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

Cyanide-Isocyanide Isomerization: Stability and Bonding in Noble Gas Inserted Metal Cyanides (Metal = Cu, Ag, Au)

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Supporting Information

Table S1. The IR stretching frequencies (in cm^{-1}) and the corresponding IR intensity in parentheses (in km/mol) for MNgCN molecules.

		CCSD(T)	MP2	MPWB95
Molecule	**Mode of vibrations**	**Freq (cm^{-1})**	**Freq (cm^{-1}) (Intensity)**	**Freq (cm^{-1}) (Intensity)**
	Cu-Xe-CN bending (degenerate)	41.4, 42	50 (1)	48 (2)
	CuXe-C-N bending (degenerate)	151	159 (0)	164 (0)
CuXeCN	Cu-Xe stretching	179	195 (217)	174 (11)
	Xe-C stretching	217	227.3 (110)	219 (50)
	C-N stretching	2123	2039 (85)	2122 (17)
	Cu-Rn-CN bending (degenerate)	43	50 (1)	48 (2)
	CuRn-C-N bending (degenerate)	159, 160	172 (0)	170 (0)
CuRnCN	Cu-Rn stretching	174	197 (2)	170 (0)
	Rn-C stretching	218	216 (334)	214 (68)
	C-N stretching	2129	2045 (115)	2128 (24)
	Ag-Xe-CN bending (degenerate)	47, 50	44 (2)	43 (3)
	AgXe-C-N bending (degenerate)	153, 155	153 (0)	153 (0)
AgXeCN	Ag-Xe stretching	132	159 (56)	127 (2)
	Xe-C stretching	212	203 (353)	204 (60)
	C-N stretching	2120	2038 (103)	2119 (17)

	Ag-Rn-CN bending (degenerate)	45	45 (1)	42 (2)
	AgRn-C-N bending (degenerate)	161	170 (0)	162 (0)
AgRnCN	Ag-Rn stretching	130	150 (2)	128 (0)
	Rn-C stretching	218	212 (422)	208 (68)
	C-N stretching	2128	2045 (148)	2127 (24)
	Au-Xe-CN bending (degenerate)	57	68 (4)	51 (4)
	AuXe-C-N bending (degenerate)	198	261 (1)	192 (0)
AuXeCN	Au-Xe stretching	136	168 (3)	127 (1)
	Xe-C stretching	251	303 (489)	204 (98)
	C-N stretching	2134	2066 (366)	2119 (50)
	Au-Rn-CN bending (degenerate)	54	61 (4.3)	48 (4)
AuRnCN	AuRn-C-N bending (degenerate)	207	252 (1)	194 (0)
	Au-Rn stretching	135	152 (8)	126 (1)
	Rn-C stretching	258	309 (367)	229 (96)
	C-N stretching	2144	2071 (302)	2141 (53)

Table S2. ZPE corrected dissociation energy (D_0, kcal/mol) and free energy change at 298 K (ΔG, kcal/mol) for different possible dissociation channels of MNgCN compounds computed at the MP2/cc-pVTZ/cc-pVTZ-PP level.

Processes		D_0		ΔG	
		Xe	**Rn**	**Xe**	**Rn**
MNgCN → M + Ng + CN	Cu	89.3	98.8	75.5	84.8
	Ag	31.9	42.3	18.3	28.4
	Au	75.3	89.0	60.5	74.2
MNgCN → M^+ + Ng + CN^-	Cu	111.6	121.0	98.5	107.8
	Ag	101.0	111.3	88.1	98.2
	Au	150.5	164.2	136.5	150.1
MNgCN → M^- + Ng + CN^+	Cu	322.4	331.9	309.4	318.6
	Ag	308.7	319.1	295.8	305.9
	Au	283.2	296.9	269.1	282.8
MNgCN → MNg^+ + CN^-	Cu	90.0	96.7	81.5	88.0
	Ag	85.6	93.0	77.0	84.2
	Au	119.2	127.3	109.7	117.9
MNgCN → M^+ + $NgCN^-$	Cu	108.7	117.3	99.9	108.5
	Ag	98.0	107.6	89.4	99.0
	Au	147.6	160.5	137.8	150.9
MNgCN → M^- + $NgCN^+$	Cu	282.7	281.6	276.1	274.8
	Ag	225.3	225.1	218.8	218.4
	Au	268.7	271.9	261.1	264.2

MNgCN → Ng + MCN	Cu	-84.7	-75.2	-90.8	-81.5
	Ag	-74.8	-64.4	-81.0	-70.9
	Au	-76.8	-63.1	-83.8	-70.1
MNgCN → Ng + MNC	Cu	-70.6	-61.2	-77.1	-67.8
	Ag	-59.0	-48.7	-65.8	-55.7
	Au	-46.5	-32.8	-53.9	-40.3
MNgCN → NgMCN	Cu	-99.6	-91.1	-98.8	-90.6
	Ag	-85.6	-76.7	-85.1	-76.5
	Au	-96.2	-84.5	-95.9	-84.3
NgMCN → Ng + MCN	Cu	14.9	15.9	8.0	9.0
	Ag	10.9	12.3	4.2	5.6
	Au	19.4	21.4	12.1	14.2
MNgCN → MNgNC	Cu	1.3	4.5	0.0	5.7
	Ag	3.8	5.1	5.0	6.3
	Au	12.3	12.3	13.5	11.0
NgMNC → Ng + MNC	Cu	17.1	17.9	7.7	10.9
	Ag	11.5	13.0	4.7	6.1
	Au	25.1	27.2	17.6	19.7
MNgCN → NgMNC	Cu	-87.8	-79.1	-84.7	-78.7
	Ag	-70.5	-61.6	-70.5	-61.8
	Au	-71.6	-60.0	-71.5	-59.9

Table S3. ZPE corrected dissociation energy (D_0, kcal/mol) and free energy change at 298 K (ΔG, kcal/mol) for different possible dissociation channels of MNgCN compounds computed at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level.

Processes		D_0		ΔG	
		Xe	**Rn**	**Xe**	**Rn**
MNgCN → M + Ng + CN	Cu	36.0	42.9	22.2	29.0
	Ag	29.3	36.5	15.8	22.8
	Au	33.1	42.0	18.9	27.8
MNgCN → M^+ + Ng + CN^-	Cu	149.0	155.9	136.0	142.8
	Ag	137.0	144.2	124.2	131.2
	Au	175.5	184.4	162.1	171.0
MNgCN → M^- + Ng + CN^+	Cu	346.1	353.1	333.2	340.0
	Ag	335.0	342.2	322.3	329.3
	Au	317.0	325.9	303.7	312.5
MNgCN → MNg^+ + CN^-	Cu	117.3	120.8	108.9	112.2
	Ag	114.6	118.2	106.3	109.7
	Au	137.8	141.2	129.0	132.3
MNgCN → M^+ + $NgCN^-$	Cu	146.1	152.3	137.2	143.5
	Ag	134.1	140.6	125.5	131.9
	Au	172.6	180.8	163.4	171.7
MNgCN → M^- + $NgCN^+$	Cu	221.2	218.7	215.1	212.4
	Ag	210.0	207.8	204.1	201.7
	Au	192.1	191.6	185.6	184.9

MNgCN → Ng + MCN	Cu	-62.6	-55.6	-68.6	-61.8
	Ag	-54.1	-46.9	-60.1	-53.1
	Au	-58.1	-49.2	-64.4	-55.6
MNgCN → Ng + MNC	Cu	-49.1	-42.2	-55.4	-48.6
	Ag	-38.9	-31.7	-45.3	-38.3
	Au	-33.5	-24.6	-40.1	-31.2
MNgCN → NgMCN	Cu	-75.6	-69.5	-74.9	-69.0
	Ag	-64.1	-58.0	-63.5	-57.6
	Au	-71.9	-64.3	-71.2	-63.7
NgMCN → Ng + MCN	Cu	13.1	13.8	6.3	7.1
	Ag	10.1	11.2	3.4	4.6
	Au	13.8	15.2	6.7	8.1
MNgCN → MNgNC	Cu	4.2	4.9	3.6	4.4
	Ag	4.1	4.9	3.3	4.3
	Au	7.0	7.5	6.6	7.2
NgMNC → Ng + MNC	Cu	15.4	16.1	8.5	9.3
	Ag	11.1	12.3	4.4	5.6
	Au	17.3	18.8	10.1	11.6
MNgCN → NgMNC	Cu	-64.5	-58.3	-63.9	-57.9
	Ag	-50.1	-44.1	-49.7	-43.9
	Au	-50.8	-43.4	-50.2	-42.9

Table S4. The rate constants (k, sec^{-1}) for different transformation processes MNgCN species computed at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level. .

Process	Transition states	$\Delta G^{\ddagger}$ or $\Delta G_f^{\ddagger}$ (kcal/mol)	Corresponding Rate Constants	Values (sec^{-1})
CuXeCN→XeAuNC	TS_1	11.8	k_1	1.389×10^{4}
CuXeCN→XeCuCN	TS_2 and TS_3	12.0	k_2	9.911×10^{3}
CuRnCN→RnCuNC	TS_1	15.1	k_1	5.291×10^{1}
CuRnCN→RnCuCN	TS_2 and TS_3	15.4	k_2	3.189×10^{1}
AgXeCN→XeAgNC	TS_1	9.8	k_1	4.063×10^{5}
AgXeCN→XeAgCN	TS_2 and TS_3	10.1	k_2	2.449×10^{5}
AgRnCN→RnAgNC	TS_1	13.3	k_1	1.104×10^{3}
AgRnCN→RnAgCN	TS_2 and TS_3	13.6	k_2	6.655×10^{2}
AuXeCN→XeAuNC	TS_1	19.7	k_1	2.246×10^{-2}
AuXeCN→XeAuCN	TS_2 and TS_3	19.9	k_2	1.602×10^{-2}
AuRnCN→RnAuNC	TS_1	24.4	k_1	8.052×10^{-6}
AuRnCN→RnAuCN	TS_2 and TS_3	24.7	k_2	4.853×10^{-6}

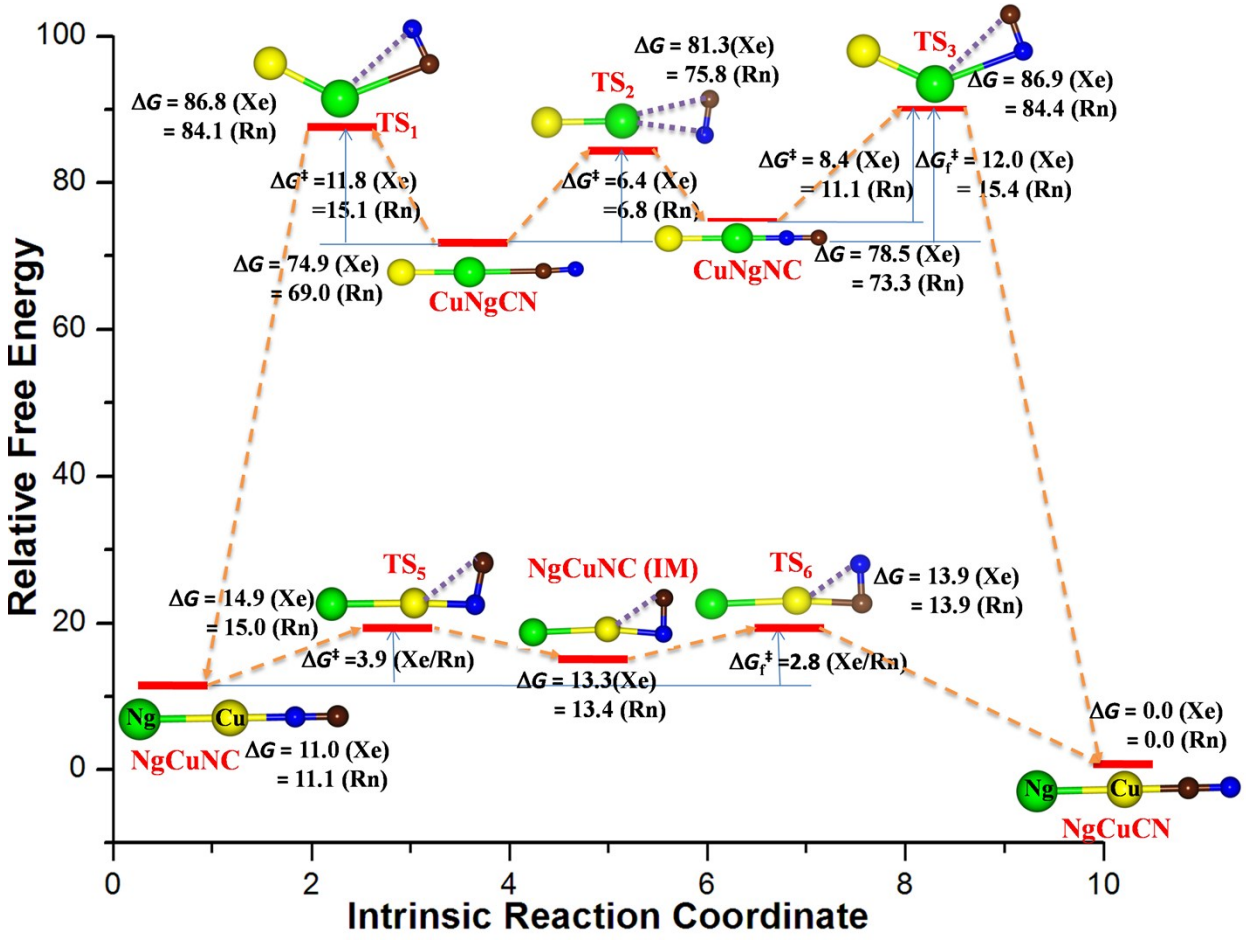


Fig. S1 The isomeric transformation occurred in CuNgCN (Ng= Xe, Rn) compounds to be converted into the most stable NgCuCN form, studied at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level. Relative free energies (ΔG) with respect to the most stable NgCuCN isomer, free energies of activation or overall final free energies of activation ($\Delta G^{\ddagger}/\Delta G_f^{\ddagger}$) are in kcal/mol.

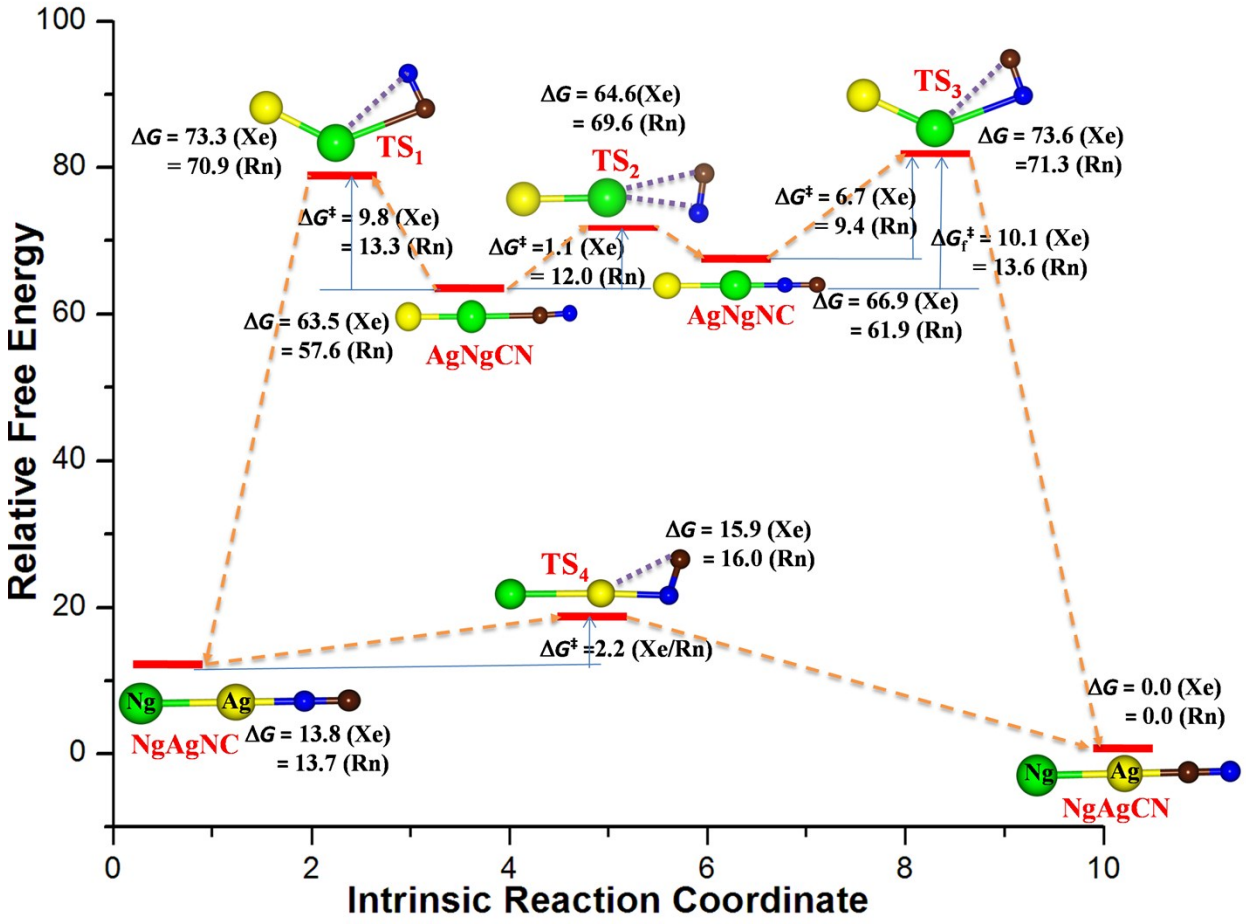
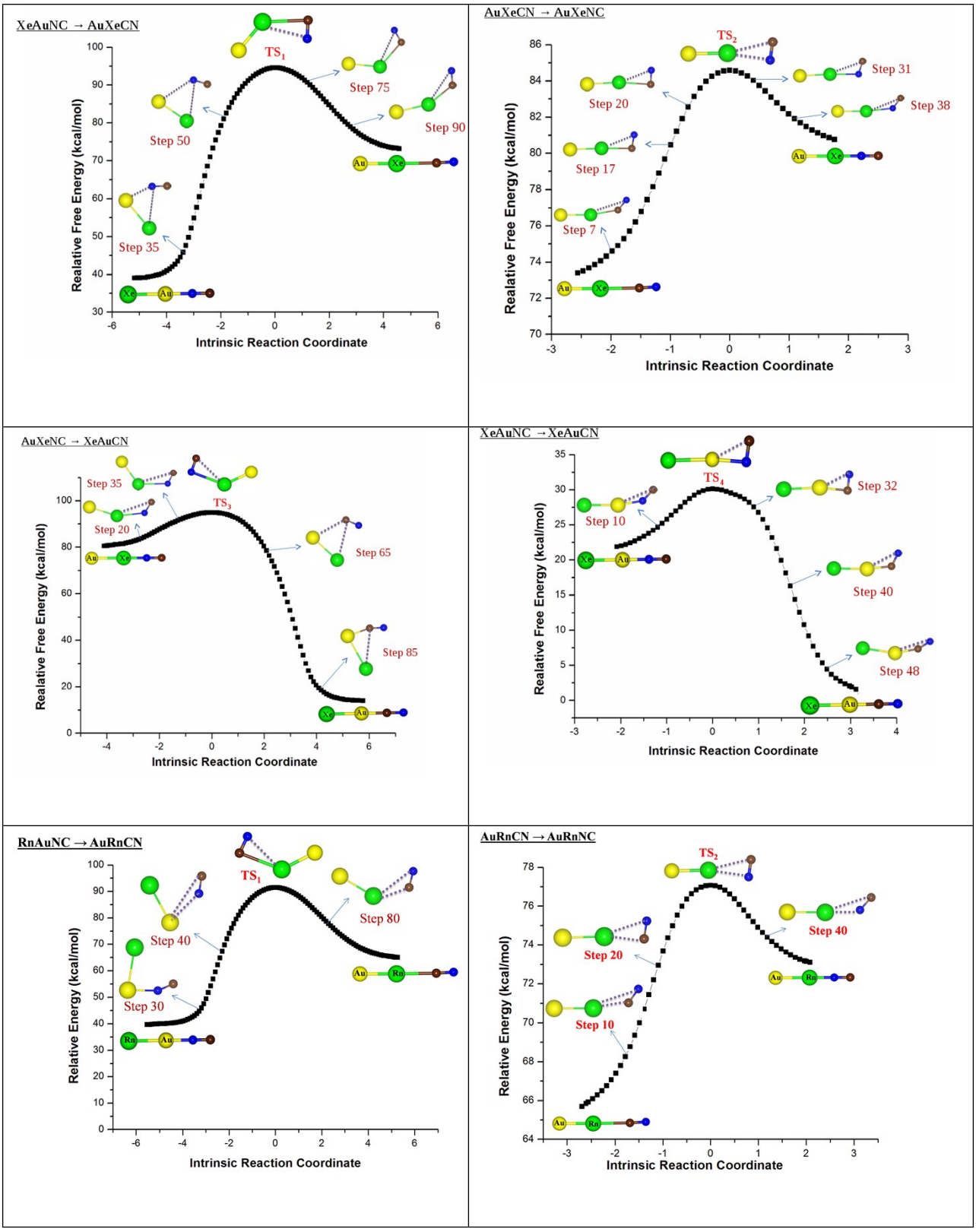
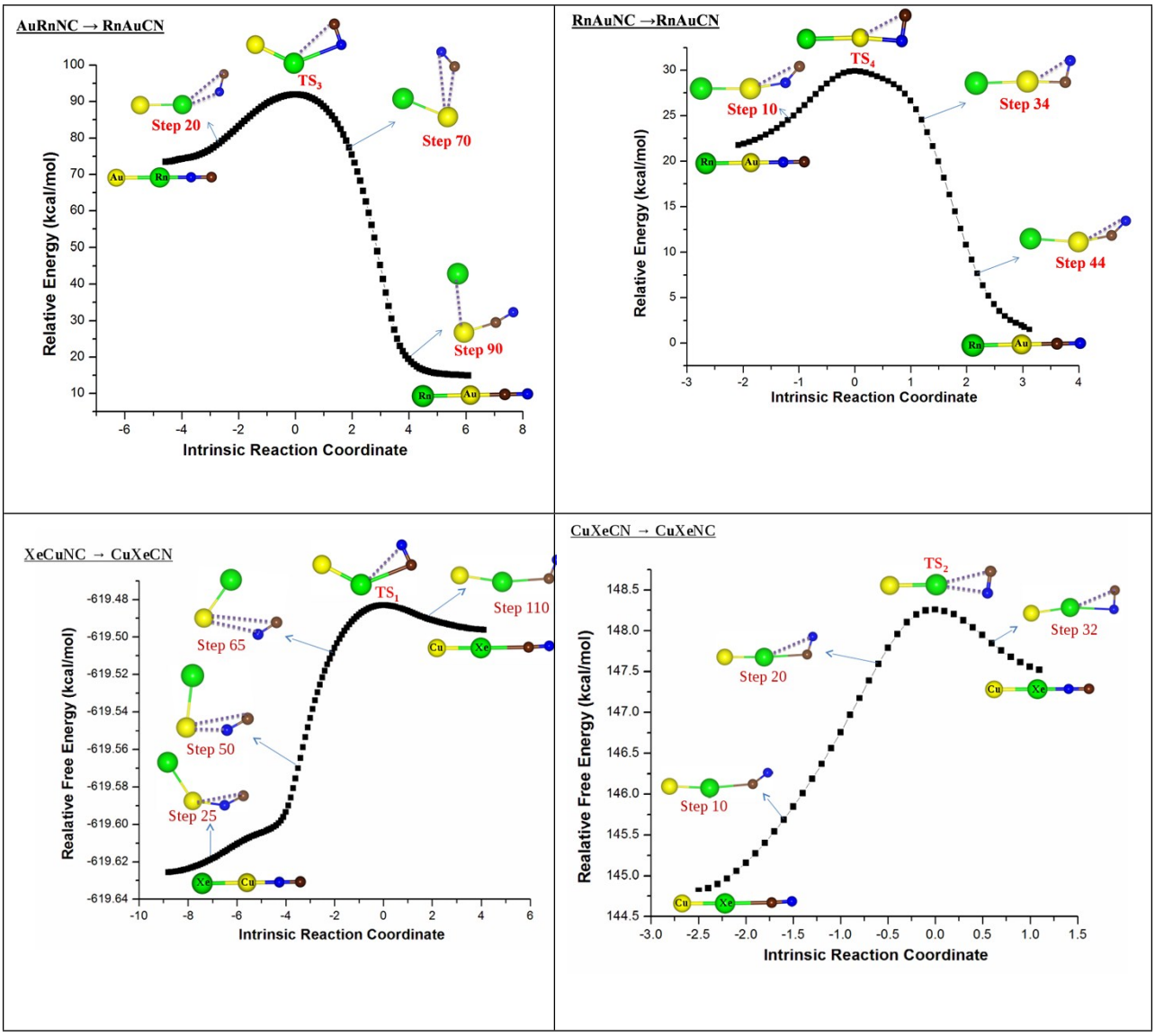
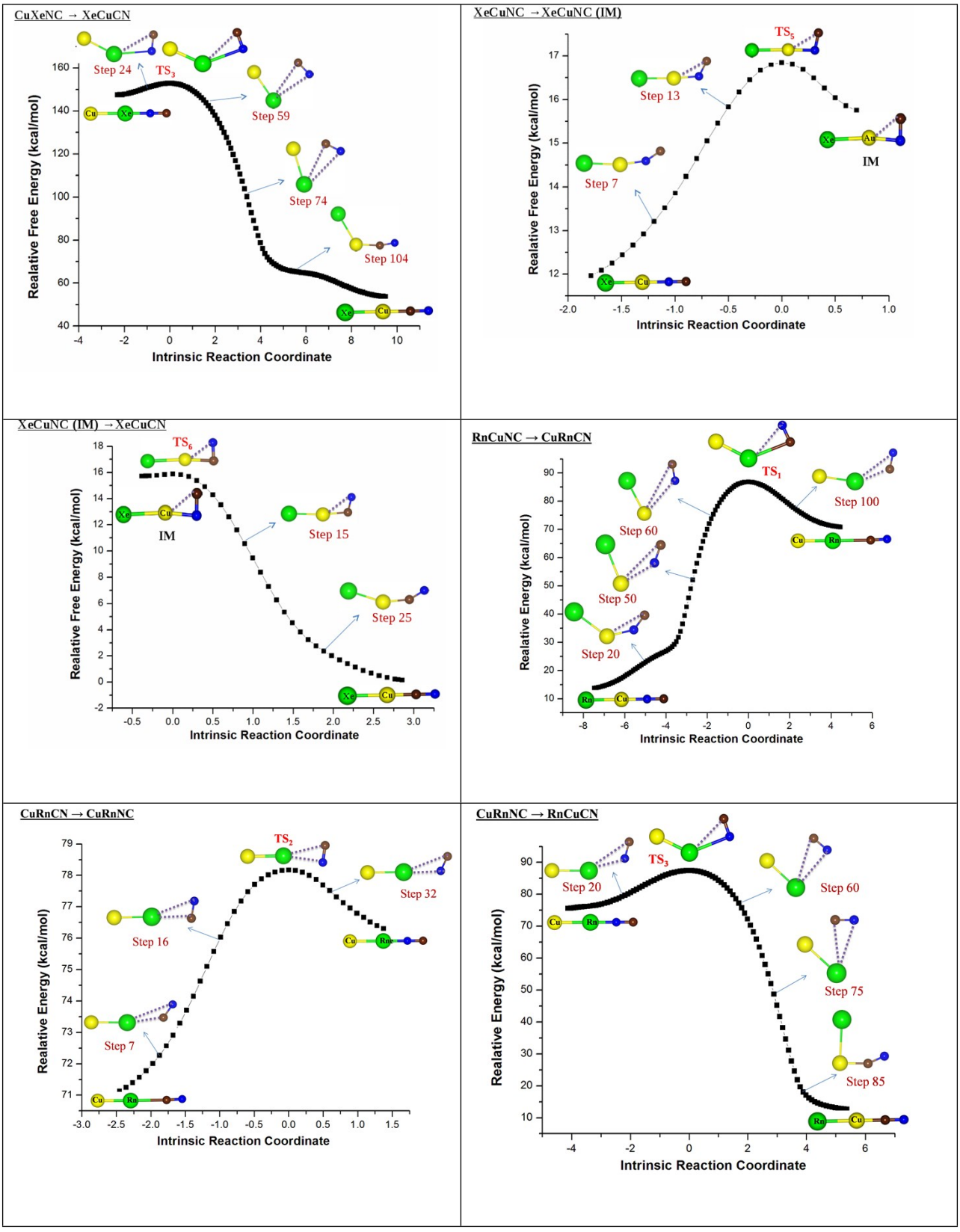
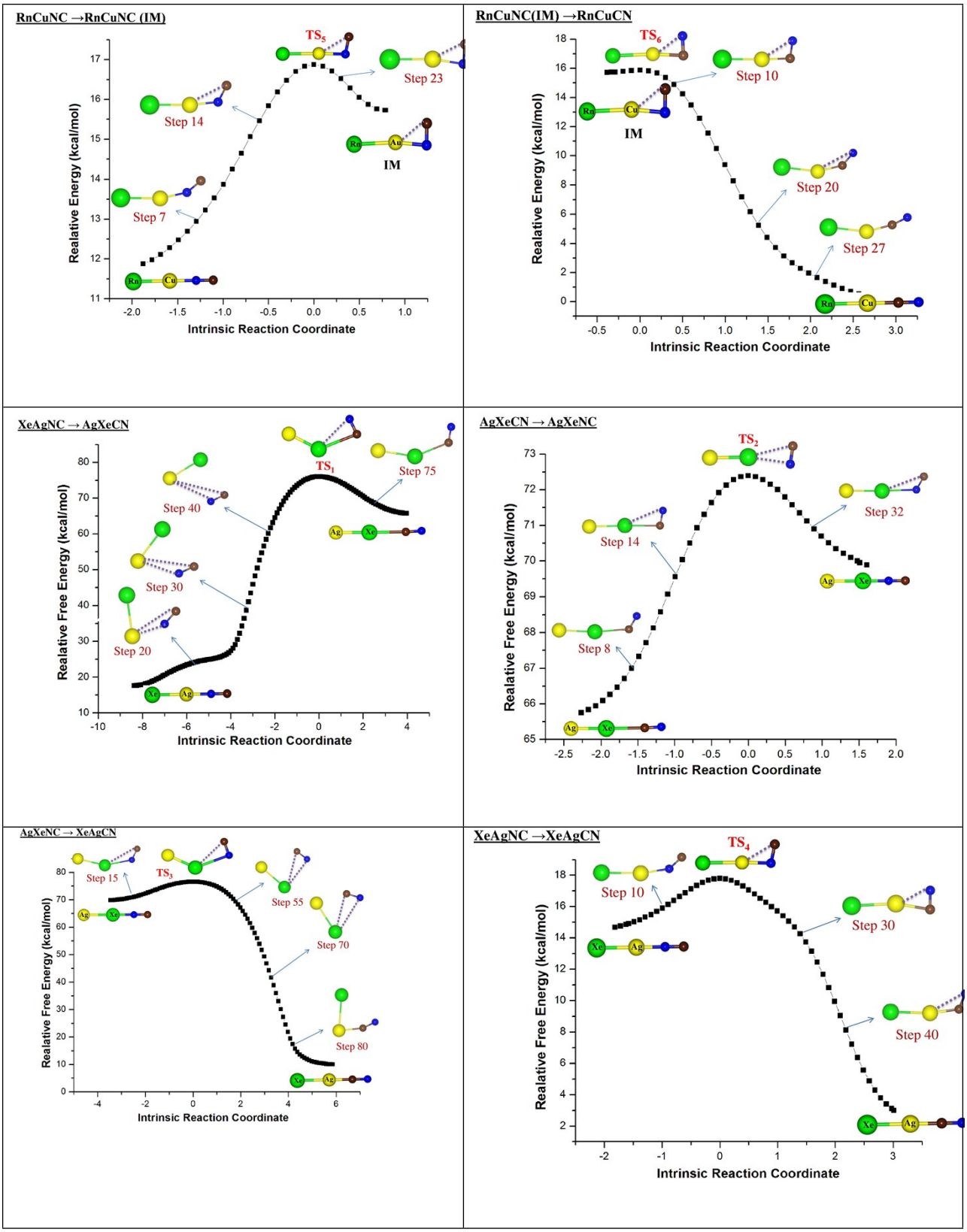


Fig. S2 The isomeric transformation occurred in AgNgCN (Ng= Xe, Rn) compounds to be converted into the most stable NgAgCN form, studied at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level. Relative free energies (ΔG) with respect to the most stable NgAgCN isomer, free energies of activation or overall final free energies of activation ($\Delta G^{\ddagger}/\Delta G_f^{\ddagger}$) are in kcal/mol.


XeAuNC → AuXeCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS1
Step 50
Step 75
Step 90
Step 35
AuXeCN → AuXeNC
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS2
Step 20
Step 31
Step 38
Step 17
Step 7
AuXeNC → XeAuCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
Step 35
TS3
Step 20
Step 65
Step 85
XeAuNC →XeAuCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS4
Step 10
Step 32
Step 40
Step 48
RnAuNC → AuRnCN
Relative Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS1
Step 40
Step 80
Step 30
AuRnCN → AuRnNC
Relative Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS2
Step 20
Step 40
Step 10


AuRnNC → RnAuCN
Relative Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS3
Step 20
Step 70
Step 90
Au
Rn
RnAuNC →RnAuCN
Relative Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS4
Step 10
Step 34
Step 44
Rn
Au
XeCuNC → CuXeCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS1
Step 65
Step 110
Step 50
Step 25
Cu
Xe
CuXeCN → CuXeNC
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS2
Step 20
Step 32
Step 10
Cu
Xe


CuXeNC → XeCuCN
Step 24
TS3
Step 59
Step 74
Step 104
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
XeCuNC →XeCuNC (IM)
TS5
Step 13
Step 7
IM
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
XeCuNC (IM) →XeCuCN
TS6
IM
Step 15
Step 25
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
RnCuNC → CuRnCN
TS1
Step 100
Step 60
Step 50
Step 20
Realative Energy (kcal/mol)
Intrinsic Reaction Coordinate
CuRnCN → CuRnNC
TS2
Step 32
Step 16
Step 7
Realative Energy (kcal/mol)
Intrinsic Reaction Coordinate
CuRnNC → RnCuCN
TS3
Step 20
Step 60
Step 75
Step 85
Realative Energy (kcal/mol)
Intrinsic Reaction Coordinate


RnCuNC →RnCuNC (IM)
Realative Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS5
Step 23
Step 14
Step 7
IM
RnCuNC(IM) →RnCuCN
Realative Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS6
Step 10
IM
Step 20
Step 27
XeAgNC → AgXeCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS1
Step 75
Step 40
Step 30
Step 20
AgXeCN → AgXeNC
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS2
Step 32
Step 14
Step 8
AgXeNC → XeAgCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
Step 15
TS3
Step 55
Step 70
Step 80
XeAgNC →XeAgCN
Realative Free Energy (kcal/mol)
Intrinsic Reaction Coordinate
TS4
Step 10
Step 30
Step 40

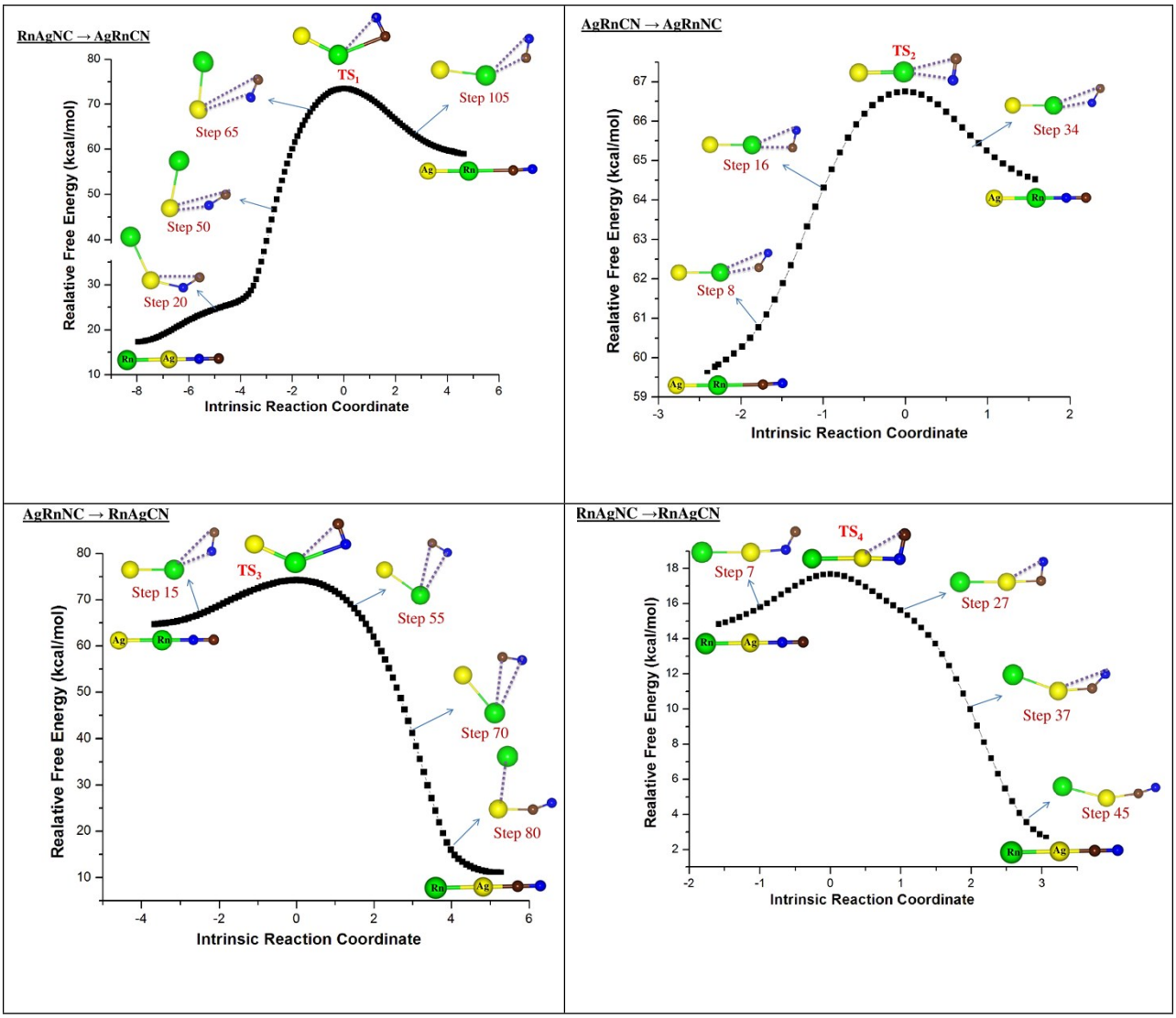


Fig. S3 The IRC plots for the isomeric transformation occurred in Ng inserted MCN (M = Cu, Ag, Au) molecules studied at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level.

Cartesian coordinates for the optimized geometries of MNgCN (M = Cu, Ag, Au; Ng =Xe-Rn) at CCSD(T)/cc-pVTZ/cc-pVTZ-PP level

1. CuXeCN geometry

Cu	0.00000000	0.00000000	-2.18039600
Xe	0.00000000	0.00000000	0.30637100
C	0.00000000	0.00000000	2.95868800
N	0.00000000	0.00000000	4.13362000

2. CuRnCN geometry

Cu	0.00000000	0.00000000	-2.31712700
Rn	0.00000000	0.00000000	0.24698900
C	0.00000000	0.00000000	2.90268700
N	0.00000000	0.00000000	4.07707000

3. AgXeCN geometry

Ag	0.00000000	0.00000000	-1.98580200
Xe	0.00000000	0.00000000	0.75491600
C	0.00000000	0.00000000	3.41092800
N	0.00000000	0.00000000	4.58595300

4. AgRnCN geometry

Ag	0.00000000	0.00000000	-2.18489800

Rn	0.00000000	0.00000000	0.60589600
C	0.00000000	0.00000000	3.25869200
N	0.00000000	0.00000000	4.43299400

5. AuXeCN geometry

Au	0.00000000	0.00000000	1.48487500
Xe	0.00000000	0.00000000	-1.15246200
C	0.00000000	0.00000000	-3.60484000
N	0.00000000	0.00000000	-4.77758400

6. AuRnCN geometry

Au	0.00000000	0.00000000	-1.72413500
Rn	0.00000000	0.00000000	0.96903400
C	0.00000000	0.00000000	3.43585100
N	0.00000000	0.00000000	4.60780600

Cartesian coordinates for the optimized geometries of NgMNC (M = Cu, Ag, Au; Ng =Xe-Rn) at MPWB95/cc-pVTZ/cc-pVTZ-PP level

1. XeCuNC geometry

Xe	0.00000000	0.00000000	1.40583100
Cu	0.00000000	0.00000000	-1.08600900
N	0.00000000	0.00000000	-2.87087500
C	0.00000000	0.00000000	-4.05407600

2. RnCuNC geometry

Cu	0.00000000	0.00000000	-1.49623400
C	0.00000000	0.00000000	-4.46544000
N	0.00000000	0.00000000	-3.28218500
Rn	0.00000000	0.00000000	1.08324100

3. XeAgNC geometry

Xe	0.00000000	0.00000000	1.71903200
Ag	0.00000000	0.00000000	-0.99652900
N	0.00000000	0.00000000	-2.99231700
C	0.00000000	0.00000000	-4.17410600

4. RnAgNC geometry

C	0.00000000	0.00000000	-4.59685900
N	0.00000000	0.00000000	-3.41518300
Rn	0.00000000	0.00000000	1.37244900
Ag	0.00000000	0.00000000	-1.41581100

5. XeAuNC geometry

Xe	0.00000000	0.00000000	-1.88959400
Au	0.00000000	0.00000000	0.75754300
N	0.00000000	0.00000000	2.69958600
C	0.00000000	0.00000000	3.88251100

6. RnAuNC geometry

Rn	0.00000000	0.00000000	1.59022800
Au	0.00000000	0.00000000	-1.13443000
N	0.00000000	0.00000000	-3.08018100
C	0.00000000	0.00000000	-4.26305500

Cartesian coordinates for the optimized geometries of MNgCN (M = Cu, Ag, Au; Ng =Xe-Rn) at MPWB95/cc-pVTZ/cc-pVTZ-PP level

1. CuXeCN geometry

C	0.00000000	0.00000000	2.94601700
N	0.00000000	0.00000000	4.11851700
Xe	0.00000000	0.00000000	0.31076900
Cu	0.00000000	0.00000000	-2.18231900

2. CuRnCN geometry

C	0.00000000	0.00000000	2.89304200
N	0.00000000	0.00000000	4.06485700
Rn	0.00000000	0.00000000	0.24977200
Cu	0.00000000	0.00000000	-2.32043700

3. AgXeCN geometry

C	0.00000000	0.00000000	3.41304600
N	0.00000000	0.00000000	4.58575200
Xe	0.00000000	0.00000000	0.75698400
Ag	0.00000000	0.00000000	-1.98841800

4. AgRnCN geometry

C	0.00000000	0.00000000	3.26244400
N	0.00000000	0.00000000	4.43426300
Rn	0.00000000	0.00000000	0.60875100
Ag	0.00000000	0.00000000	-2.19078900

5. AuXeCN geometry

C	0.00000000	0.00000000	-3.62642100
N	0.00000000	0.00000000	-4.79703300
Xe	0.00000000	0.00000000	-1.15860800
Au	0.00000000	0.00000000	1.49243800

6. AuRnCN geometry

C	0.00000000	0.00000000	3.47342900
N	0.00000000	0.00000000	4.64338100
Rn	0.00000000	0.00000000	0.98057600
Au	0.00000000	0.00000000	-1.74270600

Cartesian coordinates for the optimized geometries of MNgNC (M = Cu, Ag, Au; Ng =Xe-Rn) at MPWB95/cc-pVTZ/cc-pVTZ-PP level

1. CuXeNC geometry

Cu	0.00000000	0.00000000	-2.16011900
Xe	0.00000000	0.00000000	0.32118700
N	0.00000000	0.00000000	2.93912300
C	0.00000000	0.00000000	4.12091700

2. CuRnNC geometry

Cu	0.00000000	0.00000000	-2.29558600
Rn	0.00000000	0.00000000	0.25896400
N	0.00000000	0.00000000	2.86208100
C	0.00000000	0.00000000	4.04441900

3. AgXeNC geometry

Ag	0.00000000	0.00000000	-1.97701900
Xe	0.00000000	0.00000000	0.76474700
N	0.00000000	0.00000000	3.42579600
C	0.00000000	0.00000000	4.60716500

4. AgRnNC geometry

C	0.00000000	0.00000000	4.42737200

N	0.00000000	0.00000000	3.24546500
Ag	0.00000000	0.00000000	-2.17577200
Rn	0.00000000	0.00000000	0.61603300

5. AuXeNC geometry

Au	0.00000000	0.00000000	1.48283100
Xe	0.00000000	0.00000000	-1.16014300
N	0.00000000	0.00000000	-3.64587600
C	0.00000000	0.00000000	-4.82912700

6. AuRnNC geometry

C	0.00000000	0.00000000	4.65112800
N	0.00000000	0.00000000	3.46769000
Au	0.00000000	0.00000000	-1.72877900
Rn	0.00000000	0.00000000	0.98131300

Cartesian coordinates for the optimized geometries of NgMCN (M = Cu, Ag, Au; Ng =Xe-Rn) at MPWB95/cc-pVTZ/cc-pVTZ-PP level

1. XeCuCN geometry

C	0.00000000	0.00000000	-2.91474600
N	0.00000000	0.00000000	-4.08446400
Xe	0.00000000	0.00000000	1.44013800
Cu	0.00000000	0.00000000	-1.09268000

2. RnCuCN geometry

C	0.00000000	0.00000000	2.89433300
N	0.00000000	0.00000000	4.06612700
Cu	0.00000000	0.00000000	-2.32056500
Rn	0.00000000	0.00000000	0.24962200

3. XeAgCN geometry

C	0.00000000	0.00000000	-3.00713300
N	0.00000000	0.00000000	-4.17521700
Xe	0.00000000	0.00000000	1.74988900
Ag	0.00000000	0.00000000	-1.00478100

4. RnAgCN geometry

C	0.00000000	0.00000000	3.26320700
N	0.00000000	0.00000000	4.43506600
Ag	0.00000000	0.00000000	-2.19087500
Rn	0.00000000	0.00000000	0.60867900

5. XeAuCN geometry

C	0.00000000	0.00000000	2.71126500
N	0.00000000	0.00000000	3.87952100
Xe	0.00000000	0.00000000	-1.93916100
Au	0.00000000	0.00000000	0.77582800

6. RnAuCN geometry

C	0.00000000	0.00000000	3.47295900
N	0.00000000	0.00000000	4.64294100
Au	0.00000000	0.00000000	-1.74217800
Rn	0.00000000	0.00000000	0.98016000

Cartesian coordinates for the optimized geometries of transition states (TSs) for MNgCN → NgMNC (TS1) and MNgCN → NgMCN (TS2 and TS3) (M = Cu, Ag, Au; Ng = Xe- Rn) isomerization process at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level

1. CuXeCN → XeCuNC TS1 geometry

Cu	-1.72940300	0.69734200	0.00008000
Xe	0.31583400	-0.73335200	-0.00005900
C	2.84312600	0.93034500	0.00090500
N	2.29127100	1.97085900	-0.00065200

2. CuXeCN → CuXeNC TS2 geometry

Cu	-0.03730500	-2.10042700	0.00000000
Xe	0.00000000	0.37015200	0.00000000
C	0.71511200	3.23617800	0.00000000
N	-0.45840300	3.07244300	0.00000000

3. CuXeNC → XeCuCN TS3 geometry

Cu	-1.76144600	0.71026000	0.00001500
Xe	0.29051200	-0.71067700	-0.00001000
C	2.58122300	1.98668300	0.00002300
N	2.84385100	0.83698900	-0.00000600

1. CuRnCN → RnCuNC TS1 geometry

Cu	1.91286500	0.70632000	0.00005700
Rn	-0.32385500	-0.54808000	-0.00002100
C	-2.51785400	1.55223300	-0.00001000
N	-1.78777600	2.47688400	0.00003000

2. CuRnCN → CuRnNC TS2 geometry

Cu	-0.07862900	-2.24666000	0.00000000
C	0.80705400	3.15907800	0.00000000
N	-0.36601200	2.97951400	0.00000000
Rn	0.00000000	0.29467500	0.00000000

3. CuRnNC → RnCuCN TS3 geometry

Cu	-1.91697200	0.77888300	0.00002200
C	2.18925100	2.43294300	0.00002000
N	2.61542300	1.33294400	0.00000600
Rn	0.28079900	-0.54088200	-0.00000900

1. AgXeCN → XeAgNC TS1 geometry

Ag	1.70714300	0.35056100	0.00001200
Xe	-0.84586200	-0.75643500	-0.00001100
C	-3.02354500	1.35630100	-0.00000500
N	-2.34541300	2.31904400	0.00000800

2. AgXeCN → AgXeNC TS2 geometry

Ag	-0.01810100	-1.92643100	0.00000000
Xe	0.00000000	0.80367300	0.00000000
C	0.69595500	3.72067300	0.00000000
N	-0.47499600	3.54570100	0.00000000

3. AgXeNC → XeAgCN TS3 geometry

Ag	-1.73647200	0.39328000	0.00001300
Xe	0.80237100	-0.75814300	-0.00001300
C	2.77046400	2.33764300	0.00001700
N	3.09476600	1.20424300	-0.00000300

1. AgRnCN → RnAgNC TS1 geometry

Ag	1.94996800	0.29098800	0.00001500
C	-2.46974900	1.98021200	-0.00000200
N	-1.61954000	2.79527300	0.00001100
Rn	-0.76154900	-0.52470500	-0.00000900

2. AgRnCN → AgRnNC TS2 geometry

Ag	-0.03533500	-2.13263700	0.00000000
C	0.75788000	3.54277000	0.00000000
N	-0.41236400	3.34820200	0.00000000
Rn	0.00000000	0.64581300	0.00000000

3. AgRnNC → RnAgCN TS3 geometry

Ag	-1.96543600	0.37068100	0.00001600
C	2.05791000	2.79704300	0.00001700
N	2.65354600	1.77905800	0.00000000
Rn	0.71457200	-0.54253100	-0.00001000

1. AuXeCN → XeAuNC TS1 geometry

Au	-1.28597900	0.16806000	-0.00001000
Xe	1.26782900	-0.76804800	0.00001400
C	3.03533100	1.76287500	0.00000700
N	2.13108200	2.51722300	-0.00000600

2. AuXeCN → AuXeNC TS2 geometry

Au	-0.01446500	-1.44676100	0.00000000
Xe	0.00000000	1.18900500	0.00000000
C	0.72159400	3.94403600	0.00000000

N	-0.45526500	3.77480500	0.00000000

3. AuXeNC → XeAuCN TS3 geometry

Au	-1.30479000	0.20789500	0.00001200
Xe	1.22145200	-0.79733800	-0.00001800
C	2.51656200	2.58519500	0.00000800
N	3.14580900	1.58877200	-0.00000200

1. AuRnCN → RnAuNC TS1 geometry

Au	1.55241300	0.09186600	0.00001300
Rn	-1.15698900	-0.48570200	-0.00001300
C	-2.34250400	2.36169700	-0.00000300
N	-1.29779600	2.90611100	0.00000800

2. AuRnCN → AuRnNC TS2 geometry

Au	-0.02059600	-1.69686400	0.00000000
Rn	0.00000000	1.00440500	0.00000000
C	0.75862600	3.76467200	0.00000000
N	-0.41780600	3.58362900	0.00000000

3. AuRnNC → RnAuCN TS3 geometry

Au	-1.56904400	0.15588300	0.00001700
Rn	1.11337700	-0.53158200	-0.00001600
C	1.72870500	3.02610400	0.00000400
N	2.54739800	2.17780900	0.00000600

Cartesian coordinates for the optimized geometries of transition states (TSs) and intermediates(IMs) for NgCuNC → NgCuCN (TS5 and TS6) and NgMNC → NgMCN (TS4) (M = Ag, Au; Ng = Xe- Rn) isomerization process at the MPW1B95/cc-pVTZ/cc-pVTZ-PP level

1. XeCuNC → XeCuCN TS5 geometry

Cu	1.12812300	-0.14854100	0.00000700
Xe	-1.35843900	0.04131500	-0.00000500
C	3.33203700	0.76925500	-0.00001100
N	2.94970000	-0.36269300	0.00001900

2. XeCuNC → XeCuCN TS6 geometry

Cu	1.15017400	-0.14460200	0.00009600
Xe	-1.35814900	0.03516300	-0.00005500
C	3.02744400	-0.46255800	0.00003200
N	3.11719400	0.72429000	-0.00000100

3. IM geometry

Cu	-1.15694900	-0.02750400	0.00000200
Xe	1.35578900	0.00622600	-0.00000300
C	-3.05489200	-0.60844600	-0.00000900
N	-3.04738900	0.58743800	0.00002300

1. RnCuNC → RnCuCN TS5 geometry

Cu	-0.11462000	-1.53019500	0.00000000
C	0.87100000	-3.70770200	0.00000000
N	-0.27171700	-3.35875600	0.00000000
Rn	0.00000000	1.04806000	0.00000000

2. RnCuNC → RnCuCN TS6 geometry

Cu	-0.11563400	-1.55303600	0.00000000
Rn	0.00000000	1.04854600	0.00000000
C	-0.38198300	-3.43761900	0.00000000
N	0.80646800	-3.50160300	0.00000000

3. IM geometry

Cu	-1.55517000	-0.02712900	0.00000300
C	-3.45344400	-0.60855100	-0.00000700
N	-3.44684800	0.58745100	0.00002500
Rn	1.04591300	0.00379000	-0.00000300

1. XeAgNC → XeAgCN TS4 geometry

Ag	1.03439800	-0.11270400	-0.00038100
Xe	-1.68731100	0.04990400	0.00014300
C	3.49609900	0.80078100	0.00011900
N	3.07449800	-0.31463100	0.00135100

2. RnAgNC → RnAgCN TS4 geometry

Ag	-1.44798700	-0.11829900	-0.00238000

C	-3.90575400	0.81685400	0.00068500
N	-3.49171800	-0.30117800	0.00859400
Rn	1.34804600	0.03217700	0.00055300

1. XeAuNC → XeAuCN TS4 geometry

Au	0.78678400	-0.06442900	-0.00039500
Xe	-1.85712100	0.04587700	0.00025400
C	3.06670100	0.83380000	0.00047300
N	2.81833400	-0.34147200	0.00209600

2. RnAuNC → RnAuCN TS4 geometry

Rn	1.56368700	0.02932800	0.00001100
Au	-1.15790700	-0.06676600	-0.00002700
N	-3.19273600	-0.33050900	0.00014700
C	-3.44220600	0.84431900	0.00003300