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Electronic Supplementary Information

Prediction of Neutral Noble Gas Insertion Compounds with Heavier Pnictides: FNgY (Ng = Kr and Xe; Y = As, Sb and Bi)

Ayan Ghosh, Debashree Manna, and Tapan K. Ghanty

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Table S1. Optimized Structural Parameters (Bond Length, R In Å, Bond Angle, θ in Degree) for Minima (Min) of ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Compounds by B3LYP, MP2, CCSD(T) and MRCI Based Methods with B1, B2, and B3 Basis sets.

Bond	Methods	FKrAs	FKrSb	FKrBi	FXeAs	FXeSb	FXeBi
R(F-Ng)	B3LYP/B1	2.144	2.184	…[a]	2.198	2.227	…[a]
	B3LYP/B2	2.150	2.196	2.220	2.197	2.229	2.244
	MP2/B1	2.078	2.117	…[a]	2.152	2.176	…[a]
	MP2/B2	2.085	2.130	2.158	2.158	2.186	2.212
	CCSD(T)/B1	2.119	2.152	2.177	2.165	2.190	2.217
	CCSD(T)/B3	2.132	2.162	2.181	2.193	2.218	2.229
	MRCI/B3	2.054	2.094	2.113	2.165	2.180	2.192
R(Ng-Y)	B3LYP/B1	2.545	2.749	…[a]	2.701	2.907	…[a]
	B3LYP/B2	2.550	2.755	2.839	2.698	2.907	2.978
	MP2/B1	2.490	2.683	…[a]	2.656	2.859	…[a]
	MP2/B2	2.489	2.683	2.766	2.650	2.857	2.939
	CCSD(T)/B1	2.597	2.788	2.882	2.698	2.903	2.994
	CCSD(T)/B3	2.627	2.768	2.860	2.752	2.922	3.001
	MRCI/B3	2.563	2.680	2.741	2.772	2.945	3.021
θ(F-Ng-Y)	B3LYP/B1	180.0	180.0	…[a]	180.0	180.0	…[a]
	B3LYP/B2	180.0	180.0	180.0	180.0	180.0	180.0
	MP2/B1	180.0	180.0	…[a]	180.0	180.0	…[a]
	MP2/B2	180.0	180.0	180.0	180.0	180.0	180.0
	CCSD(T)/B1	180.0	180.0	180.0	180.0	180.0	180.0
	CCSD(T)/B3	180.0	180.0	180.0	180.0	180.0	180.0
	MRCI/B3	180.0	180.0	180.0	180.0	180.0	180.0

[a]Calculations for Bi-containing species could not be performed using B1 basis sets (aug-cc-pVTZ-PP) in the GAMESS software where ECP integrals are limited up to core potentials corresponding to the *g* angular momentum.

Table S2. Optimized Structural Parameters (Bond Length, R In Å, Bond Angle, θ in Degree) for Transition States (TS) of ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Compounds by B3LYP, MP2, CCSD(T) and MRCI Based Methods with B1, B2, and B3 Basis sets.

Bond	Methods	FKrAs	FKrSb	FKrBi	FXeAs	FXeSb	FXeBi
R(F-Rg)	B3LYP/B1	2.448	2.459	…[a]	2.442	2.477	…[a]
	B3LYP/B2	2.464	2.478	2.485	2.450	2.477	2.494
	MP2/B1	2.358	2.378	…[a]	2.403	2.432	…[a]
	MP2/B2	2.372	2.397	2.414	2.421	2.453	2.473
	CCSD(T)/B1	2.359	2.383	2.402	2.396	2.428	2.449
	CCSD(T)/B3	2.374	2.390	2.405	2.429	2.452	2.467
	MRCI/B3	2.377	2.391	2.400	2.442	2.462	2.476
R(Ng-Y)	B3LYP/B1	2.486	2.700	…[a]	2.598	2.819	…[a]
	B3LYP/B2	2.490	2.706	2.797	2.596	2.813	2.904
	MP2/B1	2.394	2.612	…[a]	2.552	2.768	…[a]
	MP2/B2	2.398	2.617	2.716	2.545	2.768	2.865
	CCSD(T)/B1	2.416	2.636	2.747	2.563	2.781	2.880
	CCSD(T)/B3	2.462	2.654	2.742	2.618	2.808	2.894
	MRCI/B3	2.454	2.645	2.721	2.623	2.813	2.893
θ(F-Ng-Y)	B3LYP/B1	100.8	104.8	…[a]	94.4	96.9	…[a]
	B3LYP/B2	100.9	105.2	107.6	94.0	97.1	98.4
	MP2/B1	107.5	111.6	…[a]	101.0	103.5	…[a]
	MP2/B2	108.1	112.2	114.9	101.3	103.7	105.3
	CCSD(T)/B1	103.8	107.5	109.0	99.4	101.5	102.7
	CCSD(T)/B3	105.4	109.0	110.0	101.3	103.2	103.6
	MRCI/B3	108.5	112.5	115.4	102.3	104.5	105.7

[a]Calculations for Bi-containing species could not be performed using B1 basis sets (aug-cc-pVTZ-PP) in the GAMESS software where ECP integrals are limited up to core potentials corresponding to the *g* angular momentum.

Table S3. Harmonic Vibrational Frequencies (in cm^{-1}) Calculated Using B3LYP, MP2 and CCSD(T) Based Methods Using B1 and B2 Basis sets for ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Compounds. Corresponding IR Intensity Values are Given within the Parentheses (in km mol^{-1}).

Species	State	Normal Modes	B3LYP/B1	B3LYP/B2	MP2/B1	MP2/B2	CCSD(T) /B1
FKrAs	Min	F-Ng Str.	378.2 (199.2)	374.8 (196.2)	417.5 (425.9)	408.9 (428.7)	398.3
		Ng-Y Str.	185.1 (4.9)	183.1 (4.7)	207.2 (2.0)	207.9 (1.8)	134.7
		F-Ng-Y Bend[a]	101.5 (8.1)	105.8 (8.3)	119.2 (9.0)	121.6 (9.4)	106.7
	TS	F-Ng Str.	247.8 (20.7)	243.0 (19.4)	316.7 (95.3)	312.2 (88.1)	311.6
		Ng-Y Str.	177.2 (2.1)	172.9 (1.8)	241.3 (84.4)	239.5 (91.6)	230.4
		F-Ng-Y Bend	-89.6 (6.4)	-87.4 (5.8)	-115.0 (10.4)	-114.3 (10.6)	-126.6
FKrSb	Min	F-Ng Str.	354.7 (198.6)	349.5 (193.5)	384.8 (513.6)	372.8 (521.7)	376.7
		Ng-Y Str.	151.6 (5.6)	148.9 (5.3)	175.9 (0.01)	174.3 (0.005)	118.9
		F-Ng-Y Bend[a]	87.0 (8.6)	91.1 (8.6)	103.3 (10.0)	103.8 (10.2)	94.6
	TS	F-Ng Str.	236.3 (17.4)	229.5 ()	299.6 (122.2)	292.2 (118.4)	296.4
		Ng-Y Str.	148.3 (1.7)	143.9 ()	196.7 (57.5)	192.3 (58.4)	185.8
		F-Ng-Y Bend	-86.3 (10.7)	-79.6 ()	-102.3 (11.1)	-101.0 (11.4)	-112.8
FKrBi	Min	F-Ng Str.	…[b]	337.1 (187.0)	…[b]	355.4 (565.3)	364.8
		Ng-Y Str.	…[b]	130.8 (4.7)	…[b]	156.9 (0.7)	108.4
		F-Ng-Y Bend[a]	…[b]	84.6 (8.7)	…[b]	94.7 (10.5)	87.7
	TS	F-Ng Str.	…[b]	221.2 (13.1)	…[b]	282.3 (129.0)	285.0
		Ng-Y Str.	…[b]	128.2 (0.6)	…[b]	168.1 (45.9)	162.0
		F-Ng-Y Bend	…[b]	-78.4 (12.9)	…[b]	-92.3 (12.4)	-106.3
FXeAs	Min	F-Ng Str.	380.3 (222.3)	377.2 (220.4)	424.4 (320.1)	410.9 (318.1)	407.2
		Ng-Y Str.	173.4 (1.1)	174.0 (1.2)	197.2 (0.03)	197.6 (0.01)	173.8
		F-Ng-Y Bend[a]	95.7 (8.3)	105.6 (8.5)	110.7 (9.0)	111.5 (9.5)	105.1
	TS	F-Ng Str.	261.4 (53.8)	256.3 (45.1)	303.9 (151.0)	298.7 (137.9)	304.1
		Ng-Y Str.	197.7 (8.6)	195.6 (7.4)	225.7 (55.8)	228.1 (59.9)	221.9
		F-Ng-Y Bend	-85.8 (4.2)	-90.9 (4.0)	-111.2 (8.3)	-109.7 (9.0)	-118.2

FXeSb	Min	F-Ng Str.	360.4 (232.1)	355.9 (228.7)	404.6 (380.8)	389.3 (382.3)	407.2
		Ng-Y Str.	138.8 (1.5)	138.0 (1.5)	160.7 (0.1)	159.8 (0.1)	173.8
		F-Ng-Y Bend[a]	84.1 (8.5)	94.5 (8.4)	99.6 (9.3)	99.5 (9.5)	105.1
	TS	F-Ng Str.	248.7 (49.0)	252.5 (53.6)	290.8 (160.6)	283.7 (153.6)	304.1
		Ng-Y Str.	153.6 (4.2)	154.9 (5.0)	181.1 (36.3)	178.9 (36.8)	221.9
		F-Ng-Y Bend	-85.7 (5.3)	-85.1 (6.0)	-101.5 (8.9)	-100.5 (9.4)	-118.2
FXeBi	Min	F-Ng Str.	…[b]	350.3 (252.2)	…[b]	474.2 (588.9)	465.1
		Ng-Y Str.	…[b]	124.4 (2.1)	…[b]	138.4 (0.02)	122.8
		F-Ng-Y Bend[a]	…[b]	89.8 (8.7)	…[b]	92.1 (9.4)	87.1
	TS	F-Ng Str.	…[b]	243.1 (53.7)	…[b]	275.1 (158.7)	285.3
		Ng-Y Str.	…[b]	131.8 (3.0)	…[b]	150.8 (25.7)	150.6
		F-Ng-Y Bend	…[b]	-80.6 (7.2)	…[b]	-94.5 (10.0)	-99.6

[a]It is doubly degenerate mode for minima energy structure

[b]Calculations for Bi-containing species could not be performed using B1 basis sets (aug-cc-pVTZ-PP) in the GAMESS software where ECP integrals are limited up to core potentials corresponding to the *g* angular momentum.

Table S4. B3LYP and MP2 Calculated Values of the Harmonic Vibrational Frequencies (in cm^{-1}) and Intrinsic Force Constants in the Parentheses (in N m^{-1}) Corresponding to Individual Internal Coordinates in the ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Using B1 and B2 Basis sets.

Internal Coordinates	Methods	FKrAs	FKrSb	FKrBi	FXeAs	FXeSb	FXeBi
F-Ng stretch	B3LYP/B1	368.3 (123.8)	345.9 (109.1)	…[b]	376.8 (138.9)	357.1 (124.7)	…[b]
	B3LYP/B2	364.8 (121.4)	340.6 (105.9)	328.7 (98.6)	373.7 (136.7)	352.5 (121.6)	347.6 (118.2)
	MP2/B1	415.3 (157.4)	382.4 (133.4)	…[b]	423.4 (175.5)	403.7 (159.4)	…[b]
	MP2/B2	406.6 (150.9)	370.3 (125.2)	352.3 (113.3)	409.8 (164.3)	388.4 (147.6)	474.9 (220.6)
Ng-Y stretch	B3LYP/B1	203.9 (97.0)	170.6 (85.0)	…[b]	180.8 (92.0)	147.2 (80.5)	…[b]
	B3LYP/B2	202.3 (95.4)	168.1 (82.5)	150.7 (80.0)	181.4 (92.6)	146.4 (79.7)	131.7 (82.7)
	MP2/B1	211.6 (104.5)	181.1 (95.8)	…[b]	199.3 (111.8)	163.0 (98.7)	…[b]
	MP2/B2	212.4 (105.2)	179.4 (93.9)	163.6 (94.5)	200.0 (112.6)	162.0 (97.6)	135.8 (88.0)
F-Ng-Y bend[a]	B3LYP/B1	101.5	87.0	…[b]	95.7	84.1	…[b]
	B3LYP/B2	105.8	91.1	84.6	105.6	94.5	89.8
	MP2/B1	119.2	103.2	…[b]	110.7	99.6	…[b]
	MP2/B2	121.6	103.8	94.7	111.5	99.5	92.1

[a]It is doubly degenerate mode for minima energy structure

[b]Calculations for Bi-containing species could not be performed using B1 basis sets (aug-cc-pVTZ-PP) in the GAMESS software where ECP integrals are limited up to core potentials corresponding to the *g* angular momentum.

Table S5. Energies (in kJ mol^{-1}) of the Various Dissociated Species Relative to the ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Calculated Using B3LYP, MP2, CCSD(T) and MRCI Based Methods Using B1, B2, B3 and B4[a] Basis sets.

Channels	Channels No.	Methods	FKrAs	FKrSb	FKrBi	FXeAs	FXeSb	FXeBi
^{3}FNgY		All	0.0	0.0	0.0	0.0	0.0	0.0
Ng + ^{3}FY	(1)	B3LYP/B1	–378.7	–363.0	…[b]	–301.7	–293.8	…[b]
		B3LYP/B2	–389.8	–371.7	–343.9	–306.9	–297.9	–278.2
		MP2/B1	–413.7	–393.8	…[b]	–324.2	–311.0	…[b]
		MP2/B2	–429.1	–401.7	–266.9	–338.0	–317.4	–186.9
		CCSD(T)/B1	–403.3	–377.5	–184.9	–319.4	–300.6	–112.3
		CCSD(T)/B3	–441.7	–423.1	–376.9	–367.6	–352.7	–308.7
		CCSD(T)/B4	–406.7	–380.4	–190.6	–320.8	–301.7	–116.4
^{2}FNg + ^{2}Y	(2)	B3LYP/B1	169.0	158.4	…[b]	217.9	199.5	…[b]
		B3LYP/B2	168.8	153.3	73.8	223.5	198.9	111.2
		MP2/B1	190.3	178.5	…[b]	279.5	260.9	…[b]
		MP2/B2	179.5	165.1	164.9	285.8	264.5	260.0
		CCSD(T)/B1	137.8	126.9	126.7	216.0	198.2	193.6
		CCSD(T)/B3	…	…	151.8	…	…	212.4
		CCSD(T)/B4	142.6	131.7	131.2	222.7	204.7	199.8
^{2}FNg + ^{4}Y	(3)	B3LYP/B1	20.3	29.1	…[b]	69.3	70.2	…[b]
		B3LYP/B2	14.7	24.0	30.6	69.3	69.6	68.0
		MP2/B1	–4.9	5.0	…[b]	84.3	87.5	…[b]
		MP2/B2	–19.8	–10.4	–5.2	86.4	89.0	89.9
		CCSD(T)/B1	–14.1	–4.6	1.2	64.2	66.6	68.1
		CCSD(T)/B3	–12.7	4.2	0.02	53.9	67.1	60.6
		CCSD(T)/B4	–6.3	2.9	8.1	73.9	76.0	76.6
^{2}F + ^{2}NgY	(4)	B3LYP/B1	172.2	167.2	…[b]	235.2	227.0	…[b]
		B3LYP/B2	164.5	159.1	159.5	232.8	223.5	217.2

		MP2/B1	173.9	166.9	…[b]	249.3	240.1	…[b]
		MP2/B2	164.6	155.1	155.6	242.6	230.6	227.2
		CCSD(T)/B1	137.4	126.8	126.9	214.0	200.9	197.5
		CCSD(T)/B3	162.4	164.3	152.0	235.6	233.2	219.4
		CCSD(T)/B4	141.2	130.7	130.3	217.5	204.3	200.7
$F^- + {}^3[NgY]^+$	**(5)**	**B3LYP/B1**	548.4	505.9	…[b]	585.2	545.0	…[b]
		B3LYP/B2	547.1	500.4	479.4	587.5	543.2	518.1
		MP2/B1	524.5	474.5	…[b]	569.0	523.5	…[b]
		MP2/B2	513.5	465.7	437.3	570.5	521.7	493.8
		CCSD(T)/B1	540.0	491.1	464.2	582.9	538.7	512.1
		CCSD(T)/B3	518.2	475.8	458.5	556.6	517.9	499.7
		CCSD(T)/B4	541.0	492.0	464.3	586.2	541.4	514.0
$F^- + {}^1[NgY]^+$	**(6)**	**B3LYP/B1**	668.6	608.6	…[b]	703.1	646.4	…[b]
		B3LYP/B2	679.5	616.6	589.9	715.4	656.5	626.4
		MP2/B1	668.3	602.2	…[b]	713.8	654.0	…[b]
		MP2/B2	663.1	594.7	563.2	709.8	647.9	617.5
		CCSD(T)/B1	652.1	586.5	554.6	582.9	634.4	603.1
		CCSD(T)/B3	651.6	593.4	568.4	690.5	636.5	609.6
		CCSD(T)/B4	651.1	585.7	553.5	695.6	635.3	603.6
$^2F + Ng + {}^2Y$	**(7)**	**B3LYP/B1**	185.2	174.6	…[b]	262.2	243.7	…[b]
		B3LYP/B2	183.4	167.9	88.4	266.3	241.7	154.1
		MP2/B1	191.6	179.8	…[b]	281.1	262.5	…[b]
		MP2/B2	180.8	166.4	166.2	271.9	250.6	246.1
		CCSD(T)/B1	139.5	128.6	128.4	223.4	205.5	201.0
		CCSD(T)/B3	…	…	152.4	…	…	220.5
		CCSD(T)/B4	144.4	133.6	133.1	230.3	212.3	207.3
$^2F + Ng + {}^4Y$	**(8)**	**B3LYP/B1**	36.5	45.3	…[b]	113.5	114.5	…[b]
		B3LYP/B2	29.3	38.6	45.2	112.2	112.4	110.9
		MP2/B1	–3.6	6.3	…[b]	85.9	89.1	…[b]
		MP2/B2	–18.5	–9.2	–3.9	72.5	75.1	76.0

		CCSD(T)/B1	–12.4	–2.9	2.9	71.5	73.9	75.4
		CCSD(T)/B3	–12.1	4.8	0.6	62.0	75.2	68.8
		CCSD(T)/B4	–4.4	4.8	9.9	81.4	83.5	84.1
^{3}FNgY [TS]		**B3LYP/B1**	72.3	59.0	…[b]	102.7	85.4	…[b]
		B3LYP/B2	70.1	56.1	50.2	99.3	89.2	78.4
		MP2/B1	83.7	60.7	…[b]	107.7	93.8	…[b]
		MP2/B2	77.0	53.0	47.8	113.2	92.1	81.3
		CCSD(T)/B1	90.4	68.9	59.8	113.5	95.8	86.7
		CCSD(T)/B3	83.8	62.6	57.1	108.2	90.6	83.5
		CCSD(T)/B4	88.7	67.2	58.0	113.3	95.3	85.8
		MRCI/B3	78.8	55.1	48.9	112.6	91.9	82.9

[a]aug–cc–pVQZ–PP (B4) Basis sets calculations are the single point energy calculations based on the optimized minima and transitions state structures as obtained by aug–cc–pVTZ–PP (B1)

[b]Calculations for Bi-containing species could not be performed using B1 basis sets (aug-cc-pVTZ-PP) in the GAMESS software where ECP integrals are limited up to core potentials corresponding to the *g* angular momentum.

Table S6. B3LYP and MP2 Calculated Values of the Mulliken Atomic Charges (in au) in ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Using B1 and B2 Basis sets.

Species	Methods	*q*(F)		*q*(Ng)		*q*(Y)	
		Minima	TS	Minima	TS	Minima	TS
FKrAs	B3LYP/B1	-0.645	-0.621	0.354	0.230	0.291	0.391
	B3LYP/B2	-0.645	-0.600	0.479	0.313	0.166	0.287
	MP2/B1	-0.668	-0.874	0.448	0.331	0.220	0.543
	MP2/B2	-0.660	-0.863	0.606	0.432	0.054	0.431
FKrSb	B3LYP/B1	-0.654	-0.651	0.252	0.135	0.402	0.516
	B3LYP/B2	-0.672	-0.633	0.395	0.273	0.277	0.360
	MP2/B1	-0.698	-0.881	0.313	0.178	0.385	0.703
	MP2/B2	-0.709	-0.878	0.509	0.362	0.200	0.517
FKrBi	B3LYP/B1	…[a]	…[a]	…[a]	…[a]	…[a]	…[a]
	B3LYP/B2	-0.677	-0.644	0.353	0.234	0.324	0.410
	MP2/B1	…[a]	…[a]	…[a]	…[a]	…[a]	…[a]
	MP2/B2	-0.727	-0.884	0.437	0.303	0.290	0.581
FXeAs	B3LYP/B1	-0.673	-0.686	0.626	0.483	0.047	0.203
	B3LYP/B2	-0.631	-0.645	0.579	0.467	0.052	0.178
	MP2/B1	-0.702	-0.830	0.653	0.485	0.049	0.345
	MP2/B2	-0.649	-0.816	0.666	0.554	-0.016	0.262
FXeSb	B3LYP/B1	-0.674	-0.690	0.446	0.303	0.228	0.387
	B3LYP/B2	-0.650	-0.677	0.516	0.400	0.133	0.277
	MP2/B1	-0.710	-0.846	0.485	0.277	0.225	0.569
	MP2/B2	-0.671	-0.836	0.623	0.464	0.049	0.371
FXeBi	B3LYP/B1	…[a]	…[a]	…[a]	…[a]	…[a]	…[a]
	B3LYP/B2	-0.663	-0.683	0.470	0.343	0.193	0.340
	MP2/B1	…[a]	…[a]	…[a]	…[a]	…[a]	…[a]
	MP2/B2	-0.687	-0.844	0.544	0.386	0.142	0.457

[a]Calculations for Bi-containing species could not be performed using B1 basis sets (aug-cc-pVTZ-PP) in the GAMESS software where ECP integrals are limited up to core potentials corresponding to the *g* angular momentum.

Table S7. MP2 (B3LYP) Calculated Values (in au) of the BCP Properties of the F–Ng and Ng–Y Bonds in ^{3}FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Compounds with B1 Basis Sets for FNgAs and FNgSb Molecules and B2 Basis Sets for FNgBi Molecules.

F−Ng Bond				
Complexes	**$\rho(r)$**	**$\nabla^2\rho(r)$**	**$E_d(r)$**	**$G(r)/\rho(r)$**
F−Kr−As	0.092 (0.077)	0.271 (0.259)	–0.022 (–0.009)	0.975 (0.954)
F−Kr−Sb	0.084 (0.071)	0.267 (0.248)	–0.016 (–0.006)	0.989 (0.958)
F−Kr−Bi	0.077 (0.065)	0.240 (0.222)	–0.014 (–0.007)	0.961 0.937
F−Xe−As	0.086 (0.082)	0.231 (0.219)	–0.026 (–0.019)	0.968 (0.900)
F−Xe−Sb	0.087 (0.077)	0.217 (0.215)	–0.026 (–0.016)	0.926 (0.895)
F−Xe−Bi	0.079 (0.074)	0.200 (0.198)	–0.021 (–0.015)	0.897 (0.876)
Ng−Y Bond				
Complexes	**$\rho(r)$**	**$\nabla^2\rho(r)$**	**$E_d(r)$**	**$G(r)/\rho(r)$**
F−Kr−As	0.075 (0.067)	0.014 (0.033)	–0.028 (–0.019)	0.415 (0.410)
F−Kr−Sb	0.060 (0.053)	0.039 (0.043)	–0.019 (–0.013)	0.476 (0.447)
F−Kr−Bi	0.055 (0.047)	0.066 (0.063)	–0.013 (–0.008)	0.537 (0.507)
F−Xe−As	0.079 (0.065)	-0.017 (0.017)	–0.031 (–0.018)	0.337 (0.339)
F−Xe−Sb	0.058 (0.052)	0.013 (0.023)	–0.018 (–0.013)	0.362 (0.353)
F−Xe−Bi	0.052 (0.048)	0.037 (0.041)	–0.012 (–0.009)	0.417 (0.406)

Table S8. Various Topological Properties at the Local Electron Energy Density Critical Points [(3,+1) HCP] for the FNgY (Ng = Kr and Xe; Y = As, Sb and Bi) Ions Calculated Using the B3LYP and MP2 Methods with B1 Basis Sets for FNgAs and FNgSb Molecules and B2 Basis Sets for FNgBi Molecules.

F−Ng Bond							
Molecules	**Methods**	R_{F-Ng}[a]	R(F)[b]	R(Ng)[b]	$E_{d\,(HCP)}$[c]	$\rho_{(HCP)}$[d]	$-E_{d\,(HCP)}/\rho_{(HCP)}$
F−Kr−As	B3LYP	2.144	0.992	1.152	–0.009	0.078	0.116
	MP2	2.078	0.964	1.114	–0.022	0.092	0.233
F−Kr−Sb	B3LYP	2.184	1.007	1.177	–0.005	0.071	0.077
	MP2	2.117	0.981	1.136	–0.016	0.084	0.188
F−Kr−Bi	B3LYP	2.220	0.979	1.241	–0.005	0.067	0.077
	MP2	2.158	0.949	1.209	–0.012	0.080	0.157
F−Xe−As	B3LYP	2.198	0.985	1.213	–0.018	0.083	0.215
	MP2	2.167	0.985	1.182	–0.025	0.087	0.281
F−Xe−Sb	B3LYP	2.227	0.993	1.234	–0.014	0.078	0.185
	MP2	2.176	0.982	1.194	–0.025	0.088	0.280
F−Xe−Bi	B3LYP	2.244	0.917	1.327	–0.012	0.083	0.143
	MP2	2.212	0.927	1.285	–0.018	0.086	0.208
Ng−Y Bond							
Molecules	**Methods**	R_{Ng-Y}[a]	R(Ng)[b]	R(Y)[b]	$E_{d\,(HCP)}$[c]	$\rho_{(HCP)}$[d]	$-E_{d\,(HCP)}/\rho_{(HCP)}$
F−Kr−As	B3LYP	2.545	1.275	1.270	–0.017	0.069	0.251
	MP2	2.490	1.256	1.234	–0.025	0.077	0.327
F−Kr−Sb	B3LYP	2.749	1.346	1.403	–0.012	0.055	0.218
	MP2	2.683	1.346	1.338	–0.018	0.062	0.293
F−Kr−Bi	B3LYP	2.839	1.401	1.438	–0.008	0.048	0.167
	MP2	2.766	1.411	1.355	–0.013	0.055	0.232
F−Xe−As	B3LYP	2.701	1.402	1.299	–0.017	0.065	0.263
	MP2	2.597	1.367	1.230	–0.030	0.080	0.376
F−Xe−Sb	B3LYP	2.907	1.475	1.432	–0.012	0.053	0.230
	MP2	2.859	1.471	1.388	–0.017	0.058	0.295
F−Xe−Bi	B3LYP	2.978	1.511	1.467	–0.009	0.048	0.187
	MP2	2.939	1.514	1.425	–0.012	0.052	0.235

[a]Calculated optimized bond length (Å) with aug-cc-pVTZ-PP basis set.

[b]Distance (Å) of the HCP from the atom in parentheses.

[c]Energy density (hartree a_0^{-3}) at the HCP.

[d]Electron density (e a_0^{-3}) at the HCP.