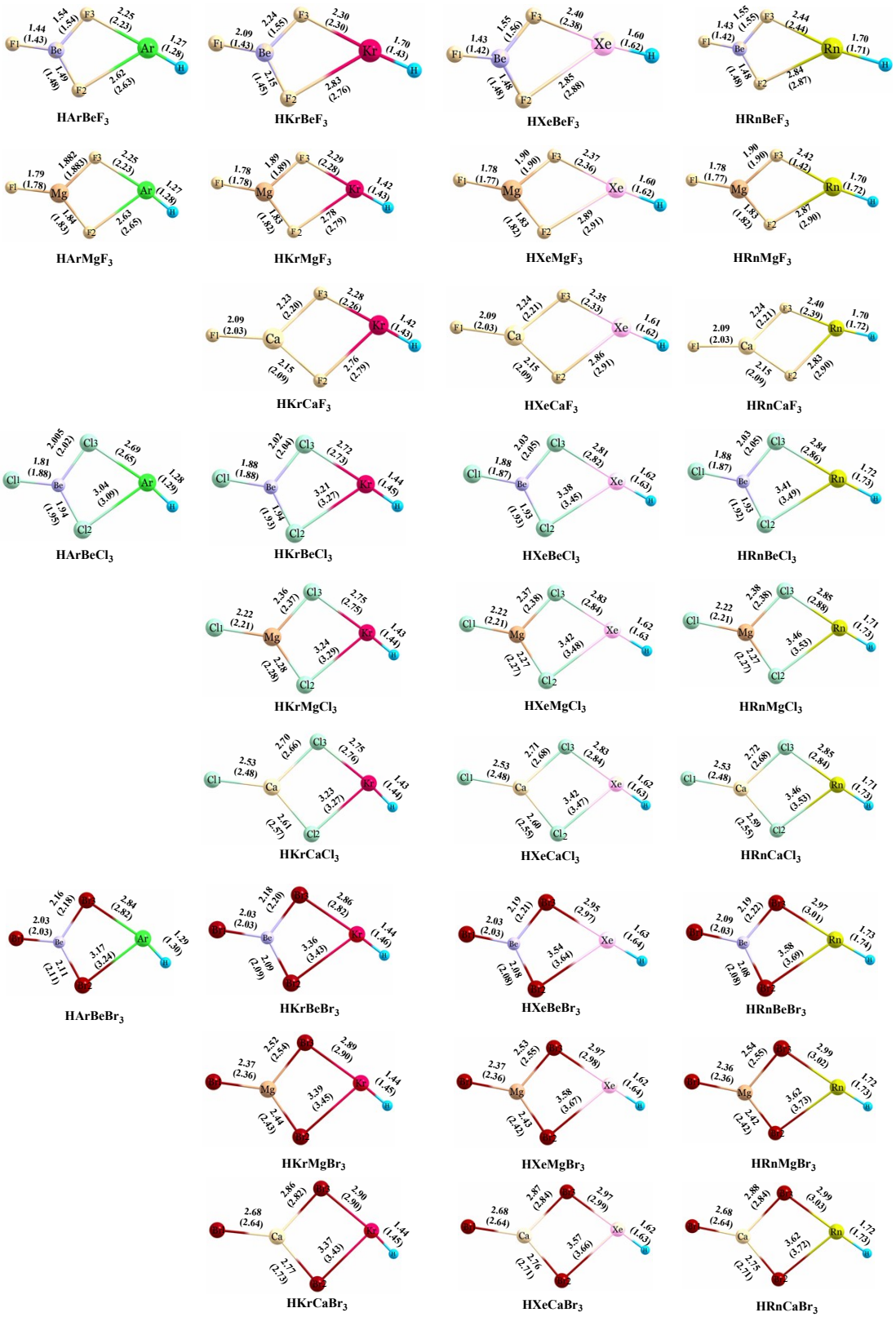

Fig. S3 The optimized structures and selected bond lengths (in Å) of the HNgY at MP2/def2-TZVP level (The bond lengths at ωB97XD/def2-TZVP level are shown in the parentheses).

2.The dissociation process of HMX_3

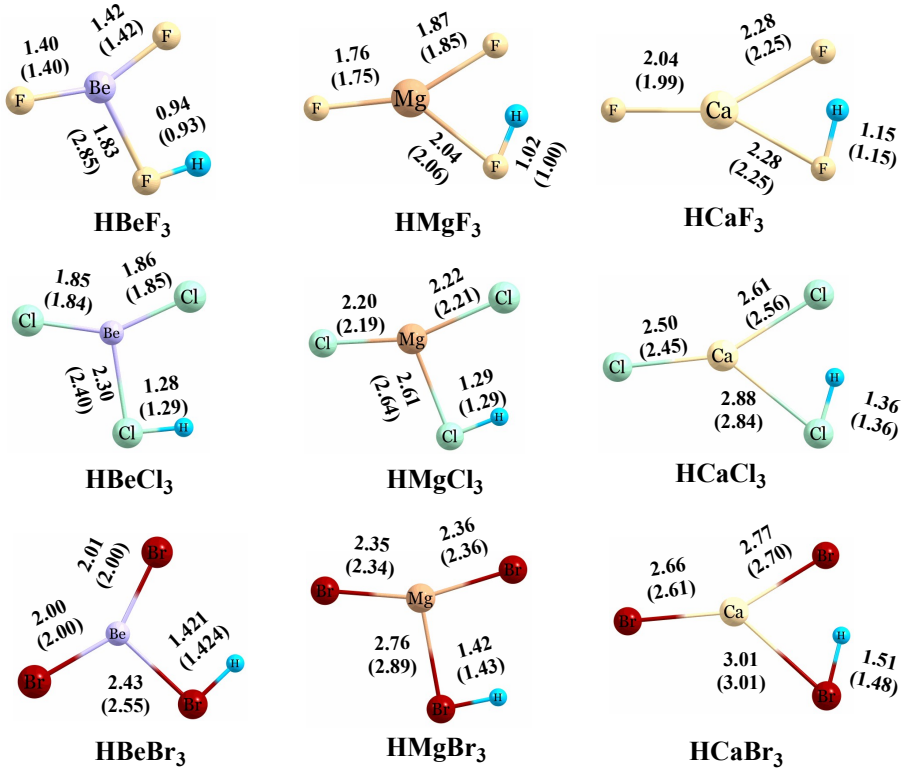

Fig. S4 The optimized structures and selected bond lengths (in Å) of the HMX_3 (M=Be, Mg, Ca; X=F, Cl, Br) at MP2/def2-TZVP level (The bond lengths at ωB97XD /def2-TZVP level are shown in the parentheses)

Table S2. The ZPE-uncorrected dissociation energy (ΔE, kcal/mol), the ZPE corrected dissociation energy (ΔE_0, kcal/mol) and dissociation free energy change (ΔG, kcal/mol) at 298.15 K for dissociation process

(a) The dissociation process: $HMX_3 \rightarrow HX+MX_2$

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HBeF_3$	BeF_2+HF	10.01	8.25	1.81	9.68	7.84	1.37	10.01	8.18
$HMgF_3$	MgF_2+HF	18.49	16.87	10.24	19.04	17.50	10.83	18.90	17.36
$HCaF_3$	CaF_2+HF	24.76	24.01	19.26	26.90	25.89	19.26	26.66	25.65
$HBeCl_3$	$BeCl_2$+HCl	4.05	2.82	-4.05	4.98	3.70	-3.30	4.12	2.84
$HMgCl_3$	$MgCl_2$+HCl	9.90	8.66	1.78	10.04	8.89	2.17	9.54	8.40
$HCaCl_3$	$CaCl_2$+HCl	12.63	11.77	6.44	12.38	11.45	6.00	11.04	10.11
$HBeBr_3$	$BeBr_2$+HBr	3.43	2.15	-1.62	5.22	4.10	-3.00	4.03	2.91
$HMgBr_3$	$MgBr_2$+HBr	9.11	8.15	1.42	9.71	8.72	1.96	9.02	8.02
$HCaBr_3$	$CaBr_2$+HBr	11.35	10.62	3.41	11.74	11.20	3.96	10.03	9.49

(b) The dissociation process: $HMX_3 \rightarrow H^+ + MX_3^-$

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HBeF_3$	$BeF_3^-+H^+$	301.27	294.85	290.26	298.25	291.85	287.22	300.07	293.66
$HMgF_3$	$MgF_3^-+H^+$	306.83	299.41	294.53	303.07	296.60	291.71	305.07	298.60
$HCaF_3$	$CaF_3^-+H^+$	318.32	312.70	308.39	317.18	311.03	306.19	319.45	313.30
$HBeCl_3$	$BeCl_3^-+H^+$	284.70	279.85	275.45	280.41	275.53	271.05	283.04	278.16
$HMgCl_3$	$MgCl_3^-+H^+$	280.72	275.78	271.29	277.07	272.16	267.82	279.42	274.50
$HCaCl_3$	$CaCl_3^-+H^+$	282.77	278.12	273.55	280.26	275.57	270.91	281.71	277.03
$HBeBr_3$	$BeBr_3^-+H^+$	279.28	274.92	270.67	274.28	269.80	265.34	277.07	272.59
$HMgBr_3$	$MgBr_3^-+H^+$	275.72	271.30	265.98	271.15	266.67	261.33	273.65	269.17
$HCaBr_3$	$CaBr_3^-+H^+$	275.65	271.46	266.99	272.57	268.52	263.88	273.77	269.72

(c) The dissociation process: $HMX_3 \rightarrow H+MX_3$

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HBeF_3$	$BeF_3^-+H^+$	141.09	157.21	156.66	132.89	151.86	144.67	127.72	146.32
$HMgF_3$	$MgF_3^-+H^+$	148.63	168.51	167.31	141.01	162.18	157.34	135.67	155.96
$HCaF_3$	$CaF_3^-+H^+$	157.68	174.83	173.46	151.01	168.66	164.72	145.03	161.95
$HBeCl_3$	$BeCl_3^-+H^+$	100.93	104.71	105.48	95.26	100.95	96.99	90.69	95.76
$HMgCl_3$	$MgCl_3^-+H^+$	107.55	113.58	113.79	101.94	109.07	106.63	97.38	103.68
$HCaCl_3$	$CaCl_3^-+H^+$	110.87	118.42	118.16	105.55	113.91	111.81	100.27	107.26
$HBeBr_3$	$BeBr_3^-+H^+$	86.34	88.89	89.99	81.32	85.43	82.59	77.32	80.36
$HMgBr_3$	$MgBr_3^-+H^+$	78.78	78.62	79.62	74.30	74.15	73.40	68.17	68.15
$HCaBr_3$	$CaBr_3^-+H^+$	95.23	102.15	101.60	90.50	98.30	96.30	86.09	91.82

ΔE_0 in CCSD(T) is equal to the electron energy plus the zero-point correction of MP2.

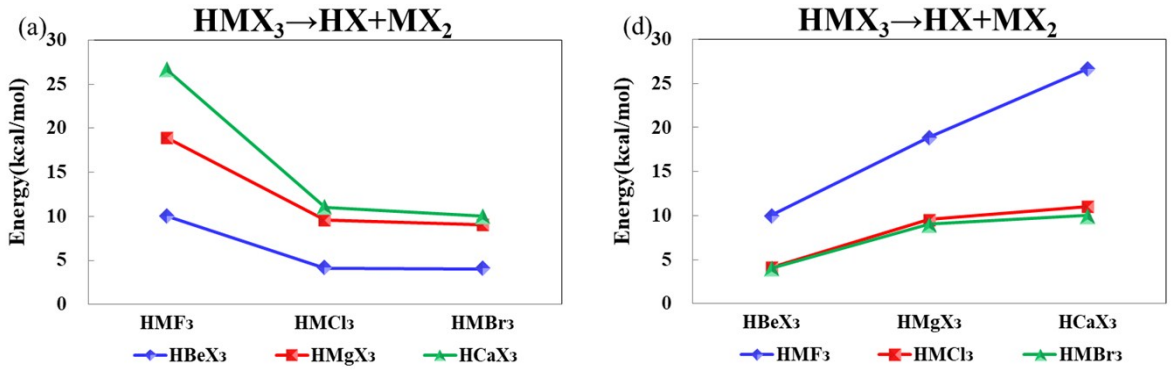

Fig. S5 Comparison of dissociation energy of $HMX_3 \rightarrow HX+MX_2$

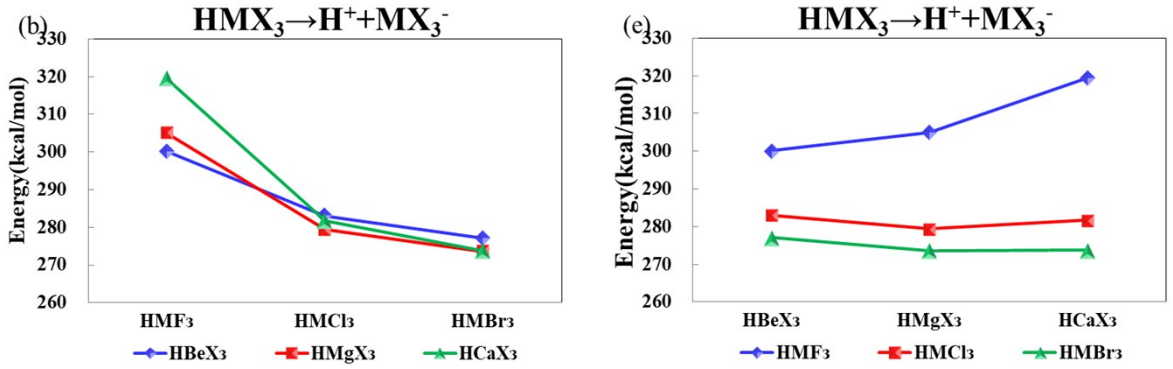

Fig. S6 Comparison of dissociation energy of $HMX_3 \rightarrow H^+ + MX_3^-$

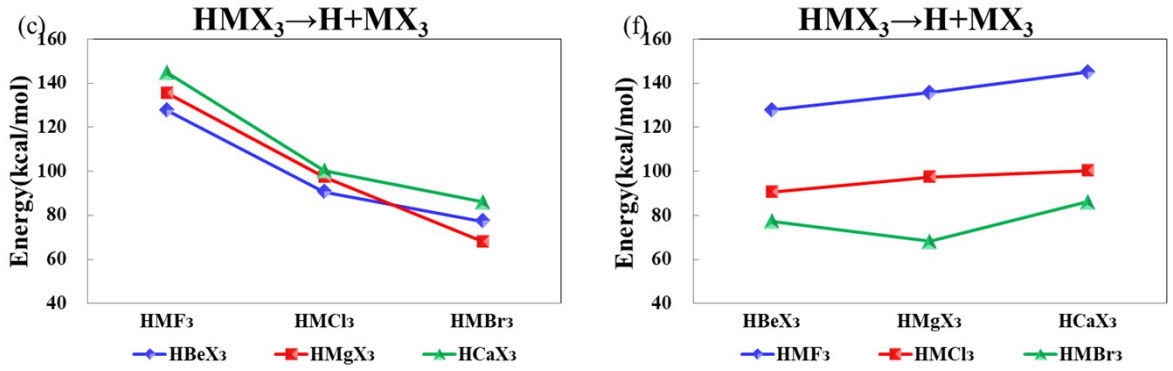

Fig. S7 Comparison of dissociation energy of $HMX_3 \rightarrow H+MX_3$

3.Geometrical parameters of stable structures

Table S3. Comparison of bond length (Å) in $HNgMX_3$ at various theoretical levels

	$HKrBeCl_3$			$HXeBeCl_3$			$HRnBeCl_3$		
	MP2	ωB97XD	Δ	MP2	ωB97XD	Δ	MP2	ωB97XD	Δ
r(M-X1)	1.878	1.876	0.002	1.877	1.874	0.003	1.875	1.873	0.002
r(M-X2)	1.936	1.933	0.003	1.927	1.925	0.002	1.926	1.924	0.002
r(M-X3)	2.021	2.037	-0.016	2.031	2.047	-0.016	2.034	2.049	-0.015
r(X2-Ng)	3.213	3.269	-0.056	3.375	3.446	-0.071	3.405	3.486	-0.081
r(X3-Ng)	2.724	2.732	-0.008	2.814	2.820	-0.006	2.840	2.863	-0.023
r(Ng-H)	1.435	1.446	-0.011	1.618	1.632	-0.014	1.715	1.728	-0.013
	$HKrMgCl_3$			$HXeMgCl_3$			$HRnMgCl_3$		
	MP2	ωB97XD	Δ	MP2	ωB97XD	Δ	MP2	ωB97XD	Δ
r(M-X1)	2.218	2.211	0.007	2.216	2.210	0.006	2.215	2.209	0.006
r(M-X2)	2.282	2.277	0.005	2.271	2.266	0.005	2.270	2.265	0.005
r(M-X3)	2.362	2.369	-0.007	2.372	2.381	-0.009	2.376	2.383	-0.007
r(X2-Ng)	3.243	3.292	-0.049	3.422	3.484	-0.062	3.460	3.531	-0.071
r(X3-Ng)	2.747	2.753	-0.006	2.832	2.838	-0.006	2.845	2.877	-0.032
r(Ng-H)	1.433	1.442	-0.009	1.615	1.629	-0.014	1.712	1.725	-0.013
	$HKrCaCl_3$			$HXeCaCl_3$			$HRnCaCl_3$		
	MP2	ωB97XD	Δ	MP2	ωB97XD	Δ	MP2	ωB97XD	Δ
r(M-X1)	2.530	2.481	0.049	2.530	2.481	0.049	2.529	2.481	0.048
r(M-X2)	2.614	2.566	0.048	2.598	2.551	0.047	2.594	2.549	0.045
r(M-X3)	2.700	2.663	0.037	2.713	2.675	0.038	2.719	2.676	0.043
r(X2-Ng)	3.228	3.269	-0.041	3.416	3.474	-0.058	3.459	3.527	-0.068
r(X3-Ng)	2.754	2.757	-0.003	2.827	2.845	-0.018	2.847	2.837	0.010
r(Ng-H)	1.430	1.442	-0.012	1.615	1.628	-0.013	1.713	1.725	-0.012

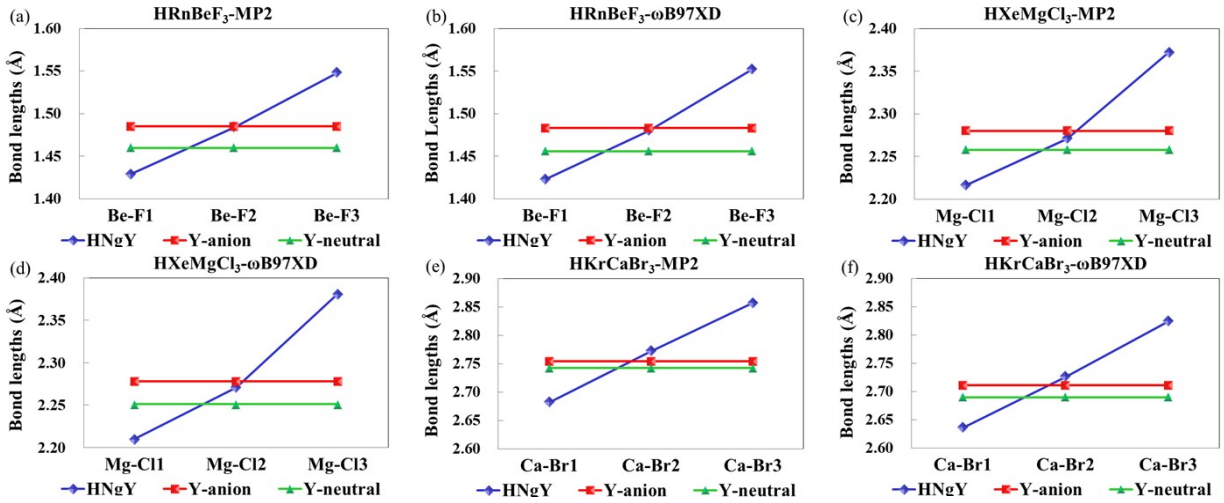

Fig. S8 Comparison of M-X bond length in HNgY with MX_3^- and MX_3 at various theoretical levels.

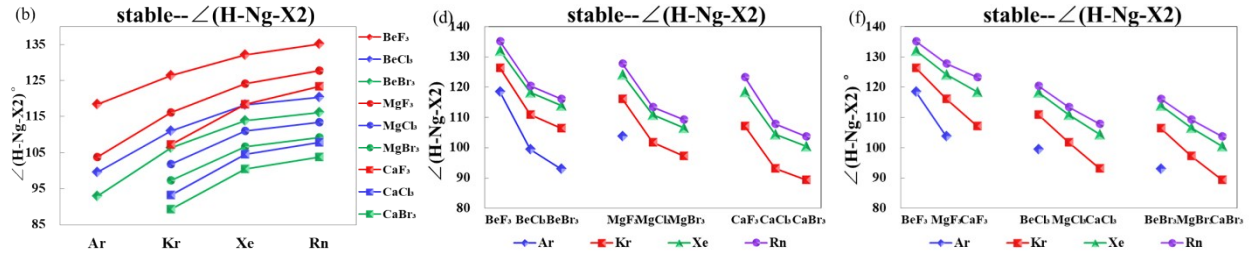

Fig. S9 Comparison of H-Ng-X2 bond angel in HNgY with MX_3^- and MX_3 at various theoretical levels

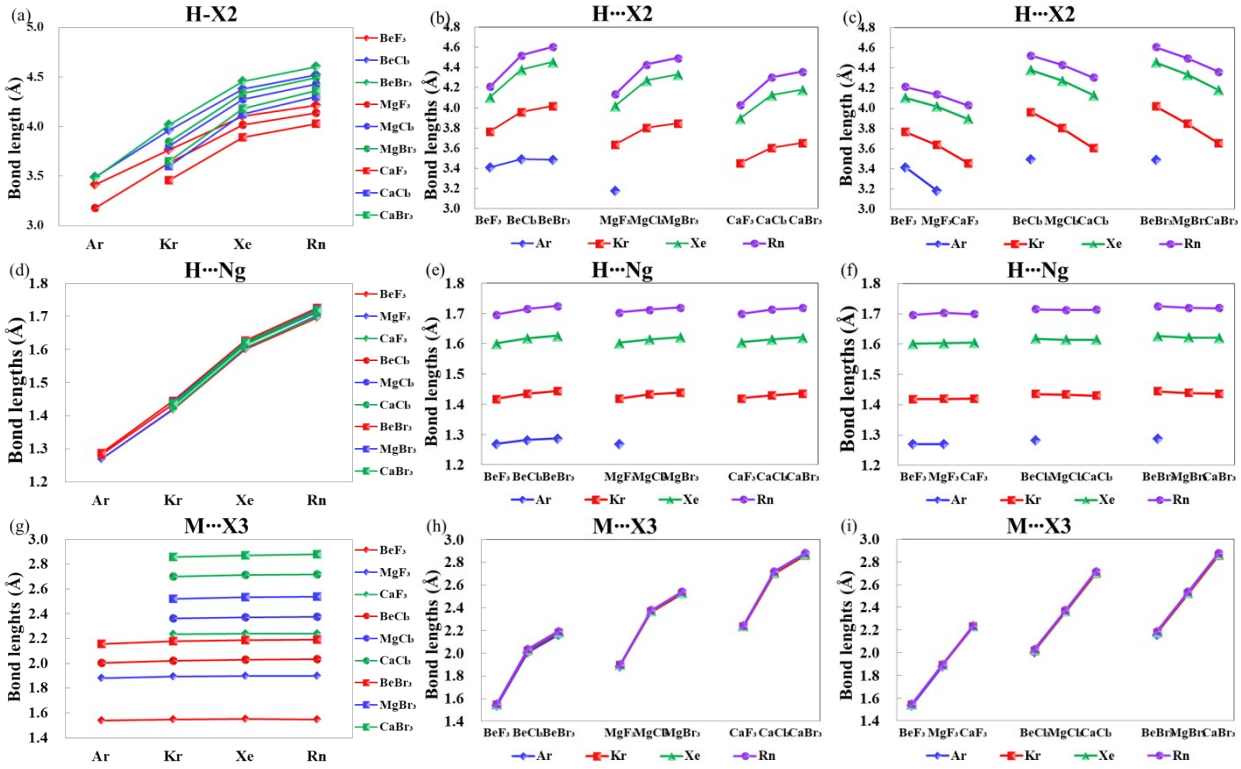

Fig. S10 The changed trend of H···Ng, H···X2 and M···X3 distances along Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca

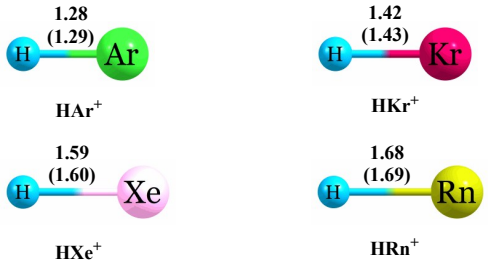

Fig. S11 The optimized structures and selected bond lengths (in Å) of the HNg^+ (Ng=Ar-Rn) at MP2/def2-TZVP level (The bond lengths at ωB97XD /def2-TZVP level are shown in the parentheses)

Table S4. Comparison of H-Ng bond length (in Å) in HNgY with HNg^+ at various theoretical levels

HNg^+				r(H-Ng)		Absolute error			r(H-Ng)		Absolute error	
	def2-TZVP			def2-TZVP		def2-TZVP			def2-TZVP		def2-TZVP	
	MP2	ωB97XD		MP2	ωB97XD	MP2	ωB97XD		MP2	ωB97XD	MP2	ωB97XD
Ar	1.283	1.285	$HArBeCl_3$	1.282	1.295	0.001	-0.010	$HArBeBr_3$	1.287	1.303	-0.004	-0.018
	1.422	1.426	$HKrBeCl_3$	1.435	1.446	-0.013	-0.020	$HKrBeBr_3$	1.444	1.455	-0.022	-0.029
Kr	1.422	1.426	$HKrMgCl_3$	1.433	1.443	-0.011	-0.017	$HKrMgBr_3$	1.439	1.450	-0.017	-0.024
	1.422	1.426	$HKrCaCl_3$	1.430	1.442	-0.008	-0.016	$HKrCaBr_3$	1.436	1.448	-0.014	-0.022
	1.593	1.602	$HXeBeCl_3$	1.618	1.632	-0.025	-0.030	$HXeBeBr_3$	1.626	1.640	-0.033	-0.038
Xe	1.593	1.602	$HXeMgCl_3$	1.615	1.629	-0.022	-0.027	$HXeMgBr_3$	1.622	1.636	-0.029	-0.034
	1.593	1.602	$HXeCaCl_3$	1.615	1.628	-0.022	-0.026	$HXeCaBr_3$	1.621	1.634	-0.028	-0.032
	1.680	1.688	$HRnBeCl_3$	1.715	1.728	-0.035	-0.040	$HRnBeBr_3$	1.725	1.736	-0.045	-0.048
Rn	1.680	1.688	$HRnMgCl_3$	1.712	1.725	-0.032	-0.037	$HRnMgBr_3$	1.720	1.733	-0.04	-0.045
	1.680	1.688	$HRnCaCl_3$	1.713	1.725	-0.033	-0.037	$HRnCaBr_3$	1.719	1.730	-0.039	-0.042

4.Charge distribution analysis of HngY

Table S5. Calculated natural charges of each atom (|e|) of $HNgMX_3$ at CCSD/def2-TZVP//MP2/def2-TZVP level.

	Ng+H	Ng	H	F2	F3	M	F1
$HArBeF_3$	0.971	0.579	0.392	-0.791	-0.793	1.366	-0.754
$HKrBeF_3$	0.961	0.693	0.268	-0.787	-0.791	1.369	-0.753
$HXeBeF_3$	0.952	0.843	0.109	-0.784	-0.789	1.372	-0.751
$HRnBeF_3$	0.922	0.863	0.059	-0.745	-0.741	1.269	-0.705
$HArMgF_3$	0.971	0.578	0.393	-0.909	-0.893	1.719	-0.887
$HKrMgF_3$	0.958	0.695	0.263	-0.906	-0.885	1.721	-0.887
$HXeMgF_3$	0.947	0.847	0.100	-0.904	-0.881	1.724	-0.887
$HRnMgF_3$	0.919	0.868	0.051	-0.872	-0.839	1.642	-0.850
$HKrCaF_3$	0.952	0.698	0.254	-0.928	-0.901	1.788	-0.911
$HXeCaF_3$	0.940	0.854	0.086	-0.927	-0.894	1.792	-0.912
$HRnCaF_3$	0.915	0.877	0.038	-0.917	-0.854	1.791	-0.935
	Ng+H	Ng	H	Cl2	Cl3	M	Cl1
$HArBeCl_3$	0.919	0.540	0.379	-0.586	-0.560	0.738	-0.511
$HKrBeCl_3$	0.883	0.631	0.252	-0.572	-0.543	0.740	-0.508
$HXeBeCl_3$	0.862	0.753	0.109	-0.563	-0.536	0.743	-0.505
$HRnBeCl_3$	0.856	0.801	0.055	-0.561	-0.535	0.743	-0.505
$HKrMgCl_3$	0.892	0.630	0.262	-0.764	-0.712	1.299	-0.716
$HXeMgCl_3$	0.870	0.754	0.116	-0.758	-0.700	1.303	-0.714
$HRnMgCl_3$	0.862	0.801	0.061	-0.756	-0.696	1.303	-0.713
$HKrCaCl_3$	0.891	0.626	0.265	-0.760	-0.706	1.290	-0.715
$HXeCaCl_3$	0.870	0.755	0.115	-0.754	-0.691	1.291	-0.715
$HRnCaCl_3$	0.861	0.802	0.059	-0.753	-0.687	1.294	-0.715
	Ng+H	Ng	H	Br2	Br3	M	Br1
$HArBeBr_3$	0.909	0.527	0.382	-0.527	-0.491	0.548	-0.438
$HKrBeBr_3$	0.858	0.611	0.247	-0.506	-0.465	0.550	-0.436
$HXeBeBr_3$	0.832	0.729	0.103	-0.496	-0.455	0.552	-0.433
$HRnBeBr_3$	0.823	0.775	0.048	-0.492	-0.453	0.552	-0.431
$HKrMgBr_3$	0.873	0.613	0.260	-0.721	-0.657	1.169	-0.664
$HXeMgBr_3$	0.843	0.731	0.112	-0.713	-0.640	1.172	-0.663
$HRnMgBr_3$	0.834	0.777	0.057	-0.711	-0.635	1.173	-0.662
$HKrCaBr_3$	0.875	0.609	0.266	-0.719	-0.652	1.159	-0.663
$HXeCaBr_3$	0.846	0.732	0.114	-0.710	-0.631	1.159	-0.664
$HRnCaBr_3$	0.836	0.778	0.058	-0.709	-0.626	1.162	-0.663

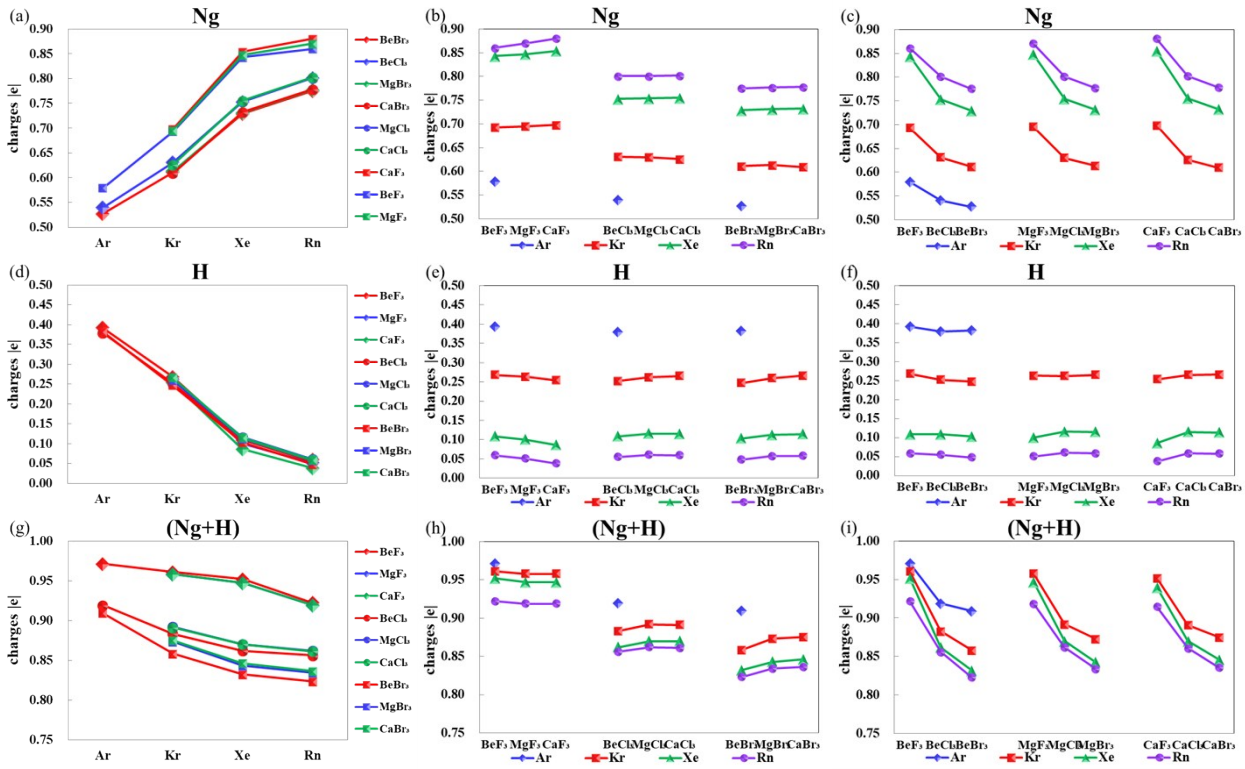

Fig. S12 The natural charges trend of Ng, H atoms and H+Ng in HNgY along Ar-Kr-Xe-Rn, Be-Mg-Ca as well as F-Cl-Br

Table S6. Wiberg bond indices (WBI) values, atom-atom overlap-weighted NAO bond order and MO bond order of HNgY bonds at CCSD/def2-TZVP // MP2/def2-TZVP level

	(a) Wiberg bond index matrix in the NAO basis:						
	H-Ng	X2-Ng	X3-Ng	M-X1	M-X2	M-X3	X2-H
$HArBeF_3$	0.7470	0.0051	0.0392	0.4674	0.3933	0.3327	0.0012
$HKrBeF_3$	0.8000	0.0069	0.0533	0.4700	0.3988	0.3179	0.0024
$HXeBeF_3$	0.8444	0.0102	0.0665	0.4735	0.3993	0.3081	0.0041
$HRnBeF_3$	0.8461	0.0141	0.0641	0.4758	0.3939	0.3115	0.0073
$HArBeCl_3$	0.7057	0.0046	0.0523	0.7397	0.6232	0.5466	0.0015
$HKrBeCl_3$	0.7469	0.0052	0.0822	0.7434	0.6446	0.5183	0.0008
$HXeBeCl_3$	0.7884	0.0067	0.1113	0.7475	0.6555	0.4994	0.0012
$HRnBeCl_3$	0.7857	0.0076	0.1159	0.7502	0.6578	0.4942	0.0024
$HArBeBr_3$	0.6915	0.0054	0.0563	0.8280	0.6949	0.6232	0.0022
$HKrBeBr_3$	0.7236	0.0057	0.0944	0.8319	0.7249	0.5868	0.0008
$HXeBeBr_3$	0.7628	0.0068	0.1304	0.8360	0.7393	0.5648	0.0007
$HRnBeBr_3$	0.7581	0.0072	0.1368	0.8388	0.7436	0.5573	0.0015
$HArMgF_3$	0.7453	0.0050	0.0403	0.2387	0.1900	0.1571	0.0008
$HKrMgF_3$	0.7987	0.0064	0.0580	0.2396	0.1949	0.1462	0.0016
$HXeMgF_3$	0.8413	0.0096	0.0733	0.2408	0.1945	0.1380	0.0032
$HRnMgF_3$	0.8425	0.0134	0.0708	0.2418	0.1905	0.1386	0.0060
$HKrMgCl_3$	0.7529	0.0047	0.0759	0.4556	0.3739	0.2930	0.0006
$HXeMgCl_3$	0.7946	0.0059	0.1056	0.4576	0.3820	0.2775	0.0008
$HRnMgCl_3$	0.7915	0.0065	0.1114	0.4592	0.3841	0.2726	0.0017
$HKrMgBr_3$	0.7337	0.0052	0.0860	0.5274	0.4330	0.3439	0.0006
$HXeMgBr_3$	0.7722	0.0060	0.1230	0.5293	0.4450	0.3249	0.0004
$HRnMgBr_3$	0.7671	0.0062	0.1305	0.6579	0.5901	0.3184	0.0009
$HKrCaF_3$	0.7984	0.0054	0.0628	0.2503	0.1897	0.1250	0.0010
$HXeCaF_3$	0.8372	0.0088	0.0807	0.2510	0.1881	0.1121	0.0027
$HRnCaF_3$	0.8371	0.0132	0.0782	0.2519	0.1801	0.1125	0.0058
$HKrCaCl_3$	0.7564	0.0045	0.0725	0.4695	0.3881	0.3098	0.0007
$HXeCaCl_3$	0.7946	0.0054	0.1058	0.4685	0.3973	0.2902	0.0006
$HRnCaCl_3$	0.7912	0.0058	0.1125	0.4687	0.3984	0.2832	0.0012
$HKrCaBr_3$	0.7397	0.0050	0.0803	0.5596	0.4609	0.3783	0.0007
$HXeCaBr_3$	0.7748	0.0058	0.1203	0.5583	0.4744	0.3561	0.0004
$HRnCaBr_3$	0.7695	0.0058	0.1287	0.5589	0.4774	0.3474	0.0007

	(b) Atom-atom overlap-weighted NAO bond order:						
	H-Ng	X2-Ng	X3-Ng	M-X1	M-X2	M-X3	X2-H
$HArBeF_3$	0.5855	-0.0032	0.0222	0.5787	0.5144	0.4545	-0.0011
$HKrBeF_3$	0.5942	0.0048	0.0501	0.5809	0.5201	0.4402	-0.0003
$HXeBeF_3$	0.6018	0.0108	0.0633	0.5835	0.5216	0.4304	0.0007
$HRnBeF_3$	0.5796	0.0123	0.0631	0.5851	0.5171	0.4347	0.0009
$HArBeCl_3$	0.5665	-0.0006	0.0397	0.8367	0.7409	0.6702	-0.0047
$HKrBeCl_3$	0.5737	0.0054	0.0840	0.8159	0.7418	0.6298	-0.0015
$HXeBeCl_3$	0.5783	0.0108	0.1113	0.8188	0.7522	0.6128	0.0009
$HRnBeCl_3$	0.5543	0.0099	0.1166	0.8208	0.7544	0.6088	0.0009
$HArBeBr_3$	0.5576	0.0002	0.0382	0.9084	0.8016	0.7391	-0.0068
$HKrBeBr_3$	0.5626	0.0058	0.0872	0.9147	0.8280	0.7068	-0.0023
$HXeBeBr_3$	0.5664	0.0101	0.1213	0.9175	0.8409	0.6881	0.0008
$HRnBeBr_3$	0.5418	0.0086	0.1286	0.9197	0.8447	0.6821	0.0008
$HArMgF_3$	0.5847	-0.0040	0.0221	0.3898	0.3386	0.2957	-0.0020
$HKrMgF_3$	0.5932	0.0039	0.0547	0.3899	0.3440	0.2818	-0.0006
$HXeMgF_3$	0.5995	0.0099	0.0700	0.3908	0.3432	0.2712	0.0008
$HRnMgF_3$	0.8425	0.0134	0.0708	0.2418	0.1905	0.1386	0.0060
$HKrMgCl_3$	0.5762	0.0055	0.0776	0.5886	0.5179	0.4367	-0.0021
$HXeMgCl_3$	0.5828	0.0097	0.1059	0.5901	0.5261	0.4206	0.0010
$HRnMgCl_3$	0.5580	0.0081	0.1117	0.5914	0.5283	0.4158	0.0010
$HKrMgBr_3$	0.5678	0.0041	0.0807	0.6550	0.5744	0.4838	-0.0030
$HXeMgBr_3$	0.5725	0.0071	0.1155	0.6564	0.5865	0.4644	0.0008
$HRnMgBr_3$	0.5472	0.0050	0.1233	0.6579	0.5901	0.4579	0.0009
$HKrCaF_3$	0.5931	0.0062	0.0515	0.3672	0.2984	0.1768	-0.0011
$HXeCaF_3$	0.5939	0.0134	0.0817	0.3663	0.3012	0.2469	0.0008
$HRnCaF_3$	0.5713	0.0161	0.0812	0.3667	0.2781	0.2471	0.0009
$HKrCaCl_3$	0.5783	0.0056	0.0786	0.6883	0.6104	0.5251	-0.0035
$HXeCaCl_3$	0.5824	0.0093	0.1115	0.6830	0.6173	0.5034	0.0009
$HRnCaCl_3$	0.5574	0.0075	0.1184	0.6834	0.6189	0.4962	0.0009
$HKrCaBr_3$	0.5709	0.0055	0.0793	0.7763	0.6831	0.5942	-0.0044
$HXeCaBr_3$	0.5742	0.0080	0.1175	0.7764	0.6986	0.5727	0.0005
$HRnCaBr_3$	0.5486	0.0055	0.1261	0.7768	0.7019	0.5638	0.0006

	(c) MO bond order						
	H-Ng	X2-Ng	X3-Ng	M-X1	M-X2	M-X3	X2-H
$HArBeF_3$	-0.0174	0.0276	-0.0037	-0.4933	-0.5096	1.3017	-0.0249
$HKrBeF_3$	-0.1794	0.0389	-0.0101	-0.5010	-0.4964	1.3059	-0.0512
$HXeBeF_3$	1.2500	-0.1602	-0.4466	0.7974	-0.1592	-0.2673	0.0627
$HRnBeF_3$	1.1640	-0.1421	-0.5103	0.7530	-0.1464	-0.2700	0.0872
$HArBeCl_3$	0.1930	0.0726	0.0035	0.9141	1.0070	-0.1419	0.0318
$HKrBeCl_3$	-0.0781	0.1288	-0.0509	0.8499	0.9917	-0.2232	0.0064
$HXeBeCl_3$	-0.9382	0.0130	-0.3136	0.2179	0.3019	0.6131	-0.0519
$HRnBeCl_3$	1.2119	-0.1025	-0.7732	0.2364	0.2533	0.6505	0.0414
$HArBeBr_3$	0.3298	0.0539	0.0192	0.9661	1.0388	-0.1234	0.0409
$HKrBeBr_3$	0.0293	0.1385	-0.0472	1.0251	1.0738	-0.1720	0.0276
$HXeBeBr_3$	-0.1255	0.1422	-0.0297	1.0516	1.0972	-0.1940	-0.0162
$HRnBeBr_3$	-0.9332	-0.0167	-0.3625	0.4592	0.2503	0.7595	-0.0507
$HArMgF_3$	0.1284	0.0461	0.0302	0.6209	0.6205	0.0395	0.0007
$HKrMgF_3$	-0.0897	0.0598	0.0313	0.6772	0.6338	0.0306	-0.0354
$HXeMgF_3$	1.2981	-0.0744	-0.4820	0.1108	0.0821	0.4080	0.0218
$HRnMgF_3$	0.5772	0.0101	0.0694	0.3908	0.3384	0.2719	0.0009
$HKrMgCl_3$	0.2139	0.0461	-0.1046	0.5370	0.6406	-0.2572	-0.0050
$HXeMgCl_3$	-0.9105	0.0317	-0.3038	-0.1385	-0.0526	0.4654	-0.0122
$HRnMgCl_3$	1.2555	-0.0366	-0.7976	0.1043	-0.2266	0.4695	0.0119
$HKrMgBr_3$	0.1562	0.1188	-0.1053	0.6243	0.7492	-0.1526	0.0246
$HXeMgBr_3$	-0.0258	0.1326	-0.0827	-0.0019	0.1326	-0.0827	-0.0161
$HRnMgBr_3$	-0.9084	-0.0146	-0.3503	-0.0972	-0.1142	0.5287	-0.0146
$HKrCaF_3$	1.4175	-0.0142	-0.3466	0.3189	0.4491	0.4020	-0.0286
$HXeCaF_3$	1.4704	-0.0534	-0.3588	0.3387	0.4336	0.3895	0.0084
$HRnCaF_3$	1.2227	-0.0430	-0.5997	-0.4758	0.3557	0.1492	0.0274
$HKrCaCl_3$	0.1694	0.1100	-0.0887	0.9919	0.8681	-0.1476	0.0343
$HXeCaCl_3$	-0.8733	0.0627	-0.3306	0.6044	-0.2974	-0.0176	0.0225
$HRnCaCl_3$	-0.9807	0.0569	-0.2376	0.3107	-0.6313	-0.1422	0.0077
$HKrCaBr_3$	0.2516	0.1050	-0.1078	0.9787	0.9198	-0.2510	0.0372
$HXeCaBr_3$	0.0418	0.1429	-0.0892	0.9198	0.9708	-0.3069	0.0006
$HRnCaBr_3$	-0.8806	0.0385	-0.3585	0.6057	-0.3769	0.0147	0.0284

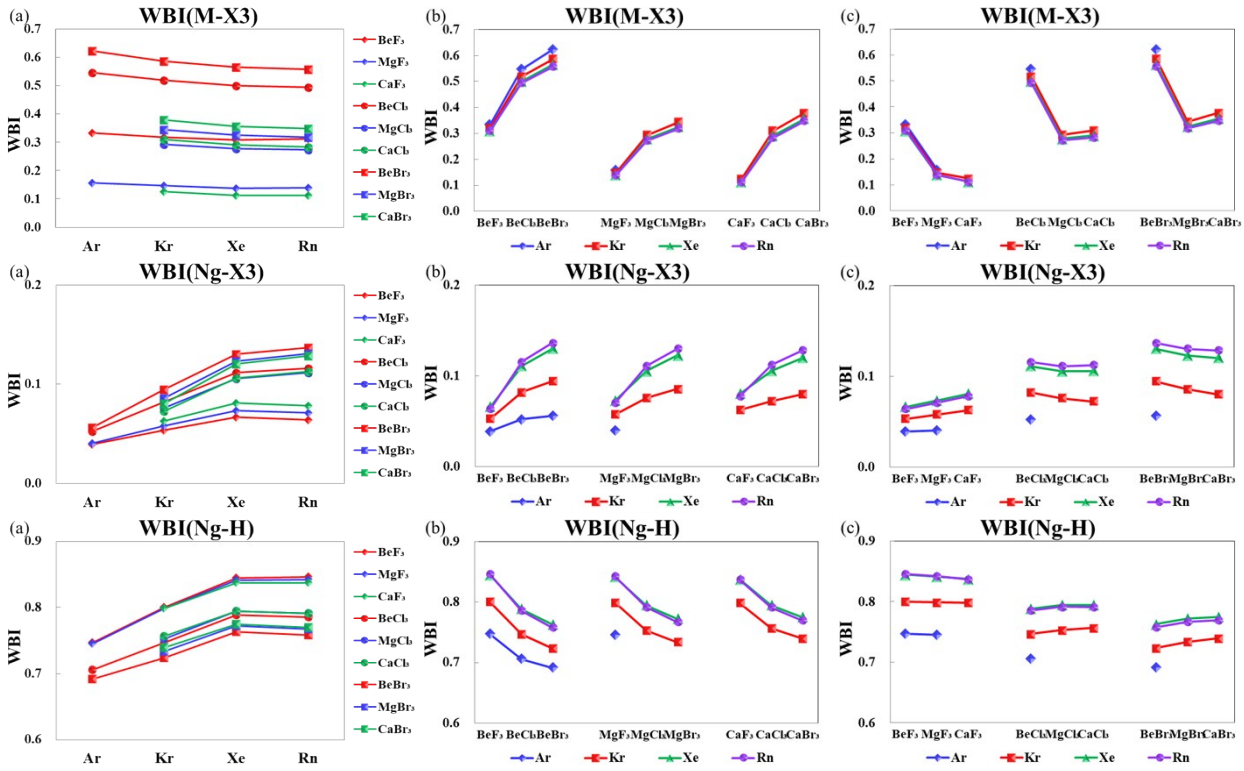

Fig. S13 Comparison of Wiberg bond indices (WBI) values for M-X3, Ng-X3 and Ng-H along Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca

Table S7 MO bond order (Occupancy) Bond orbital

	BD		BD*	
	Ng	H	Ng	H
$HArBeF_3$	70.64%	29.36%	29.36%	70.64%
$HArBeCl_3$	72.11%	27.89%	27.89%	72.11%
$HArBeBr_3$	72.62%	27.38%	27.38%	72.62%
$HKrBeF_3$	64.66%	35.34%	35.34%	64.66%
$HXeBeF_3$	56.73%	43.27%	43.27%	56.73%
$HRnBeF_3$	55.14%	44.86%	44.86%	55.14%
$HKrBeCl_3$	66.62%	33.38%	33.38%	66.62%
$HXeBeCl_3$	59.39%	40.61%	40.61%	59.39%
$HRnBeCl_3$	56.82%	43.18%	43.18%	56.82%
$HKrBeBr_3$	67.18%	32.82%	32.82%	67.18%
$HXeBeBr_3$	59.97%	40.03%	40.03%	59.97%
$HRnBeBr_3$	57.43%	42.57%	42.57%	57.43%
$HArMgF_3$	70.71%	29.29%	29.29%	70.71%
$HKrMgF_3$	64.48%	35.52%	35.52%	64.48%
$HXeMgF_3$	56.41%	43.59%	43.59%	56.41%
$HKrMgCl_3$	66.80%	33.20%	33.20%	66.80%
$HXeMgCl_3$	59.53%	40.47%	40.47%	59.53%
$HRnMgCl_3$	56.97%	43.03%	43.03%	56.97%
$HKrMgBr_3$	67.33%	32.67%	32.67%	67.33%
$HXeMgBr_3$	60.08%	39.92%	39.92%	60.08%
$HRnMgBr_3$	57.56%	42.44%	42.44%	57.56%
$HKrCaF_3$	64.19%	35.81%	35.81%	64.19%
$HXeCaF_3$	55.87%	44.13%	44.13%	55.87%

Table S8 Analysis of charge density descriptors (a.u.) at the bond critical point (BCPs) of the part of $HNgMX_3$ molecules by AIM at CCSD/def2-TZVP // MP2/def2-TZVP level.

		ρ(r)	∇^2	$G(r_c)$	$V(r_c)$	$H(r_c)$
	H-Ar					
$HArBeCl_3$	Ar-Cl2	0.016	0.068	0.015	-0.012	0.002
	Ar-Cl3	0.034	0.113	0.028	-0.028	0.000
	H-Kr	0.200	-0.469	0.049	-0.216	-0.166
$HKrBeCl_3$	Kr-Cl2	0.015	0.053	0.012	-0.010	0.002
	Kr-Cl3	0.039	0.103	0.028	-0.031	-0.002
	H-Xe	0.162	-0.267	0.057	-0.182	-0.124
$HXeBeCl_3$	Xe-Cl2	0.014	0.045	0.010	-0.008	0.001
	Xe-Cl3	0.040	0.092	0.027	-0.031	-0.004
	H-Rn	0.141	-0.122	0.064	-0.158	-0.094
$HRnBeCl_3$	Rn-Cl2	0.014	0.044	0.010	-0.008	0.001
	Rn-Cl3	0.041	0.093	0.028	-0.033	-0.005
	H-Ar					
$HArBeBr_3$	Ar-Br2	0.016	0.057	0.013	-0.011	0.002
	Ar-Br3	0.030	0.088	0.022	-0.022	0.000
	H-Kr	0.196	-0.449	0.049	-0.210	-0.161
$HKrBeBr_3$	Kr-Br2	0.014	0.043	0.010	-0.009	0.001
	Kr-Br3	0.036	0.081	0.023	-0.025	-0.003
	H-Xe	0.159	-0.258	0.056	-0.176	-0.120
$HXeBeBr_3$	Xe-Br2	0.013	0.036	0.008	-0.007	0.001
	Xe-Br3	0.037	0.073	0.022	-0.026	-0.004
	H-Rn	0.138	-0.117	0.062	-0.153	-0.091
$HRnBeBr_3$	Rn-Br2	0.013	0.035	0.008	-0.007	0.001
	Rn-Br3	0.038	0.073	0.023	-0.028	-0.005

(Carried out at CCSD/def2-TZVP//MP2/def2-TZVP level of theory with the help of Multiwfn software)

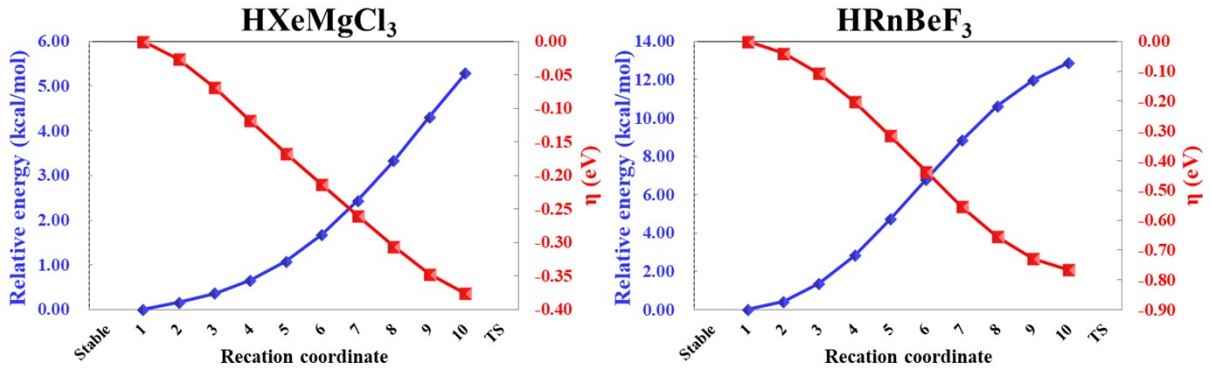

Fig. S14 Variation of relative energy (ΔE, kcal/mol) and hardness (η, eV), of HNgBeF3 and HXeMgCl3 with reaction coordinates corresponding to trace the the IRC path. The most stable structure has been taken as the reference for calculating the rotational barrier.

Table S9 The LUMO and HOMO energy of $HNgMX_3$ as well as the energy gap and chemical hardness at CCSD/def2-TZVP // MP2/def2-TZVP level.

	LUMO(a.u.)	HOMO(a.u.)	gap (eV)	η(eV)
$HArBeF_3$	-0.00549	-0.51255	13.80	6.90
$HKrBeF_3$	0.00671	-0.51687	14.25	7.12
$HXeBeF_3$	0.02124	-0.52065	14.75	7.37
$HRnBeF_3$	0.02223	-0.50581	14.37	7.18
$HArBeCl_3$	-0.02047	-0.38592	9.94	4.97
$HKrBeCl_3$	-0.01070	-0.38803	10.27	5.13
$HXeBeCl_3$	0.00245	-0.39144	10.72	5.36
$HRnBeCl_3$	0.00501	-0.39358	10.85	5.42
$HArBeBr_3$	-0.02400	-0.35539	9.02	4.51
$HKrBeBr_3$	-0.01605	-0.35695	9.28	4.64
$HXeBeBr_3$	-0.00322	-0.35981	9.70	4.85
$HRnBeBr_3$	-0.00046	-0.36184	9.83	4.92
$HArMgF_3$	0.00234	-0.49465	13.52	6.76
$HKrMgF_3$	0.01338	-0.49753	13.90	6.95
$HXeMgF_3$	0.02740	-0.50229	14.41	7.21
$HRnMgF_3$	0.02791	-0.49247	14.16	7.08
$HKrMgCl_3$	-0.01059	-0.39194	10.38	5.19
$HXeMgCl_3$	0.00144	-0.39439	10.77	5.39
$HRnMgCl_3$	0.00395	-0.39628	10.89	5.45
$HKrMgBr_3$	-0.01596	-0.36272	9.44	4.72
$HXeMgBr_3$	-0.00446	-0.36474	9.80	4.90
$HRnMgBr_3$	-0.00174	-0.36647	9.92	4.96
$HKrCaF_3$	0.02400	-0.47167	13.49	6.74
$HXeCaF_3$	0.03563	-0.47566	13.91	6.96
$HRnCaF_3$	0.03357	-0.46883	13.67	6.84
$HKrCaCl_3$	-0.00410	-0.38212	10.29	5.14
$HXeCaCl_3$	0.00668	-0.38365	10.62	5.31
$HRnCaCl_3$	0.00837	-0.38515	10.71	5.35
$HKrCaBr_3$	-0.01102	-0.35577	9.38	4.69
$HXeCaBr_3$	-0.00093	-0.35696	9.69	4.84
$HRnCaBr_3$	0.00115	-0.35830	9.78	4.89

$gap=(\epsilon_{LUMO}-\epsilon_{HOMO})$; $\eta=(\epsilon_{LUMO}-\epsilon_{HOMO})/2$

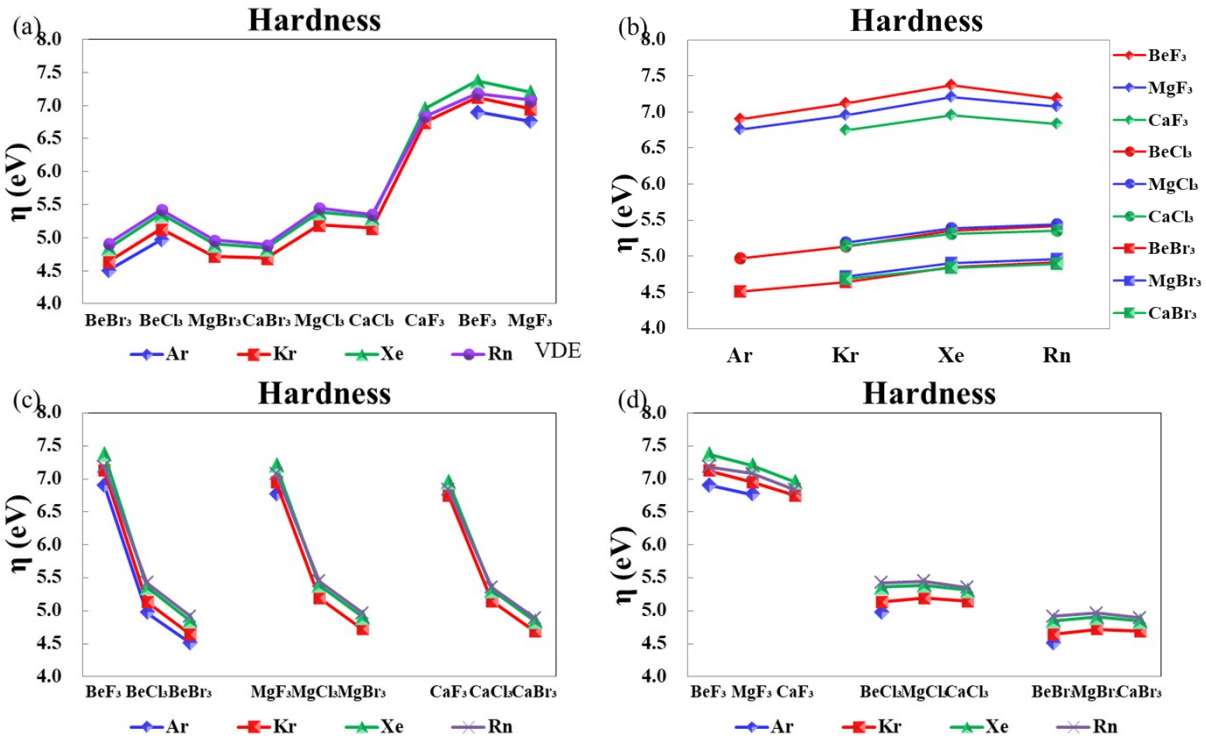

Fig. S15 Comparison of chemical hardness (η) values for HNgMX3 along VDE, Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca.

5.Thermodynamic and kinetic stability of HNgY

Table S10. The fragment energies of $HNgMX_3$ (Ng=Ar-Rn; M=Be, Mg, Ca; X=F, Cl, Br) along six pathways (kcal/mol)

(a) The fragment energies of HNgBeF3 (Ng=Ar - Rn) along six pathways kcal/mol

Molecule	Dissociation processes	ωB97X-D			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HArBeF_3$	$HBeF_3$+Ar	-96.33	-95.79	-103.19	-98.28	-97.89	-105.31	-97.96	-97.57
	BeF_3+H+Ar	44.75	37.10	24.53	58.93	53.97	41.00	58.70	53.74
	BeF_2+HF+Ar	-86.32	-87.54	-101.38	-88.61	-90.05	-103.94	-87.94	-89.39
	HAr_++BeF_3^-	109.65	107.67	100.15	108.18	106.06	98.50	108.35	106.23
	HArF+BeF_2	46.42	45.38	37.53	49.94	48.66	40.78	50.31	49.02
	H^++Ar+BeF_3^-	204.93	199.06	187.07	199.97	193.96	181.91	202.11	196.09
$HKrBeF_3$	$HBeF_3$+Kr	-82.38	-81.44	-88.89	-84.56	-83.79	-91.24	-83.96	-83.19
	BeF_3+H+Kr	58.71	51.45	38.84	72.65	68.07	55.07	72.70	68.12
	BeF_2+HF+Kr	-72.37	-73.19	-87.07	-74.88	-75.94	-89.88	-73.95	-75.01
	HKr^++BeF_3^-	111.89	110.02	102.34	110.48	108.50	100.77	110.70	108.71
	HKrF+BeF_2	42.03	41.01	33.14	44.51	43.32	35.42	44.91	43.73
	H^++Kr+BeF_3^-	218.89	213.42	201.37	213.69	208.06	195.98	216.11	210.48
$HXeBeF_3$	$HBeF_3$+Xe	-63.27	-61.92	-69.34	-67.19	-65.98	-73.39	-65.58	-64.38
	BeF_3+H+Xe	77.82	70.97	58.38	90.02	85.88	72.93	91.07	86.93
	BeF_2+HF+Xe	-53.26	-53.68	-67.52	-57.51	-58.14	-72.02	-55.57	-56.20
	HXe_++BeF_3^-	115.09	113.30	105.51	113.34	111.51	103.70	113.50	111.67
	HXeF+BeF_2	37.37	36.44	28.57	40.38	39.29	31.39	40.56	39.47
	H^++Xe+$BeF3^-$	238.00	232.93	220.92	231.06	225.87	213.83	234.48	229.28
$HRnBeF_3$	$HBeF_3$+Rn	-54.52	-52.93	-60.35	-57.36	-55.86	-63.27	-55.87	-54.38
	BeF_3+H+Rn	86.57	79.96	67.37	99.86	96.00	83.05	100.79	96.93
	BeF_2+HF+Rn	-44.51	-44.69	-58.53	-47.68	-48.02	-61.90	-45.86	-46.20
	HRn^++BeF_3^-	117.44	115.76	107.92	116.47	114.75	106.88	116.33	114.61
	HRnF+BeF_2	38.85	37.60	29.67	41.49	40.30	32.36	41.64	40.45
	H^++Rn+BeF_3^-	246.75	241.92	229.91	240.90	235.99	223.95	244.20	239.29

(b) The fragment energies of $HNgBeCl_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HArBeCl_3$	$HBeCl_3$+Ar	-92.37	-92.37	-100.32	-92.31	-92.96	-100.28	-93.68	-94.33
	$BeCl_3$+H+Ar	8.56	2.31	-9.63	12.39	7.99	-4.52	11.80	11.80
	$BeCl_2$+HCl+Ar	-88.32	-90.13	-104.38	-87.33	-89.26	-103.58	-89.56	-91.49
	HAr^++$BeCl_3^-$	97.05	95.50	88.21	96.31	94.68	87.37	95.60	93.97
	HArCl+$BeCl_2$	29.52	28.55	20.43	34.33	32.81	24.64	31.86	30.33
	H^++Ar+$BeCl_3^-$	192.33	186.90	172.39	188.10	182.57	168.50	189.35	183.83
$HKrBeCl_3$	$HBeCl_3$+Kr	-79.13	-79.39	-86.87	-78.87	-79.19	-86.60	-80.04	-80.36
	$BeCl_3$+H+Kr	21.80	15.86	3.83	25.84	21.76	9.16	25.44	21.36
	$BeCl_2$+HCl+Kr	-75.08	-76.57	-90.92	-73.89	-75.49	-89.90	-75.92	-77.52
	HKr^++BeCl3$^-$	98.57	97.06	89.55	98.34	96.78	89.25	97.59	96.03
	HKrCl+$BeCl_2$	30.33	25.66	17.46	30.51	28.48	20.91	28.26	26.24
	H^++Kr+$BeCl_3^-$	205.57	200.46	185.79	201.55	196.34	182.06	203.00	197.80
$HXeBeCl_3$	$HBeCl_3$+Xe	-61.17	-61.08	-68.52	-62.29	-62.24	-69.60	-62.70	-62.65
	$BeCl_3$+H+Xe	39.77	34.17	22.17	42.42	38.71	26.16	42.78	39.07
	$BeCl_2$+HCl+Xe	-57.12	-58.26	-72.58	-57.31	-58.54	-72.90	-58.57	-59.81
	HXe^++$BeCl_3^-$	100.62	99.13	91.52	100.40	98.93	91.32	99.36	97.89
	HXeCl+$BeCl_2$	23.43	22.77	14.58	27.70	26.05	19.48	25.58	23.93
	H^++Xe+$BeCl_3^-$	223.54	218.77	206.92	218.13	213.29	201.45	220.34	215.51
$HRnBeCl_3$	$HBeCl_3$+Rn	-52.68	-52.50	-59.99	-52.62	-52.32	-59.70	-53.36	-53.06
	$BeCl_3$+H+Rn	48.25	42.75	30.70	52.09	48.63	36.06	52.12	48.66
	$BeCl_2$+HCl+Rn	-48.63	-49.68	-64.05	-49.68	-48.62	-63.00	-49.24	-50.22
	HRn^++$BeCl_3^-$	102.72	101.19	93.46	103.36	101.98	94.28	101.81	100.42
	HRnCl+$BeCl_2$	23.41	22.43	14.14	27.18	27.18	18.09	25.19	24.37
	H^++Rn+$BeCl_3^-$	232.02	227.35	215.45	227.79	223.22	211.35	229.67	225.10

(c) The fragment energies of $HNgBeBr_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HArBeBr_3$	$HBeBr_3$+Ar	-89.82	-90.67	-98.28	-88.76	-89.55	-96.84	-90.41	-91.19
	$BeBr_3$+H+Ar	-3.48	-9.35	-20.97	0.13	-4.12	-16.47	-0.42	-4.67
	$BeBr_2$+HBr+Ar	-86.39	-88.53	-99.90	-83.55	-85.45	-99.84	-86.38	-88.28
	HAr^++$BeBr_3^-$	94.17	92.85	85.47	93.73	92.36	85.09	92.91	91.54
	HArBr+$BeBr_2$	25.73	24.50	19.31	31.00	29.20	21.02	27.35	25.55
	H^++Ar+$BeBr_3^-$	189.46	184.25	172.39	185.52	180.25	168.50	186.67	181.40
$HKrBeBr_3$	$HBeBr_3$+Kr	-76.75	-77.28	-84.88	-77.28	-75.84	-83.27	-76.82	-77.31
	$BeBr_3$+H+Kr	9.59	4.04	-7.56	13.55	13.55	-2.91	13.17	9.21
	$BeBr_2$+HBr+Kr	-73.32	-75.13	-86.49	-70.13	-71.74	-86.27	-72.79	-74.40
	HKr^++$BeBr_3^-$	95.53	94.25	86.76	95.72	94.39	86.86	94.85	93.52
	HKrBr+$BeBr_2$	23.13	21.30	16.75	27.69	26.54	18.26	24.65	23.50
	H^++Kr+$BeBr_3^-$	202.53	197.64	185.79	198.94	193.96	182.06	200.26	195.28
$HXeBeBr_3$	$HBeBr_3$+Xe	-58.96	-59.23	-66.81	-58.71	-58.86	-66.25	-59.48	-59.63
	$BeBr_3$+H+Xe	27.38	22.09	10.51	30.18	26.57	14.11	26.57	26.89
	$BeBr_2$+HBr+Xe	-55.53	-57.08	-68.43	-53.50	-54.76	-69.25	-55.46	-56.72
	HXe^++$BeBr_3^-$	97.41	96.06	88.45	97.84	96.58	88.95	96.61	95.34
	HXeBr+$BeBr_2$	20.53	19.60	14.48	25.54	24.81	16.55	22.80	22.07
	H^++Xe+$BeBr_3^-$	220.32	215.70	203.86	215.57	210.94	199.09	217.59	212.96
$HRnBeBr_3$	$HBeBr_3$+Rn	-50.45	-50.55	-58.23	-48.89	-48.77	-56.21	-50.06	-49.95
	$BeBr_3$+H+Rn	35.89	30.77	19.08	40.01	36.65	24.15	39.92	36.57
	$BeBr_2$+HBr+Rn	-47.02	-48.40	-59.85	-48.40	-44.67	-59.21	-46.04	-47.04
	HRn^++$BeBr_3^-$	99.53	98.22	90.44	100.97	99.78	92.05	99.14	97.96
	HRnBr+$BeBr_2$	20.34	19.26	14.00	24.98	23.58	15.74	22.42	21.02
	H^++Rn+$BeBr_3^-$	228.83	224.37	212.44	225.39	221.02	209.12	227.01	222.64

(d) The fragment energies of HNgMgF3 (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97X-D			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HArMgF_3$	$HMgF_3$+Ar	-101.02	-100.41	-107.72	-103.61	-103.09	-110.34	-103.31	-102.80
	MgF_3+H+Ar	47.61	40.59	27.96	64.90	59.09	45.63	64.00	58.18
	MgF_2+HF	-82.53	-83.54	-97.48	-84.57	-85.59	-99.50	-84.41	-85.43
	HAr^++MgF_3^-	110.52	107.59	99.89	107.67	105.61	97.96	108.00	105.94
	HArF+MgF_2	50.22	49.38	41.44	53.98	53.12	45.22	53.84	52.98
	H^++Ar+MgF_3^-	205.81	198.99	186.81	199.46	193.50	181.37	201.76	195.80
$HKrMgF_3$	$HMgF_3$+Kr	-87.29	-86.26	-93.60	-90.17	-89.33	-96.64	-89.57	-88.72
	MgF_3+H+Kr	61.34	54.75	42.08	78.33	72.86	59.33	77.74	72.26
	MgF_2+HF	-68.80	-69.39	-83.36	-71.13	-71.82	-85.80	-70.67	-71.36
	HKr^++MgF_3^-	112.54	109.75	101.90	109.68	107.70	99.87	110.10	108.12
	HKrF+MgF_2	45.60	44.82	36.85	48.26	47.45	39.50	48.19	47.38
	H^++Kr+MgF_3^-	219.54	213.15	200.93	212.89	207.27	195.07	215.50	209.88
$HXeMgF_3$	$HMgF_3$+Xe	-68.16	-66.66	-73.77	-72.99	-71.70	-78.95	-71.34	-70.05
	MgF_3+H+Xe	80.47	74.35	61.90	95.52	90.48	77.02	95.97	90.93
	MgF_2+HF	-49.68	-49.79	-63.53	-53.95	-54.20	-68.11	-52.44	-52.69
	HXe^++MgF_3^-	115.76	113.12	105.35	112.35	110.53	102.63	112.75	110.94
	HXeF+MgF_2	40.95	40.33	32.56	43.95	43.23	35.30	43.69	42.98
	H^++Xe+MgF_3^-	238.67	232.75	220.76	230.08	224.90	212.77	233.73	228.55
$HRnMgF_3$	$HMgF_3$+Rn	-72.64	-69.76	-76.29	-63.20	-61.62	-68.88	-61.65	-60.07
	MgF_3+H+Rn	75.99	71.25	59.38	105.31	100.56	87.09	105.66	100.91
	MgF_2+HF	-54.15	-52.89	-66.06	-44.16	-44.12	-58.04	-42.75	-42.71
	HRn^++MgF_3^-	104.89	103.49	96.24	115.44	113.74	105.76	115.56	113.85
	HRnF+MgF_2	29.21	29.40	22.15	45.01	44.20	36.22	44.74	43.94
	H^++Rn+MgF_3^-	234.19	229.65	218.24	239.87	234.98	222.84	243.42	238.53

(e) The fragment energies of $HNgMgCl_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HKrMgCl_3$	$HMgCl_3$+Kr	-77.01	-77.17	-84.71	-77.54	-77.81	-85.48	-78.43	-78.70
	$MgCl_3$+H+Kr	30.53	24.77	12.68	36.03	31.26	18.20	35.35	30.58
	$MgCl_2$+HCl+Kr	-67.12	-68.51	-82.93	-67.12	-67.12	-83.31	-68.89	-70.30
	HKr^++$MgCl_3^-$	96.71	95.22	87.55	96.31	94.79	87.14	95.57	94.04
	HKrCl+$MgCl_2$	34.44	33.72	25.45	36.89	35.07	27.49	35.28	33.46
	H^++Kr+$MgCl_3^-$	203.71	198.61	186.59	199.52	194.35	182.34	200.98	195.81
$HXeMgCl_3$	$HMgCl_3$+Xe	-59.35	-59.17	-66.61	-61.36	-61.25	-68.86	-61.46	-61.35
	$MgCl_3$+H+Xe	48.20	42.76	30.77	52.22	47.82	34.82	52.33	47.93
	$MgCl_2$+HCl+Xe	-49.45	-50.51	-64.83	-51.32	-52.36	-66.69	-51.92	-52.95
	HXe^++$MgCl_3^-$	98.46	96.97	89.27	97.99	96.54	88.83	96.98	95.54
	HXeCl+$MgCl_2$	31.09	30.52	22.32	33.69	32.24	25.69	32.24	30.79
	H^++Xe+$MgCl_3^-$	221.37	216.61	204.68	215.71	210.91	198.96	217.96	213.15
$HRnMgCl_3$	$HMgCl_3$+Rn	-50.90	-50.45	-57.87	-51.84	-51.48	-59.09	-52.25	-51.89
	$MgCl_3$+H+Rn	56.64	51.48	39.51	61.74	57.59	44.59	61.54	57.39
	$MgCl_2$+HCl+Rn	-41.00	-41.79	-56.09	-41.80	-41.79	-56.92	-42.71	-43.49
	HRn^++$MgCl_3^-$	100.51	99.17	91.43	100.80	99.44	91.66	99.30	99.30
	HRnCl+$MgCl_2$	31.03	30.32	22.10	33.02	32.39	24.17	31.73	31.10
	H^++Rn+$MgCl_3^-$	229.82	225.33	213.42	225.23	220.68	208.73	227.16	222.62

(f) The fragment energies of $HNgMgBr_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HKrMgBr_3$	$HMgBr_3$+Kr	-74.80	-75.28	-82.95	-74.05	-74.53	-82.26	-75.26	-75.74
	$MgBr_3$+H+Kr	3.98	-0.99	-14.78	4.57	-0.38	-14.11	4.36	-0.59
	$MgBr_2$+HBr	-65.69	-67.14	-81.53	-64.34	-65.81	-80.30	-66.24	-67.71
	HKr^++$MgBr_3^-$	93.91	92.62	84.00	93.89	92.57	83.87	92.99	91.67
	HKrBr+$MgBr_2$	30.75	29.30	21.72	33.48	32.46	24.24	31.20	30.18
	HKrBr+$MgBr_2$	200.92	196.02	183.03	197.11	192.14	179.07	198.40	193.43
$HXeMgBr_3$	$HMgBr_3$+Xe	-57.29	-57.51	-65.18	-57.79	-57.93	-65.60	-58.27	-58.41
	$MgBr_3$+H+Xe	21.50	16.79	2.99	20.82	16.22	2.55	21.35	16.75
	$MgBr_2$+HBr	-48.17	-49.36	-63.76	-48.08	-49.21	-63.64	-49.25	-50.38
	HXe^++$MgBr_3^-$	95.52	94.16	85.39	95.64	94.38	85.60	94.40	93.15
	HXeBr+$MgBr_2$	27.89	27.32	19.14	30.96	30.36	22.17	29.00	28.40
	H^++Xe+$MgBr_3^-$	218.43	213.79	200.80	213.36	208.74	195.73	215.38	210.76
$HRnMgBr_3$	$HMgBr_3$+Rn	-48.81	-48.71	-56.38	-48.12	-47.99	-55.68	-48.98	-48.85
	$MgBr_3$+H+Rn	29.97	25.59	11.79	30.49	26.15	12.46	30.64	26.30
	$MgBr_2$+HBr	-39.69	-40.56	-54.96	-38.41	-39.28	-53.72	-39.96	-40.83
	HRn^++$MgBr_3^-$	97.61	96.43	87.60	98.61	97.44	88.57	96.81	95.64
	HRnBr+$MgBr_2$	27.66	27.10	18.89	30.25	28.98	21.23	28.50	27.23
	H^++Rn+$MgBr_3^-$	226.91	222.59	209.60	223.03	218.68	205.64	224.68	220.32

(g) The fragment energies of $HNgCaF_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97X-D			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HKrCaF_3$	$HCaF_3$+Kr	-96.81	-96.67	-104.40	-101.16	-100.70	-108.11	-100.24	-100.24
	CaF_3+H+Kr	60.87	54.35	40.64	73.67	67.96	53.84	72.75	67.05
	CaF_2+HF	-72.05	-72.65	-85.14	-74.25	-74.81	-88.86	-74.04	-74.60
	HKr^++CaF_3^-	114.51	112.64	104.97	112.81	110.77	102.88	113.33	111.29
	HKrF+CaF_2	42.35	41.55	35.08	45.14	44.46	36.44	44.82	44.14
	H^++Kr+CaF_3^-	221.51	216.04	204.00	216.02	210.33	198.08	218.74	213.06
$HXeCaF_3$	$HCaF_3$+Xe	-77.43	-76.90	-84.58	-83.64	-82.70	-90.04	-82.09	-81.16
	CaF_3+H+Xe	80.24	74.11	60.45	91.19	85.96	71.91	91.37	86.13
	CaF_2+HF+Xe	-52.68	-52.89	-65.33	-56.73	-56.82	-70.79	-55.43	-55.51
	HXe^++CaF_3^-	117.97	116.17	108.40	115.82	113.97	106.02	116.38	114.53
	HXeF+CaF_2	37.95	37.23	30.77	41.16	40.61	32.62	40.71	40.15
	H^++Xe+CaF_3^-	240.89	235.80	223.81	233.55	228.33	216.15	237.36	232.14
$HRnCaF_3$	$HCaF_3$+Rn	-68.60	-67.73	-75.36	-73.81	-72.59	-79.93	-72.36	-71.14
	CaF_3+H+Rn	89.08	83.28	69.67	101.02	96.07	82.02	101.10	96.15
	CaF_2+HF+Rn	-43.84	-43.72	-56.10	-46.91	-46.70	-60.68	-45.70	-45.49
	HRn^++CaF_3^-	120.42	118.81	111.04	118.94	117.20	109.19	119.22	117.48
	HRnF+CaF_2	39.52	38.57	32.11	42.26	41.62	33.58	41.79	41.15
	H^++Rn+CaF_3^-	249.72	244.97	233.04	243.37	238.44	226.26	247.09	242.16

(h) The fragment energies of $HNgCaCl_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HKrCaCl_3$	$HCaCl_3$+Kr	-78.31	-78.81	-86.20	-79.82	-80.34	-87.69	-79.83	-80.35
	$CaCl_3$+H+Kr	32.56	26.74	14.06	38.59	33.57	19.57	38.33	33.31
	$CaCl_2$+HCl+Kr	-65.68	-67.04	-79.77	-67.44	-67.44	-81.68	-67.44	-70.24
	HKr^++$CaCl_3^-$	97.45	95.92	88.32	97.22	95.67	88.02	96.47	94.92
	HKrCl+$CaCl_2$	35.87	35.19	28.61	36.95	35.09	29.12	35.38	33.52
	H^++Kr+$CaCl_3^-$	204.45	199.31	187.35	200.43	195.24	183.22	201.87	196.68
$HXeCaCl_3$	$HCaCl_3$+Xe	-60.81	-60.91	-68.19	-63.81	-63.92	-71.18	-63.02	-63.02
	$CaCl_3$+H+Xe	50.06	44.65	32.08	54.61	49.99	36.08	55.15	50.53
	$CaCl_2$+HCl+Xe	-48.17	-49.14	-61.75	-51.42	-52.47	-65.18	-51.97	-53.02
	HXe^++$CaCl_3^-$	99.05	97.58	89.95	98.72	97.29	89.59	97.71	96.28
	HXeCl+$CaCl_2$	32.37	31.89	25.40	33.59	32.13	27.20	32.18	30.73
	H^++Xe+$CaCl_3^-$	221.96	217.21	205.36	216.45	211.66	199.72	218.69	213.90
$HRnCaCl_3$	$HCaCl_3$+Rn	-52.41	-52.41	-59.91	-54.37	-54.22	-61.48	-53.88	-53.74
	$CaCl_3$+H+Rn	58.46	53.14	40.36	64.05	59.69	45.78	64.28	59.91
	$CaCl_2$+HCl+Rn	-39.78	-40.65	-53.47	-41.98	-42.77	-55.48	-42.84	-43.63
	HRn^++$CaCl_3^-$	101.05	99.55	91.65	101.46	100.11	92.35	99.96	98.61
	HRnCl+$CaCl_2$	32.26	31.46	24.72	32.84	32.20	25.61	31.59	30.96
	H^++Rn+$CaCl_3^-$	230.36	225.71	213.65	225.89	221.35	209.42	227.82	223.29

(i) The fragment energies of $HNgCaBr_3$ (Ng=Ar - Rn) along six pathways

Molecule	Dissociation processes	ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
$HKrCaBr_3$	$HCaBr_3$+Kr	-74.59	-75.29	-82.68	-75.08	-76.04	-83.43	-75.07	-76.03
	$CaBr_3$+H+Kr	20.63	15.21	3.41	27.07	22.27	8.40	26.53	21.73
	$CaBr_2$+HBr	-63.25	-64.66	-79.27	-63.35	-64.83	-79.46	-65.05	-66.53
	HKr^++$CaBr_3^-$	94.05	92.77	85.27	94.28	92.92	85.26	93.29	91.93
	HKrBr+$CaBr_2$	33.20	31.77	23.98	34.47	33.44	25.07	32.39	31.36
	H^++Kr+$CaBr_3^-$	201.06	196.17	184.30	197.49	192.48	180.46	198.70	193.69
$HXeCaBr_3$	$HCaBr_3$+Xe	-57.28	-57.68	-65.02	-59.06	-59.61	-66.93	-58.32	-58.87
	$CaBr_3$+H+Xe	37.95	32.82	21.07	43.09	38.69	24.90	43.29	38.89
	$CaBr_2$+HBr+Xe	-45.93	-47.06	-61.61	-47.32	-48.41	-62.96	-48.29	-49.37
	HXe^++$CaBr_3^-$	95.46	94.14	86.55	95.79	94.54	86.82	94.54	93.23
	HXeBr+$CaBr_2$	30.13	29.62	21.30	31.72	31.16	22.84	29.97	29.41
	H^++Xe+$CaBr_3^-$	218.37	213.78	201.96	213.51	208.90	196.96	215.46	210.85
$HRnCaBr_3$	$HCaBr_3$+Rn	-48.87	-49.01	-56.49	-49.50	-49.79	-57.11	-49.13	-49.42
	$CaBr_3$+H+Rn	46.35	41.49	29.60	52.65	48.51	34.71	52.47	48.34
	$CaBr_2$+HBr+Rn	-37.53	-38.39	-53.08	-37.76	-38.59	-53.15	-39.10	-39.93
	HRn^++$CaBr_3^-$	97.47	96.29	88.50	98.64	97.48	89.70	96.78	95.62
	HRnBr+$CaBr_2$	27.23	29.27	20.77	30.89	29.67	21.81	29.36	29.36
	H^++Rn+$CaBr_3^-$	226.77	222.44	210.49	223.07	218.72	206.77	224.64	220.30

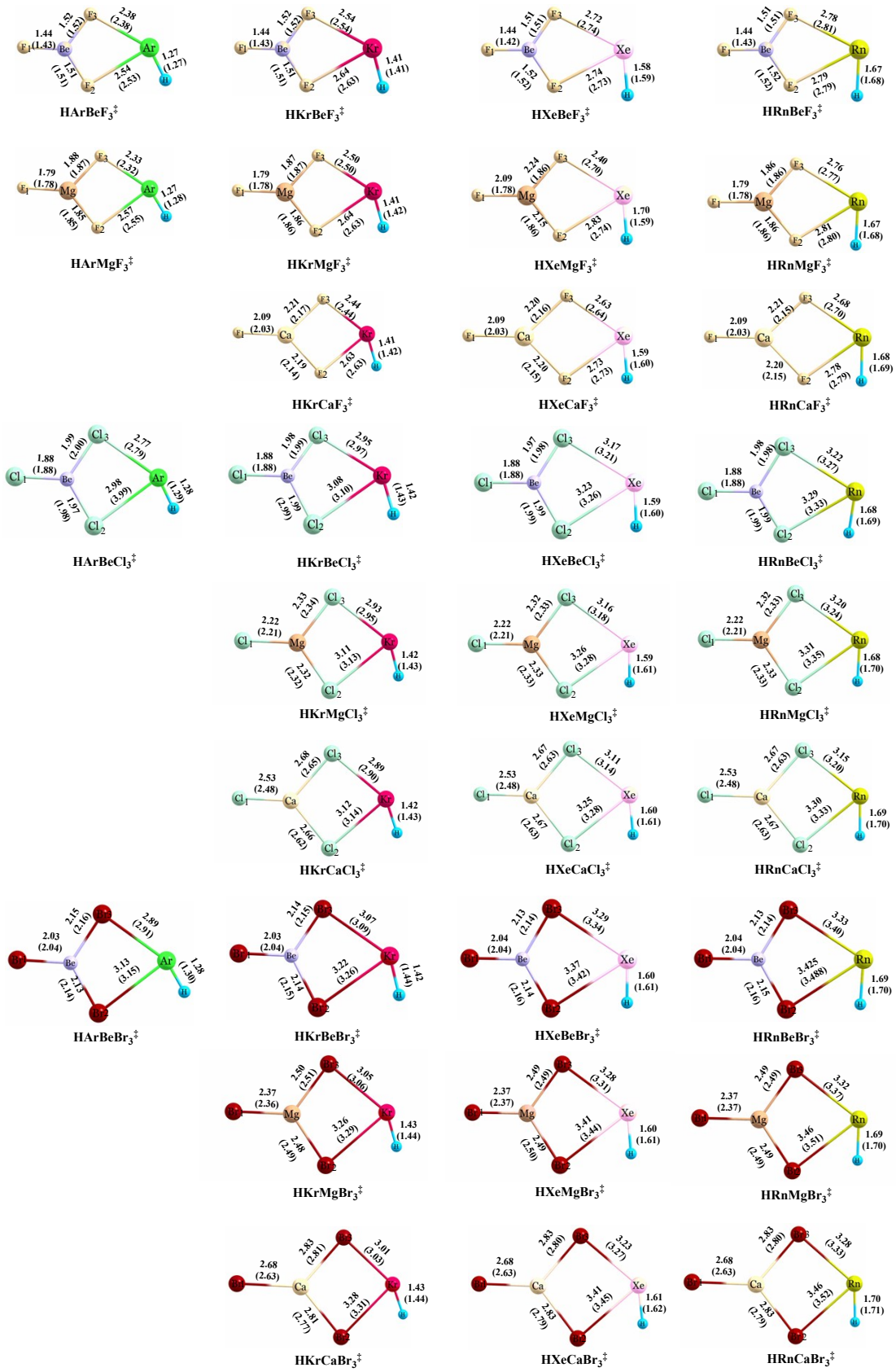

Fig. S16 The optimized geometries of transition state in $HNgMX_3$ (Ng=Ar-Rn) are performed at the MP2/def2-TZVP level (the corresponding value from ωB97XD/def2-TZVP level in parentheses).

Table S11. The energy barriers of $HNgMX_3$ along channel 5 at various levels (in kcal/mol).

M	HNgY	ωB97XD			MP2			CCSD(T)-SP		
		$\Delta E^{\ddagger}$	$\Delta E_0^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E_0^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E_0^{\ddagger}$	$\Delta G^{\ddagger}$
Be	$HArBeF_3$	2.01	1.40	1.53	1.28	0.64	0.76	1.31	0.67	0.79
	$HKrBeF_3$	6.01	5.32	5.36	5.14	4.34	4.35	5.32	4.52	4.53
	$HXeBeF_3$	11.64	10.74	10.56	10.20	9.34	9.22	10.64	9.78	9.66
	$HRnBeF_3$	14.90	13.71	13.75	13.72	12.88	12.70	14.07	13.24	13.05
	$HArBeCl_3$	0.81	0.26	0.49	0.81	0.26	0.49	0.30	-0.15	-0.02
	$HKrBeCl_3$	4.19	3.50	3.54	3.59	2.94	3.00	3.73	3.09	3.14
	$HXeBeCl_3$	9.57	8.69	8.41	8.57	7.82	7.62	8.92	8.17	7.97
	$HRnBeCl_3$	12.56	11.59	11.21	12.56	11.59	11.21	12.27	11.52	10.92
	$HArBeBr_3$	0.42	-0.12	0.14	0.07	-0.28	0.12	0.08	-0.27	0.13
	$HKrBeBr_3$	3.61	2.94	3.10	3.11	2.52	2.65	3.29	2.70	2.83
	$HXeBeBr_3$	9.02	8.18	8.06	8.16	7.47	7.37	8.57	7.88	7.78
	$HRnBeBr_3$	11.80	10.81	10.39	11.44	10.75	10.62	11.74	11.05	10.92
Mg	$HArMgF_3$	0.66	0.13	0.36	0.24	-0.23	0.04	0.27	-0.20	0.07
	$HKrMgF_3$	4.24	3.54	3.64	3.52	2.80	2.93	3.71	3.00	3.12
	$HXeMgF_3$	10.06	9.22	9.30	8.69	7.88	7.90	9.21	8.40	8.42
	$HRnMgF_3$	13.32	12.05	11.29	12.23	12.09	12.18	12.67	12.54	12.62
	$HKrMgCl_3$	2.37	1.73	1.90	1.94	1.36	1.54	2.08	1.50	1.68
	$HXeMgCl_3$	7.36	6.56	6.60	6.51	5.82	5.83	6.89	6.19	6.21
	$HRnMgCl_3$	10.17	9.29	9.12	9.71	9.00	8.98	10.00	9.30	9.27
	$HKrMgBr_3$	1.95	1.35	1.65	1.60	1.06	1.29	1.76	1.21	1.45
	$HXeMgBr_3$	6.93	6.09	6.14	6.18	5.52	5.59	6.58	5.92	5.99
	$HRnMgBr_3$	9.53	8.76	8.72	9.16	8.50	8.55	9.51	8.85	8.9
Ca	$HKrCaF_3$	3.10	2.37	2.55	2.27	1.62	1.80	2.43	1.78	1.96
	$HXeCaF_3$	9.28	8.39	8.48	7.85	7.09	7.18	8.42	7.66	7.75
	$HRnCaF_3$	12.58	11.71	11.75	11.43	10.73	10.80	12.00	11.29	11.37
	$HKrCaCl_3$	1.32	0.76	0.96	0.93	0.40	0.65	1.05	0.52	0.77
	$HXeCaCl_3$	6.06	5.37	5.47	5.26	4.60	4.72	5.65	4.99	5.11
	$HRnCaCl_3$	8.76	7.95	7.83	8.27	7.59	7.68	8.63	7.96	8.04
	$HKrCaBr_3$	0.98	0.46	0.91	0.69	0.19	0.49	0.81	0.31	0.61
	$HXeCaBr_3$	5.58	4.84	5.04	4.86	4.22	4.36	5.27	4.62	4.77
	$HRnCaBr_3$	8.05	7.27	7.26	7.62	7.24	7.68	8.01	7.63	8.07

$\Delta E^{\ddagger}$ is the ZPVE-uncorrected reaction energy; $\Delta E_0^{\ddagger}$ is the ZPVE-corrected reaction energy; $\Delta G^{\ddagger}$ is the reaction free energy change

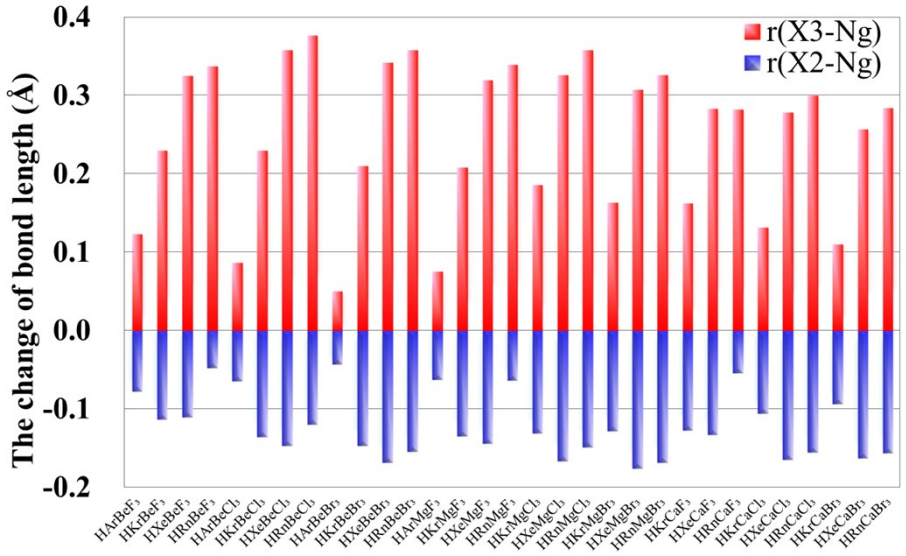

Fig. S17 The comparison of the change in X2-Ng and X3-Ng bond length from stable configuration to transition state (Å)

Table S12. Comparison of bond length (Å) in HNgY with stable and transition state at various theoretical levels

		MP2			ωB97XD		
		stable	TS	difference	stable	TS	difference
$HKrBeCl_3$	r(M-X1)	1.878	1.883	-0.005	1.876	1.880	-0.004
	r(M-X2)	1.936	1.985	-0.049	1.933	1.989	-0.056
	r(M-X3)	2.021	1.981	0.040	2.037	1.989	0.048
	r(X2-Ng)	3.213	3.078	0.135	3.269	3.098	0.171
	r(X3-Ng)	2.724	2.954	-0.230	2.732	2.973	-0.241
	r(Ng-H)	1.435	1.418	0.017	1.446	1.427	0.019
	r(X2-H)	3.961	2.845	1.116	4.040	2.853	1.187
$HXeBeCl_3$	r(M-X1)	1.877	1.884	-0.007	1.874	1.883	-0.009
	r(M-X2)	1.927	1.987	-0.060	1.925	1.994	-0.069
	r(M-X3)	2.031	1.974	0.057	2.047	1.979	0.068
	r(X2-Ng)	3.375	3.229	0.146	3.446	3.259	0.187
	r(X3-Ng)	2.814	3.172	-0.358	2.820	3.205	-0.385
	r(Ng-H)	1.618	1.589	0.029	1.632	1.601	0.031
	r(X2-H)	4.378	2.754	1.624	4.477	2.772	1.705
$HRnBeCl_3$	r(M-X1)	1.875	1.884	-0.009	1.873	1.883	-0.010
	r(M-X2)	1.926	1.987	-0.061	1.924	1.993	-0.069
	r(M-X3)	2.034	1.975	0.059	2.049	1.980	0.069
	r(X2-Ng)	3.405	3.286	0.119	3.486	3.330	0.156
	r(X3-Ng)	2.840	3.216	-0.376	2.863	3.267	-0.404
	r(Ng-H)	1.715	1.679	0.036	1.728	1.689	0.039
	r(X2-H)	4.521	2.672	1.849	4.630	2.718	1.912

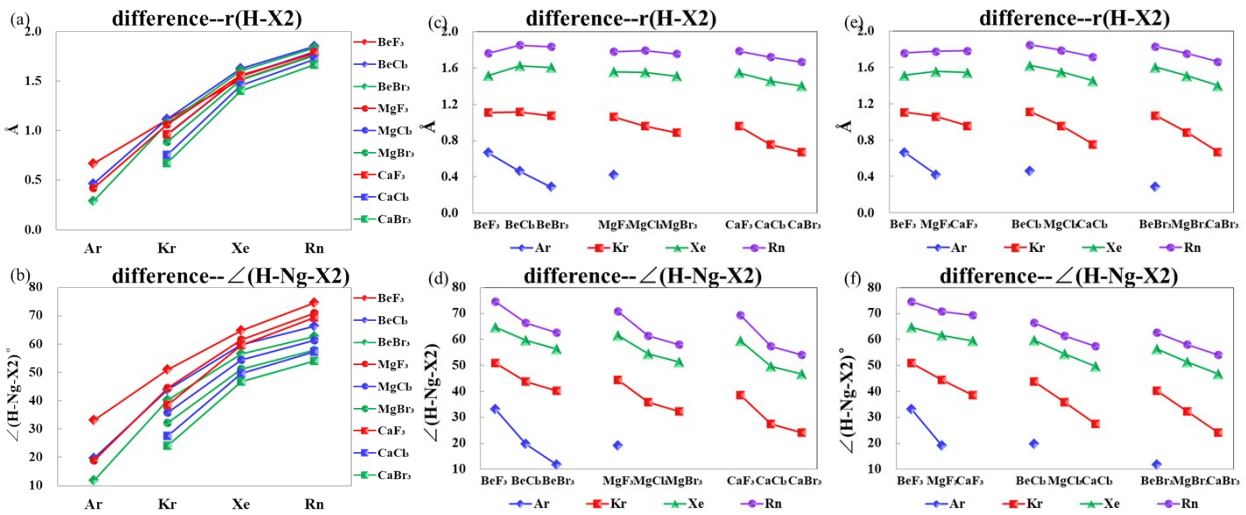

Fig. S18 Comparison of the difference of H-Ng bond length and H-Ng-X2 Angle from stable configuration to transition state along Ar-Kr-Xe-Rn, F-Cl-Br as well as Be-Mg-Ca

Table S13. The natural charges of the transition state at CCSD/def2-TZVP //MP2/def2-TZVP level (|e|)

	HNgY	M	F1	F2	F3	Ng	H	Ng+H
Be	HArBeF3	1.367	-0.755	-0.802	-0.799	0.553	0.435	0.988
	HKrBeF3	1.369	-0.756	-0.804	-0.800	0.639	0.352	0.991
	HXeBeF3	1.369	-0.756	-0.806	-0.801	0.761	0.233	0.994
	HRnBeF3	1.264	-0.714	-0.772	-0.765	0.778	0.208	0.986
Mg	HArMgF3	1.719	-0.888	-0.912	-0.901	0.560	0.422	0.982
	HKrMgF3	1.719	-0.888	-0.913	-0.906	0.641	0.347	0.988
	HXeMgF3	1.719	-0.888	-0.913	-0.909	0.755	0.236	0.991
	HRnMgF3	1.641	-0.852	-0.883	-0.879	0.763	0.209	0.972
Ca	HKrCaF3	1.783	-0.910	-0.933	-0.922	0.644	0.338	0.982
	HXeCaF3	1.781	-0.909	-0.931	-0.927	0.750	0.237	0.987
	HRnCaF3	1.771	-0.934	-0.912	-0.906	0.770	0.210	0.980
	HNgY	M	Cl1	Cl2	Cl3	Ng	H	Ng+H
Be	$HArBeCl_3$	0.741	-0.512	-0.602	-0.574	0.534	0.414	0.948
	$HKrBeCl_3$	0.743	-0.513	-0.607	-0.582	0.614	0.344	0.958
	$HXeBeCl_3$	0.744	-0.514	-0.608	-0.590	0.727	0.241	0.968
	$HRnBeCl_3$	0.744	-0.514	-0.604	-0.591	0.755	0.211	0.966
Mg	$HKrMgCl_3$	1.300	-0.716	-0.781	-0.754	0.612	0.339	0.951
	$HXeMgCl_3$	1.300	-0.717	-0.779	-0.766	0.722	0.239	0.961
	$HRnMgCl_3$	1.300	-0.717	-0.774	-0.767	0.749	0.209	0.958
Ca	$HKrCaCl_3$	1.288	-0.713	-0.771	-0.739	0.609	0.327	0.936
	$HXeCaCl_3$	1.281	-0.713	-0.767	-0.753	0.719	0.233	0.952
	$HRnCaCl_3$	1.281	-0.713	-0.761	-0.754	0.745	0.202	0.947
	HNgY	M	Br1	Br2	Br3	Ng	H	Ng+H
Be	$HArBeBr_3$	0.550	-0.438	-0.539	-0.501	0.524	0.404	0.928
	$HKrBeBr_3$	0.553	-0.438	-0.544	-0.511	0.602	0.338	0.940
	$HXeBeBr_3$	0.555	-0.441	-0.545	-0.522	0.717	0.237	0.954
	$HRnBeBr_3$	0.554	-0.441	-0.538	-0.523	0.745	0.203	0.948
Mg	$HKrMgBr_3$	1.170	-0.665	-0.738	-0.701	0.601	0.333	0.934
	$HXeMgBr_3$	1.171	-0.666	-0.735	-0.717	0.712	0.234	0.946
	$HRnMgBr_3$	1.170	-0.665	-0.727	-0.718	0.740	0.200	0.940
Ca	$HKrCaBr_3$	1.161	-0.662	-0.730	-0.686	0.596	0.321	0.917
	$HXeCaBr_3$	1.156	-0.662	-0.723	-0.704	0.707	0.227	0.934
	$HRnCaBr_3$	1.159	-0.660	-0.713	-0.704	0.727	0.191	0.918

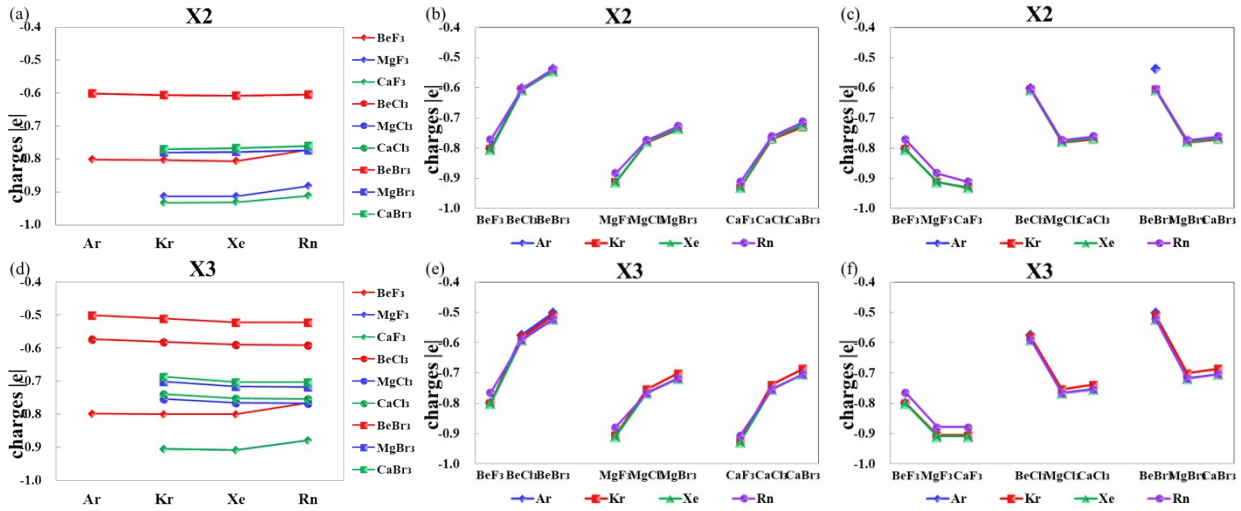

Fig. S19 The natural charges trend of X2 , X3 atoms in transition state along Ar-Kr-Xe-Rn, Be-Mg-Ca, as well as the F-Cl-Br

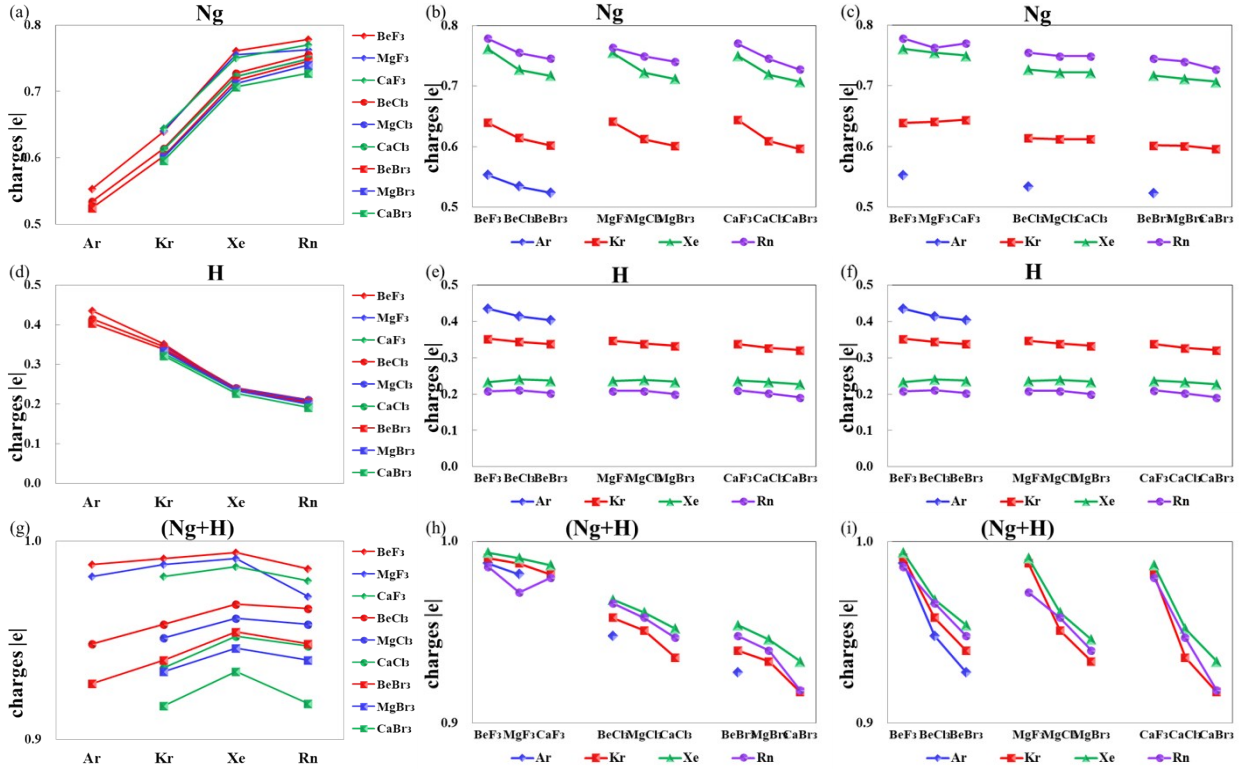

Fig. S20 The natural charges trend of Ng, H atoms and Ng+H in transition state along Ar-Kr-Xe-Rn, Be-Mg-Ca, as well as the F-Cl-Br

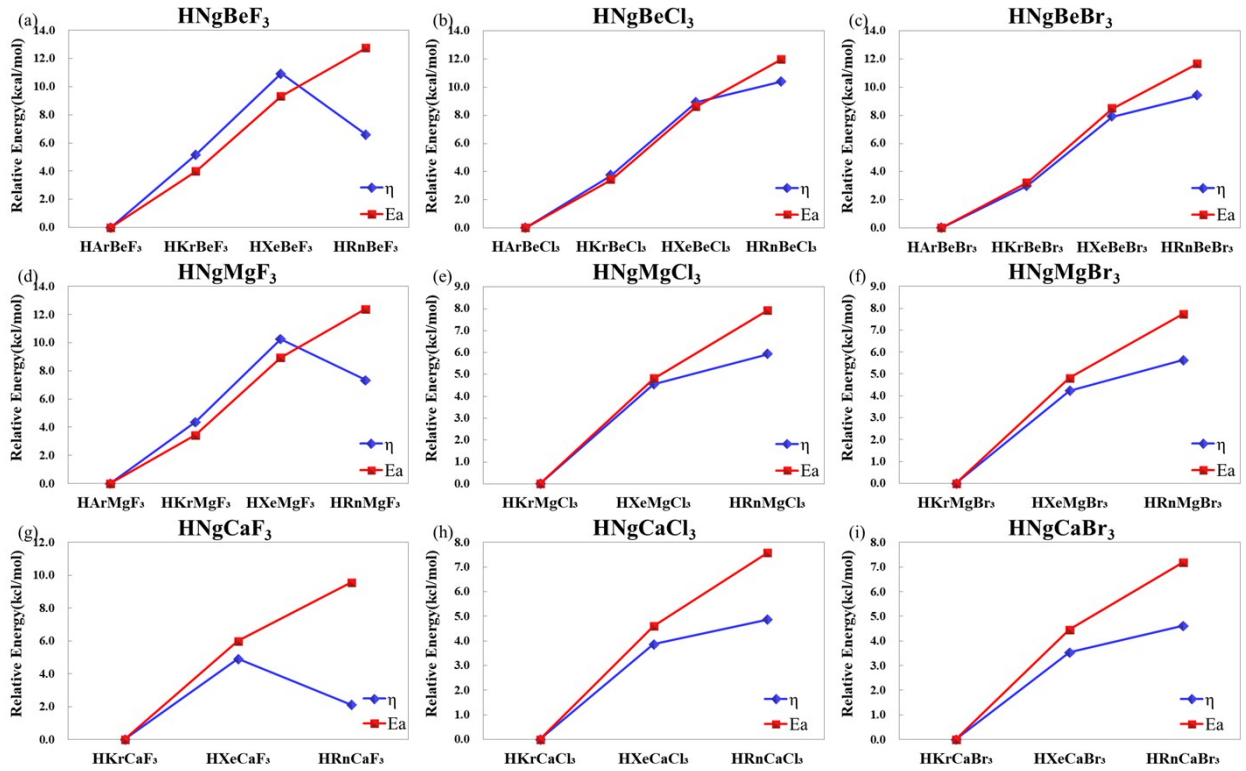

Fig. S21 The relative energy barriers obtained from CCSD(T) calculation and chemical hardness

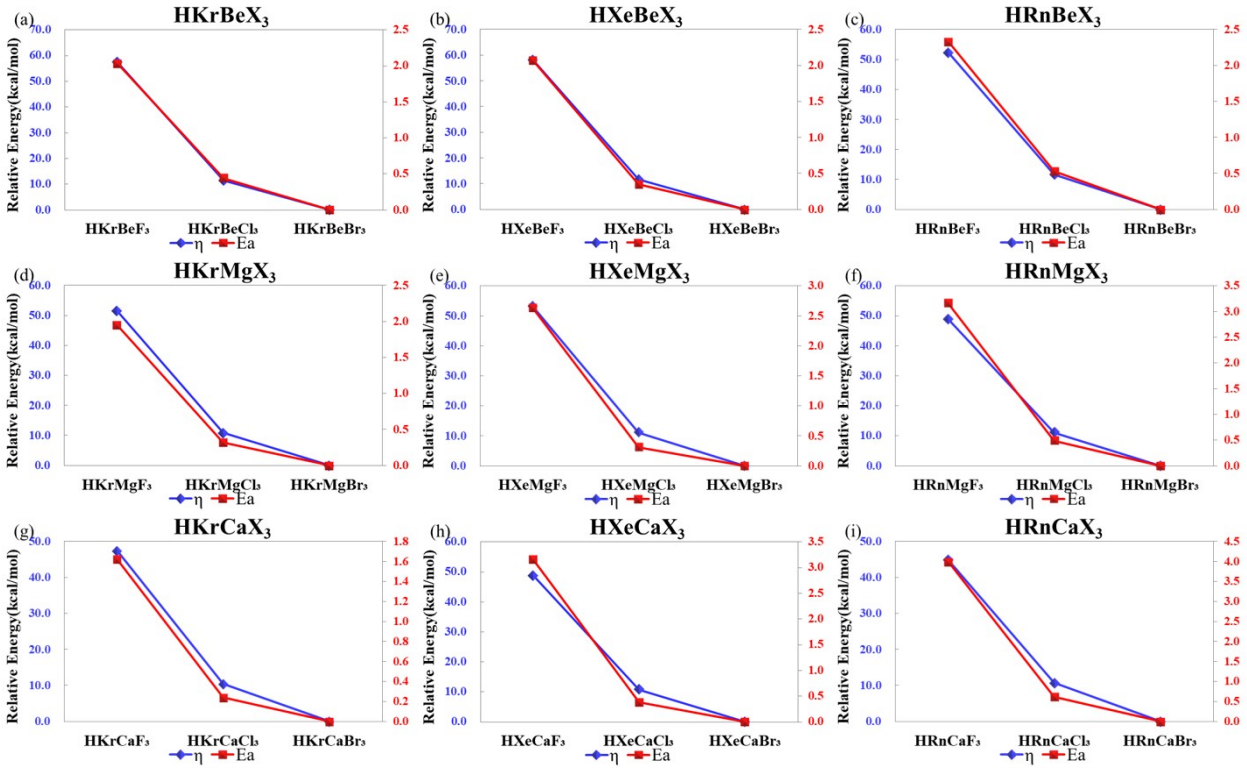

Fig. S22 The relative energy barriers obtained from CCSD(T) calculation and chemical hardness

6.Geometry and stability of HNgX

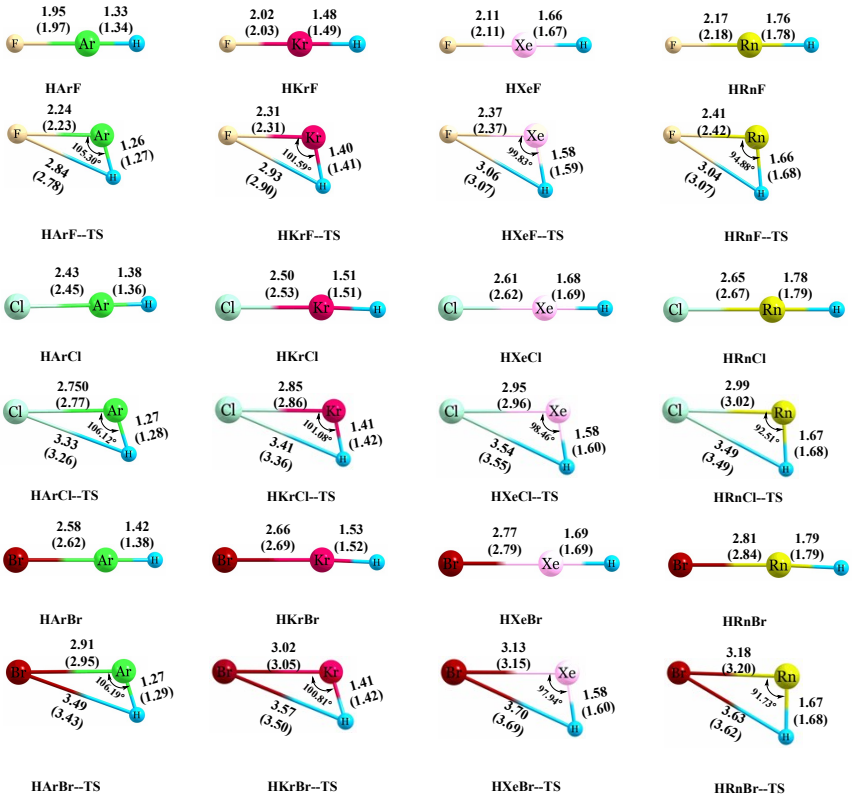

Fig. S23 The optimized geometries of transition state in $HNgMX_3$ (Ng=Ar-Rn) are performed at the MP2/def2-TZVP level (the corresponding value from ωB97XD/def2-TZVP level in parentheses).

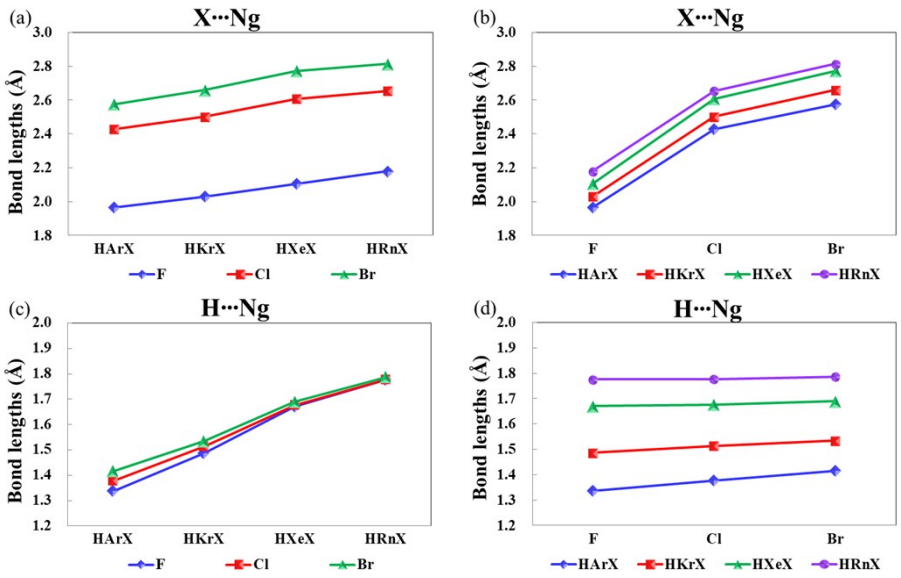

Fig. S24 Comparison of the change of H-Ng and X-Ng bond length from stable configuration to transition state along F-Cl-Br and Ar-Kr-Xe-Rn

Table S14. The fragment energies of HNgX (Ng=Ar-Rn; X=F, Cl, Br) (kcal/mol)

HNgX		ωB97XD			MP2			CCSD(T)	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
HArF	HF+Ar	-132.75	-132.93	-138.91	-138.55	-138.71	-144.72	-138.25	-138.41
HKrF	HF+Kr	-114.40	-114.20	-120.21	-119.39	-119.27	-125.30	-118.86	-118.74
HXeF	HF+Xe	-90.62	-90.12	-96.09	-97.89	-97.43	-103.41	-96.13	-95.67
HRnF	HF+Rn	-83.36	-82.29	-88.20	-89.17	-88.32	-94.26	-87.49	-86.64
HArCl	HCl+Ar	-117.84	-118.68	-124.80	-121.67	-122.07	-128.22	-121.42	-121.82
HKrCl	HCl+Kr	-101.55	-102.23	-108.38	-104.39	-103.98	-110.81	-104.18	-103.76
HXeCl	HCl+Xe	-80.55	-81.03	-87.15	-85.01	-84.60	-92.38	-84.15	-83.74
HRnCl	HCl+Rn	-72.04	-72.11	-78.19	-74.82	-74.97	-81.09	-74.44	-74.59
HArBr	HBr+Ar	-112.12	-113.02	-119.20	-114.55	-114.64	-120.86	-113.73	-113.82
HKrBr	HBr+Kr	-96.44	-96.43	-103.25	-97.82	-98.27	-104.54	-97.44	-97.90
HXeBr	HBr+Xe	-76.06	-76.68	-82.90	-79.04	-79.57	-85.80	-78.26	-78.78
HRnBr	HBr+Rn	-67.36	-67.66	-73.85	-68.66	-68.26	-74.95	-68.46	-68.0603

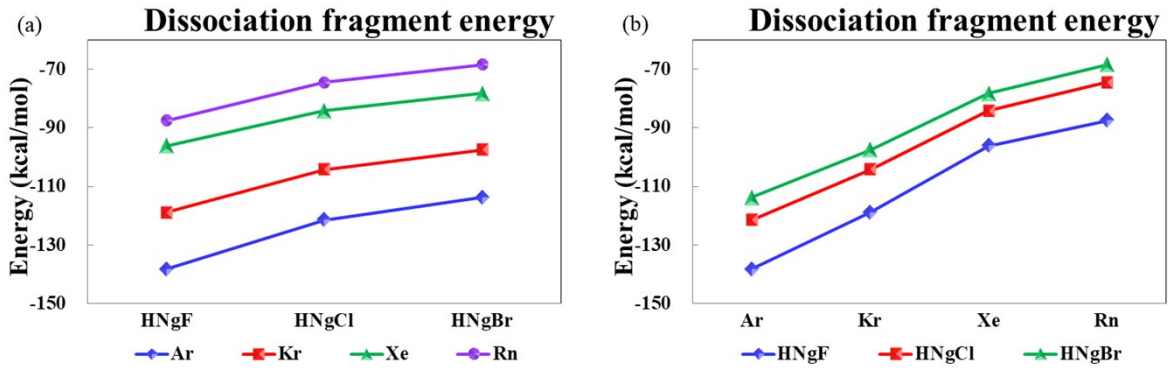

Fig. S25 Comparison of dissociation energy of HNgX→HX+Ng along F-Cl-Br and Ar-Kr-Xe-Rn

Table S15. The activation energies of HNgX (Ng=Ar-Rn; X=F, Cl, Br) (kcal/mol)

		ωB97XD			MP2			CCSD	
		ΔE	ΔE_0	ΔG	ΔE	ΔE_0	ΔG	ΔE	ΔE_0
HArF	HF+Ar	29.86	28.19	26.87	27.86	26.54	25.20	28.65	27.33
HKrF	HF+Kr	35.96	34.32	32.90	35.32	33.90	32.47	36.31	34.89
HXeF	HF+Xe	41.38	39.80	38.33	40.20	38.75	37.29	40.20	38.75
HRnF	HF+Rn	43.38	42.14	40.68	42.84	41.55	40.08	44.25	42.96
HArCl	HCl+Ar	22.71	21.45	20.10	21.10	20.74	19.41	21.10	20.74
HKrCl	HCl+Kr	28.63	27.48	26.02	28.08	28.24	26.15	28.08	28.24
HXeCl	HCl+Xe	34.01	32.76	31.25	33.48	33.31	30.16	33.48	33.31
HRnCl	HCl+Rn	37.17	36.17	34.66	37.53	36.59	35.06	37.53	36.59
HArBr	HBr+Ar	21.00	19.76	18.42	19.76	19.98	18.65	19.76	19.98
HKrBr	HBr+Kr	26.84	26.69	24.68	26.52	26.13	24.68	26.52	26.13
HXeBr	HBr+Xe	32.11	31.03	29.52	31.71	30.93	29.42	31.71	30.93
HRnBr	HBr+Rn	35.38	34.47	32.94	35.81	35.76	33.75	35.81	35.76

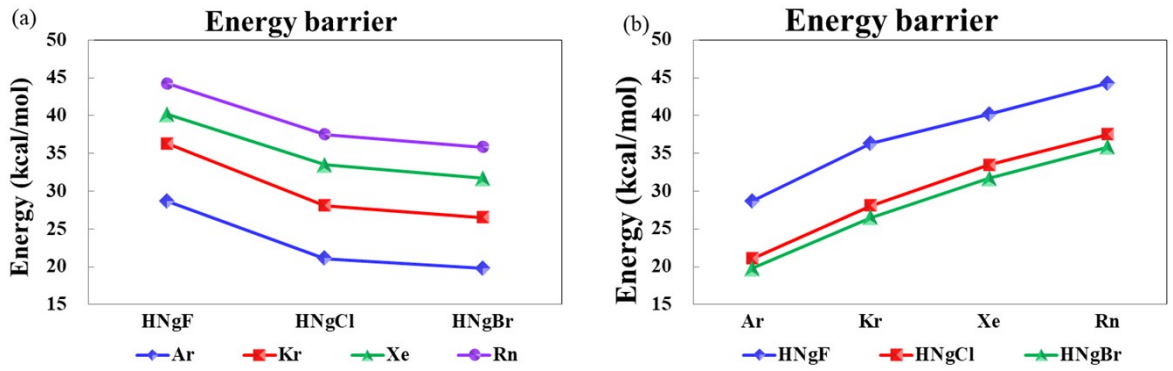

Fig. S26 Comparison of energy barrier of HNgX→HX+Ng along F-Cl-Br and Ar-Kr-Xe-Rn

Cartesian coordinates

Optimized coordinates at MP2/ def2-TZVP level

$BeCl_3$				**$BeCl_3^-$**			
Cl	0.00000000	1.89714100	0.00000000	Cl	0.00000000	1.94541300	0.00000000
Cl	1.64297200	-0.94857000	0.00000000	Cl	1.68477700	-0.97270600	0.00000000
Cl	-1.64297200	-0.94857000	0.00000000	Cl	-1.68477700	-0.97270600	0.00000000
Be	0.00000000	0.00000000	0.00000000	Be	0.00000000	0.00000000	0.00000000
$HArBeCl_3$				**$HArBeCl_3$(TS)**			
Cl	-0.27780400	2.80157000	0.00000000	Cl	-0.10650800	2.80188700	0.00000000
Cl	1.74741400	0.06921500	0.00000000	Cl	1.71988500	-0.04611300	0.00000000
Cl	-1.57206200	-0.30211000	0.00000000	Cl	-1.64432000	-0.19732500	0.00000000
Be	0.00000000	0.94160100	0.00000000	Be	0.00000000	0.92359800	0.00000000
Ar	0.04275900	-2.45001200	0.00000000	Ar	-0.03279300	-2.45423400	0.00000000
H	0.97202700	-3.33367700	0.00000000	H	1.11629600	-3.01181600	0.00000000
$HKrBeCl_3$				**$HKrBeCl_3$(TS)**			
Cl	-0.39754500	3.32616800	0.00000000	Cl	-0.03688400	3.33906700	0.00000000
Cl	1.75748100	0.67724400	0.00000000	Cl	1.71396500	0.45603300	0.00000000
Cl	-1.52870600	0.16920100	0.00000000	Cl	-1.67017100	0.39102800	0.00000000
Be	0.00000000	1.49039400	0.00000000 Kr	Be	0.00000000	1.45633700	0.00000000 Kr
0.05420500	-2.04728000	0.00000000		-0.04067600	-2.07289000	0.00000000	
H	0.91770600	-3.19393100	0.00000000	H	1.34687900	-2.36548600	0.00000000
$HXeBeCl_3$				**$HXeBeCl_3$(TS)**			
Cl	3.34584200	1.71761300	0.00000000	Cl	-0.06844300	-3.78271000	0.00000000
Cl	1.66128100	-1.26213200	0.00000000	Cl	1.68427200	-0.90925700	0.00000000
Cl	0.00000000	1.60936700	0.00000000	Cl	-1.70015900	-0.83227800	0.00000000
Be	1.79530600	0.66065500	0.00000000	Be	-0.03892100	-1.89890700	0.00000000
Xe	-1.65994900	-0.66322400	0.00000000	Xe	0.00000000	1.84563900	0.00000000
H	-2.66506500	-1.93095800	0.00000000	H	1.58929500	1.84329000	0.00000000
$HRnBeCl_3$				**$HRnBeCl_3$(TS)**			
Cl	-0.35919600	-4.17137100	0.00000000	Cl	-0.07695200	-4.22933600	0.00000000
Cl	1.78735200	-1.50029400	0.00000000	Cl	1.68872900	-1.36606400	0.00000000
Cl	-1.48869900	-1.02014500	0.00000000	Cl	-1.70069000	-1.27685400	0.00000000
Be	0.05603000	-2.34298100	0.00000000	Be	-0.04019600	-2.34560500	0.00000000
Rn	0.00000000	1.39790800	0.00000000	Rn	0.00000000	1.45238800	0.00000000
H	0.80511700	2.91258000	0.00000000	H	1.67230800	1.30538200	0.00000000

$BeBr_3$				**$BeBr_3^-$**			
Br	0.00000000	2.04745300	0.00000000	Br	0.00000000	2.09962100	0.00000000
Br	-1.77314600	-1.02372600	0.00000000	Br	1.81832500	-1.04981000	0.00000000
Br	1.77314600	-1.02372600	0.00000000	Br	-1.81832500	-1.04981000	0.00000000
Be	0.00000000	0.00000000	0.00000000	Be	0.00000000	0.00000000	0.00000000
$HArBeBr_3$				**$HArBeBr_3$(TS)**			
Be	0.00000000	0.59126600	0.00000000	Br	-0.17171600	2.60360600	0.00000000
Ar	0.12335500	-2.92991300	0.00000000	Br	1.88474600	-0.40785600	0.00000000
H	1.14803700	-3.70910800	0.00000000	Br	-1.75968700	-0.65546600	0.00000000
Br	1.91137300	-0.30772700	0.00000000	Be	0.00000000	0.57764500	0.00000000
Br	-0.31495800	2.59963600	0.00000000	Ar	0.02608000	-2.92767200	0.00000000
Br	-1.69265600	-0.74669500	0.00000000	H	1.16358400	-3.52245300	0.00000000
HKrBeBr3				**HKrBeBr3(TS)**			
Be	0.00000000	1.00727600	0.00000000	Br	-0.05123400	2.99279100	0.00000000
Kr	0.15070300	-2.66940100	0.00000000	Br	1.86758800	-0.08688400	0.00000000
H	1.11343600	-3.74528400	0.00000000	Br	-1.81502000	-0.17451800	0.00000000
Br	-1.63206700	-0.43304800	0.00000000	Be	0.00000000	0.95923800	0.00000000
Br	1.92346900	0.18951200	0.00000000	Kr	-0.03883100	-2.67907500	0.00000000
Br	-0.47822300	2.98109600	0.00000000	H	1.35122400	-2.98889800	0.00000000
$HXeBeBr_3$				**$HXeBeBr_3$（TS）**			
Br	-0.54316300	3.32313500	0.00000000	Br	0.00553200	3.35767500	0.00000000
Br	1.92070200	0.57113300	0.00000000	Br	1.85593500	0.24712700	0.00000000
Br	-1.61436300	-0.10813500	0.00000000	Br	-1.83166100	0.23112300	0.00000000
Be	0.00000000	1.36811100	0.00000000	Be	0.00000000	1.32154900	0.00000000
Xe	0.13342700	-2.48486000	0.00000000	Xe	-0.04795500	-2.53620800	0.00000000
H	1.08378900	-3.80466400	0.00000000	H	1.54636000	-2.58832200	0.00000000
$HRnBeBr_3$				**$HRnBeBr_3$(TS)**			
Be	1.76313900	0.35349700	0.00000000	Br	3.78932500	-0.03715500	0.00055900
Rn	-2.04230600	-0.50376800	0.00000000	Br	0.71182900	1.86339800	-0.00045800
H	-3.26744200	-1.71792500	0.00000000	Br	0.64119500	-1.83132600	-0.00110600
Br	0.00000000	1.65599100	0.00000000	Be	1.75348600	-0.01112800	-0.00031900
Br	1.33806900	-1.67880700	0.00000000	Rn	-2.15046900	-0.01679600	0.00041200
Br	3.57202200	1.26933000	0.00000000	H	-2.05585000	1.66684800	0.00096000

$MgCl_3$				$MgCl_3^-$			
Cl	0.00000000	2.25757000	0.00000000	Cl	0.00000000	2.27991100	0.00000000
Cl	-1.95511300	-1.12878500	0.00000000	Cl	1.97446100	-1.13995600	0.00000000
Cl	1.95511300	-1.12878500	0.00000000	Cl	-1.97446100	-1.13995600	0.00000000
Mg	0.00000000	0.00000000	0.00000000	Mg	0.00000000	0.00000000	0.00000000
$HKrMgCl_3$				$HKrMgCl_3$(TS)			
Cl	0.48883100	-3.69274400	0.00000000	Cl	-0.09105900	3.69820200	0.00000000
Cl	-1.96175400	-0.36294600	0.00000000	Cl	1.91484300	0.16414100	0.00000000
Cl	1.67176800	0.13854200	0.00000000	Cl	-1.83845700	0.04359800	0.00000000
Mg	0.00000000	-1.52959300	0.00000000	Mg	0.00000000	1.48125700	0.00000000
Kr	-0.06523100	2.26728500	0.00000000	Kr	-0.03040800	-2.26531800	0.00000000
H	-1.03205200	3.32436000	0.00000000	H	1.34413600	-2.62465100	0.00000000
$HXeMgCl_3$				$HXeMgCl_3$(TS)			
Cl	3.97267300	1.20630600	0.00000000	Cl	-0.01317600	4.13958500	0.00000000
Cl	1.12361400	-1.81375600	0.00000000	Cl	1.90169300	0.57647500	0.00000000
Cl	0.00000000	1.65593400	0.00000000	Cl	-1.86512400	0.53413500	0.00000000
Mg	1.94857800	0.30364500	0.00000000	Mg	0.00000000	1.91966100	0.00000000
Xe	-1.97927900	-0.36989200	0.00000000	Xe	-0.03614500	-2.04005300	0.00000000
H	-3.13874800	-1.49382500	0.00000000	H	1.55417500	-2.12641900	0.00000000
$HRnMgCl_3$				$HRnMgCl_3$(TS)			
Cl	-0.47497500	-4.58217700	0.00000000	Cl	-0.09444400	-4.60158200	0.00000000
Cl	1.98935600	-1.22951800	0.00000000	Cl	1.89874400	-1.08478600	0.00000000
Cl	-1.61306000	-0.75240900	0.00000000	Cl	-1.87806800	-0.96573300	0.00000000
Mg	0.06535000	-2.43410500	0.00000000	Mg	-0.03560300	-2.38251900	0.00000000
Rn	0.00000000	1.60158800	0.00000000	Rn	0.00000000	1.62945400	0.00000000
H	0.89333200	3.06242400	0.00000000	H	1.68128700	1.54289200	0.00000000

$MgBr_3$				**$MgBr_3^-$**			
Br	0.00000000	2.40499800	0.00000000	Br	0.00000000	2.43506100	0.00000000
Br	2.08278900	-1.20249900	0.00000000	Br	-2.10882500	-1.21753000	0.00000000
Br	-2.08278900	-1.20249900	0.00000000	Br	2.10882500	-1.21753000	0.00000000
Mg	0.00000000	0.00000000	0.00000000	Mg	0.00000000	0.00000000	0.00000000
$HKrMgBr_3$				**$HKrMgBr_3$(TS)**			
Mg	0.00000000	1.09364300	0.00000000	Br	-0.12388700	3.40174600	0.00000000
Kr	0.16789800	-2.82053000	0.00000000	Br	2.08493100	-0.31021800	0.00000000
H	1.22006300	-3.80204400	0.00000000	Br	-1.98575100	-0.47298900	0.00000000
Br	2.14355900	-0.06908400	0.00000000	Mg	0.00000000	1.03706300	0.00000000
Br	-1.78216300	-0.68785200	0.00000000	Kr	-0.01382800	-2.80319500	0.00000000
Br	-0.56895000	3.39171900	0.00000000	H	1.36253000	-3.17858900	0.00000000
$HXeMgBr_3$				**$HXeMgBr_3$(TS)**			
Br	-0.68974500	3.72871100	0.00000000	Br	-0.02525800	3.75571100	0.00000000
Br	2.14570200	0.33470400	0.00000000	Br	2.07131900	0.00762900	0.00000000
Br	-1.74477800	-0.37030600	0.00000000	Br	-2.02578400	-0.05202100	0.00000000
Mg	0.00000000	1.46524900	0.00000000	Mg	0.00000000	1.38643400	0.00000000
Xe	0.16494300	-2.64716900	0.00000000	Xe	-0.04191400	-2.66231200	0.00000000
H	1.20179800	-3.89468800	0.00000000	H	1.55367700	-2.76851100	0.00000000
$HRnMgBr_3$				**$HRnMgBr_3$(TS)**			
Mg	1.90742300	0.08025000	0.00000000	Br	-4.18631300	-0.05553100	-0.00011000
Rn	-2.25117000	-0.21431300	0.00000000	Br	-0.46768100	2.08664300	-0.00000400
H	-3.57917000	-1.30804800	0.00000000	Br	-0.36921500	-2.02648500	-0.00014400
Br	0.84607900	-2.09629100	0.00000000	Mg	-1.81786000	-0.00522400	-0.00008800
Br	0.00000000	1.75435300	0.00000000	Rn	2.27195900	-0.02057800	0.00011500
Br	4.13365500	0.87839500	0.00000000	H	2.23816000	1.67049100	0.00021500

$CaCl_3$				**$CaCl_3^-$**			
Cl	0.00000000	2.59367400	0.00000000	Cl	0.00000000	2.59793400	0.00000000
Cl	2.24618700	-1.29683700	0.00000000	Cl	2.24987700	-1.29896700	0.00000000
Cl	-2.24618700	-1.29683700	0.00000000	Cl	-2.24987700	-1.29896700	0.00000000
Ca	0.00000000	0.00000000	0.00000000	Ca	0.00000000	0.00000000	0.00000000
$HKrCaCl_3$				**$HKrCaCl_3$(TS)**			
Cl	-0.41914500	4.07300800	0.00000000	Cl	-4.05276100	-0.08334300	0.00000200
Cl	2.08170200	-0.00208200	0.00000000	Cl	0.17296600	2.06079900	0.00012600
Cl	-1.79683400	-0.43758900	0.00000000	Cl	0.28648800	-1.95157900	-0.00010000
Ca	0.00000000	1.57813800	0.00000000	Ca	-1.52830600	0.02245500	0.00003700
Kr	0.03324000	-2.49625300	0.00000000	Kr	2.46491800	-0.06051600	-0.00003400
H	1.08609100	-3.46439300	0.00000000	H	2.91527000	1.28957800	0.00003000
$HXeCaCl_3$				**$HXeCaCl_3$(TS)**			
Cl	4.51776600	0.41859700	0.00000000	Cl	4.47976000	-0.04758800	-0.00002700
Cl	0.42978900	-2.10252400	0.00000000	Cl	0.25853000	2.06022000	-0.00015600
Cl	0.00000000	1.73937300	0.00000000	Cl	0.18178400	-1.99420300	0.00013200
Ca	2.03294700	-0.05753900	0.00000000	Ca	1.95265600	0.00298600	-0.00003900
Xe	-2.24506900	0.02148200	0.00000000	Xe	-2.22828800	-0.03572800	0.00003200
H	-3.53366200	-0.95182900	0.00000000	H	-2.36683900	1.55630900	-0.00007600
$HRnCaCl_3$				**$HRnCaCl_3$(TS)**			
Cl	4.71030900	1.74844400	0.00000000	Cl	4.95076700	-0.06197100	-0.00001800
Cl	1.44327300	-1.78365200	0.00000000	Cl	0.74959300	2.07917000	-0.00019000
Cl	0.00000000	1.77734200	0.00000000	Cl	0.65333100	-1.99675800	0.00011100
Ca	2.45411600	0.60581900	0.00000000	Ca	2.42507600	0.00325400	-
Rn	-1.75387900	-0.46464900	0.00000000	0.00011500			
H	-2.85962300	-1.77283000	0.00000000	Rn	-1.79900000	-0.02417200	0.00004700
				H	-1.80031100	1.66620500	-0.00010400

$CaBr_3$				**$CaBr_3^-$**			
Br	0.00000000	2.74168500	0.00000000	Br	0.00000000	2.75433700	0.00000000
Br	2.37436900	-1.37084200	0.00000000	Br	2.38532600	-1.37716900	0.00000000
Br	-2.37436900	-1.37084200	0.00000000	Br	-2.38532600	-1.37716900	0.00000000
Ca	0.00000000	0.00000000	0.00000000	Ca	0.00000000	0.00000000	0.00000000
$HKrCaBr_3$				**$HKrCaBr_3$(TS)**			
Ca	0.00000000	1.19620700	0.00000000	Br	-3.82189600	-0.07765700	0.00001000
Kr	0.11617300	-2.99624900	0.00000000	Br	0.62370300	2.22300800	0.00010400
H	1.23235900	-3.89918400	0.00000000	Br	0.71789200	-2.11121100	-0.00010100
Br	-1.91629200	-0.92231400	0.00000000	Ca	-1.14577900	0.03605300	0.00001000
Br	2.26832700	-0.39795000	0.00000000	Kr	2.95234100	-0.08807000	-0.00001800
Br	-0.50673800	3.82997800	0.00000000	H	3.44182100	1.25458600	0.00004200
$HXeCaBr_3$				**$HXeCaBr_3$(TS)**			
Br	-0.67672200	4.17007900	0.00000000	Br	-4.15556800	-0.05707700	-0.00000800
Br	2.27970100	0.02767300	0.00000000	Br	0.26095700	2.23726500	0.00001700
Br	-1.85240100	-0.61909300	0.00000000	Br	0.34821200	-2.15959800	-0.00000400
Ca	0.00000000	1.57430400	0.00000000	Ca	-1.47746800	0.00770700	0.00001600
Xe	0.13875800	-2.82812400	0.00000000	Xe	2.79108800	-0.04493100	-0.00000900
H	1.23684600	-4.02045200	0.00000000	H	2.95457200	1.55148600	-0.00000400
$HRnCaBr_3$				**$HRnCaBr_3$(TS)**			
Ca	2.02611200	-0.18535200	0.00000000	Br	-4.58327300	-0.07330000	0.00005600
Rn	-2.43296600	0.11873900	0.00000000	Br	-0.19877700	2.26039200	0.00015500
H	-3.85209900	-0.85212700	0.00000000	Br	-0.08782300	-2.16345800	-0.00014500
Br	0.26264000	-2.29524500	0.00000000	Ca	-1.90806400	0.00875200	0.00002600
Br	0.00000000	1.85795700	0.00000000	Rn	2.39740500	-0.03103400	-0.00003400
Br	4.66778700	0.27579100	0.00000000	H	2.43002000	1.66665100	0.00008100

BeF3				**BeF_3^-**			
Be	0.00000000	0.00000000	0.00000000	Be	0.00000000	0.00000000	0.00000000
F	0.00000000	1.46002700	0.00000000	F	0.00000000	1.48534400	0.00000000
F	1.26442000	-0.73001300	0.00000000	F	-1.28634500	-0.74267200	0.00000000
F	-1.26442000	-0.73001300	0.00000000	F	1.28634500	-0.74267200	0.00000000
$HRnBeF_3$				**$HRnBeF_3$(TS)**			
Be		0.01189900	-2.43643100	Be	2.48305300	-0.00639700	-0.00023700
0.00000000				Rn	-0.85790700	-0.01853400	0.00008700
Rn	0.00000000	0.80900100	0.00000000	H	-0.78795400	1.64876500	-0.00039500
H	0.50841300	2.42727200	0.00000000	F	1.63250200	-1.25330100	0.00012300
F	1.30516200	-1.70956200	0.00000000	F	1.62891300	1.24600300	-0.00017300
F	-1.10863800	-1.36820700	0.00000000	F	3.92033700	0.00404500	-0.00063500
F	-0.25830300	-3.83952200	0.00000000				
MgF_3				**MgF_3^-**			
Mg	0.00000000	0.00000000	0.00000000	Mg	0.00000000	0.00000000	0.00000000
F	0.00000000	1.82847200	0.00000000	F	0.00000000	1.82847200	0.00000000
F	1.58350300	-0.91423600	0.00000000	F	-1.58350400	-0.91423600	0.00000000
F	-1.58350300	-0.91423600	0.00000000	F	1.58350400	-0.91423600	0.00000000
$HRnMgF_3$				**$HRnMgF_3$(TS)**			
Mg	0.01398700	-2.52964500	0.00000000	Mg	-2.52049300	-0.00640600	-0.00012000
Rn	0.00000000	1.03137600	0.00000000	Rn	1.06792600	-0.01872800	0.00004600
H	0.61650700	2.61429200	0.00000000	H	1.00840900	1.65107500	0.00033800
F	-1.19910800	-1.07245100	0.00000000	F	-1.31242200	-1.41800300	-0.00031900
F	1.47888500	-1.43103700	0.00000000	F	-1.33814000	1.43097200	0.00016300
F	-0.36692800	-4.26950100	0.00000000	F	-4.30545500	-0.00892200	-0.00015700
CaF_3				**CaF_3^-**			
Ca	0.00000000	0.00000000	0.00000000	Ca	0.00000000	0.00000000	0.00000000
F	0.00000000	2.16277100	0.00000000	F	0.00000000	2.14423400	0.00000000
F	-1.87301400	-1.08138500	0.00000000	F	1.85696100	-1.07211700	0.00000000
F	1.87301400	-1.08138500	0.00000000	F	-1.85696100	-1.07211700	0.00000000
$HRnCaF_3$				**$HRnCaF_3$(TS)**			
Ca	0.00885100	-2.60892100	0.00000000	Ca	2.53277700	-0.00244700	-0.00009400
Rn	0.00000000	1.25845800	0.00000000	Rn	-1.26248200	-0.02060200	0.00000900
H	0.67653800	2.82141000	0.00000000	H	-1.23959300	1.65675500	-0.00014600
F	1.55634300	-1.11010900	0.00000000	F	1.00622400	1.58547300	0.00001000
F	-1.27250200	-0.77244700	0.00000000	F	0.94735400	-1.53535000	-0.00001000
F	-0.37868000	-4.65859300	0.00000000	F	4.61948200	-0.03190700	0.00013400