Supplementary Information for "Theoretical Prediction of New Noble-Gas Molecules FNgBNR (Ng = Ar, Kr, and Xe; R = H, CH_3,CCH, $CHCH_2$, F, and OH)"

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Table S1 The calculated geometries (in Å) of FArBNR at various methods.

	F–Ar	Ar–B	B–N	N–R
		FArBNH		
MP2/aug-cc-pVDZ	2.041	1.794	1.244	1.004
MP2/aug-cc-pVTZ	2.009	1.775	1.236	0.995
B3LYP/aug-cc-pVDZ	2.024	1.831	1.229	1.000
B3LYP/aug-cc-pVTZ	2.018	1.816	1.225	0.994
MPW1PW91/aug-cc-pVDZ	2.000	1.807	1.228	0.998
MPW1PW91/aug-cc-pVTZ	1.991	1.796	1.223	0.992
CCSD(T)/aug-cc-pVTZ	2.019	1.791	1.234	0.996
		$FArBNCH_3$		
MP2/aug-cc-pVDZ	2.058	1.790	1.246	1.431
MP2/aug-cc-pVTZ	2.024	1.773	1.239	1.419
B3LYP/aug-cc-pVDZ	2.039	1.829	1.229	1.421
B3LYP/aug-cc-pVTZ	2.032	1.815	1.225	1.415
MPW1PW91/aug-cc-pVDZ	2.014	1.805	1.228	1.412
MPW1PW91/aug-cc-pVTZ	2.004	1.796	1.224	1.407
		FArBNCCH		
MP2/aug-cc-pVDZ	2.023	1.800	1.254	1.320
MP2/aug-cc-pVTZ	1.991	1.780	1.247	1.308
B3LYP/aug-cc-pVDZ	2.012	1.833	1.242	1.306
B3LYP/aug-cc-pVTZ	2.006	1.817	1.237	1.300
MPW1PW91/aug-cc-pVDZ	1.987	1.808	1.240	1.303
MPW1PW91/aug-cc-pVTZ	1.977	1.797	1.236	1.297
		$FArBNCHCH_2$		
MP2/aug-cc-pVDZ	2.046	1.792	1.251	1.388
MP2/aug-cc-pVTZ	2.014	1.774	1.244	1.376
B3LYP/aug-cc-pVDZ	2.029	1.830	1.235	1.377
B3LYP/aug-cc-pVTZ	2.022	1.816	1.231	1.370
MPW1PW91/aug-cc-pVDZ	2.004	1.806	1.234	1.371
MPW1PW91/aug-cc-pVTZ	1.995	1.796	1.230	1.365
		FArBNF		
MP2/aug-cc-pVDZ	2.021	1.806	1.239	1.312
MP2/aug-cc-pVTZ	1.992	1.785	1.230	1.299
B3LYP/aug-cc-pVDZ	2.014	1.843	1.225	1.307
B3LYP/aug-cc-pVTZ	2.007	1.827	1.219	1.303
MPW1PW91/aug-cc-pVDZ	1.989	1.816	1.222	1.294

MPW1PW91/aug-cc-pVTZ	1.982	1.805	1.217	1.290
		FArBNOH		
MP2/aug-cc-pVDZ	2.044	1.797	1.242	1.336
MP2/aug-cc-pVTZ	2.068	1.808	1.242	1.336
B3LYP/aug-cc-pVDZ	2.030	1.836	1.227	1.331
B3LYP/aug-cc-pVTZ	2.024	1.820	1.222	1.328
MPW1PW91/aug-cc-pVDZ	2.006	1.811	1.225	1.319
MPW1PW91/aug-cc-pVTZ	1.998	1.800	1.220	1.316

Table S2 The calculated geometries (in Å) of FKrBNR at various methods.

	F–Kr	Kr–B	B–N	N–R
		FKrBNH		
MP2/aug-cc-pVDZ	2.082	1.961	1.248	1.003
MP2/aug-cc-pVTZ	2.059	1.937	1.240	0.995
B3LYP/aug-cc-pVDZ	2.084	1.995	1.233	1.000
B3LYP/aug-cc-pVTZ	2.075	1.983	1.228	0.993
MPW1PW91/aug-cc-pVDZ	2.058	1.971	1.231	0.997
MPW1PW91/aug-cc-pVTZ	2.047	1.964	1.227	0.992
CCSD(T)/aug-cc-pVTZ	2.064	1.953	1.238	0.995
		$FKrBNCH_3$		
MP2/aug-cc-pVDZ	2.097	1.958	1.250	1.430
MP2/aug-cc-pVTZ	2.073	1.934	1.242	1.417
B3LYP/aug-cc-pVDZ	2.095	1.993	1.233	1.420
B3LYP/aug-cc-pVTZ	2.087	1.982	1.228	1.414
MPW1PW91/aug-cc-pVDZ	2.070	1.970	1.231	1.411
MPW1PW91/aug-cc-pVTZ	2.059	1.962	1.227	1.406
		FKrBNCCH		
MP2/aug-cc-pVDZ	2.068	1.966	1.258	1.319
MP2/aug-cc-pVTZ	2.045	1.940	1.250	1.307
B3LYP/aug-cc-pVDZ	2.071	1.995	1.245	1.306
B3LYP/aug-cc-pVTZ	2.062	1.983	1.241	1.299
MPW1PW91/aug-cc-pVDZ	2.045	1.972	1.244	1.302
MPW1PW91/aug-cc-pVTZ	2.033	1.964	1.239	1.296
		$FKrBNCHCH_2$		
MP2/aug-cc-pVDZ	2.086	1.960	1.255	1.386
MP2/aug-cc-pVTZ	2.063	1.935	1.247	1.373
B3LYP/aug-cc-pVDZ	2.086	1.994	1.239	1.375
B3LYP/aug-cc-pVTZ	2.078	1.982	1.234	1.368
MPW1PW91/aug-cc-pVDZ	2.059	1.970	1.237	1.369
MPW1PW91/aug-cc-pVTZ	2.050	1.962	1.233	1.363
		FKrBNF		
MP2/aug-cc-pVDZ	2.066	1.971	1.243	1.315
MP2/aug-cc-pVTZ	2.045	1.945	1.234	1.302
B3LYP/aug-cc-pVDZ	2.073	2.002	1.228	1.310
B3LYP/aug-cc-pVTZ	2.064	1.990	1.222	1.306
MPW1PW91/aug-cc-pVDZ	2.048	1.978	1.226	1.297

MPW1PW91/aug-cc-pVTZ	2.037	1.970	1.220	1.293
		FKrBNOH		
MP2/aug-cc-pVDZ	2.085	1.963	1.247	1.339
MP2/aug-cc-pVTZ	2.063	1.938	1.238	1.328
B3LYP/aug-cc-pVDZ	2.088	1.998	1.230	1.333
B3LYP/aug-cc-pVTZ	2.079	1.985	1.225	1.330
MPW1PW91/aug-cc-pVDZ	2.062	1.973	1.229	1.321
MPW1PW91/aug-cc-pVTZ	2.052	1.965	1.224	1.318

Table S3 The calculated geometries (in Å) of FXeBNR at various methods.

	F–Xe	Xe–B	B–N	N–R
		FXeBNH		
MP2/aug-cc-pVDZ	2.153	2.154	1.253	1.003
MP2/aug-cc-pVTZ	2.129	2.131	1.244	0.994
B3LYP/aug-cc-pVDZ	2.161	2.187	1.237	0.999
B3LYP/aug-cc-pVTZ	2.145	2.179	1.232	0.993
MPW1PW91/aug-cc-pVDZ	2.137	2.165	1.235	0.997
MPW1PW91/aug-cc-pVTZ	2.118	2.161	1.231	0.991
CCSD(T)/aug-cc-pVTZ	2.128	2.148	1.242	0.994
		$FXeBNCH_3$		
MP2/aug-cc-pVDZ	2.163	2.150	1.255	1.428
MP2/aug-cc-pVTZ	2.139	2.128	1.246	1.416
B3LYP/aug-cc-pVDZ	2.171	2.184	1.236	1.418
B3LYP/aug-cc-pVTZ	2.154	2.177	1.232	1.412
MPW1PW91/aug-cc-pVDZ	2.145	2.163	1.235	1.410
MPW1PW91/aug-cc-pVTZ	2.126	2.159	1.231	1.404
		FXeBNCCH		
MP2/aug-cc-pVDZ	2.142	2.152	1.263	1.317
MP2/aug-cc-pVTZ	2.118	2.129	1.254	1.305
B3LYP/aug-cc-pVDZ	2.149	2.185	1.250	1.304
B3LYP/aug-cc-pVTZ	2.132	2.178	1.245	1.298
MPW1PW91/aug-cc-pVDZ	2.124	2.163	1.248	1.301
MPW1PW91/aug-cc-pVTZ	2.105	2.159	1.244	1.295
		$FXeBNCHCH_2$		
MP2/aug-cc-pVDZ	2.155	2.150	1.260	1.383
MP2/aug-cc-pVTZ	2.131	2.128	1.251	1.371
B3LYP/aug-cc-pVDZ	2.162	2.184	1.243	1.373
B3LYP/aug-cc-pVTZ	2.146	2.177	1.238	1.366
MPW1PW91/aug-cc-pVDZ	2.137	2.163	1.242	1.367
MPW1PW91/aug-cc-pVTZ	2.118	2.159	1.237	1.361
		FXeBNF		
MP2/aug-cc-pVDZ	2.142	2.158	1.248	1.318
MP2/aug-cc-pVTZ	2.118	2.135	1.238	1.304
B3LYP/aug-cc-pVDZ	2.151	2.192	1.232	1.313
B3LYP/aug-cc-pVTZ	2.134	2.184	1.227	1.308
MPW1PW91/aug-cc-pVDZ	2.126	2.169	1.230	1.300

MPW1PW91/aug-cc-pVTZ	2.108	2.165	1.225	1.295
		FXeBNOH		
MP2/aug-cc-pVDZ	2.155	2.153	1.251	1.342
MP2/aug-cc-pVTZ	2.130	2.130	1.242	1.331
B3LYP/aug-cc-pVDZ	2.164	2.187	1.235	1.336
B3LYP/aug-cc-pVTZ	2.148	2.178	1.230	1.332
MPW1PW91/aug-cc-pVDZ	2.139	2.164	1.233	1.323
MPW1PW91/aug-cc-pVTZ	2.121	2.160	1.228	1.319

Table S4 The calculated three-body dissociation energies (in kcal/mol) of FNgBNR → F + Ng + BNR

	Ar	Kr	Xe
		R=H	
MP2/aug-cc-pVDZ	12.2	32.0	58.2
MP2/aug-cc-pVTZ	20.3	41.0	67.1
B3LYP/aug-cc-pVDZ	15.3	31.1	53.2
B3LYP/aug-cc-pVTZ	16.9	33.1	55.4
MPW1PW91/aug-cc-pVDZ	11.6	28.6	51.6
MPW1PW91/aug-cc-pVTZ	12.9	30.3	53.5
CCSD(T)/aug-cc-pVTZ	10.1	30.7	66.4
CCSD(T)/aug-cc-pVQZ[a]	11.5	31.8	59.6
		R=CH_3	
MP2/aug-cc-pVDZ	19.3	35.1	61.0
MP2/aug-cc-pVTZ	23.6	44.0	69.8
B3LYP/aug-cc-pVDZ	17.2	32.5	54.0
B3LYP/aug-cc-pVTZ	18.7	34.4	56.2
MPW1PW91/aug-cc-pVDZ	11.6	29.9	52.5
MPW1PW91/aug-cc-pVTZ	14.6	31.5	54.4
CCSD(T)/aug-cc-pVTZ[b]	11.3	32.6	58.6
		R=CCH	
MP2/aug-cc-pVDZ	17.0	37.9	65.5
MP2/aug-cc-pVTZ	23.6	45.5	72.9
B3LYP/aug-cc-pVDZ	13.0	29.7	52.7
B3LYP/aug-cc-pVTZ	14.5	31.5	54.8
MPW1PW91/aug-cc-pVDZ	9.0	26.9	51.1
MPW1PW91/aug-cc-pVTZ	10.3	28.5	52.9
CCSD(T)/aug-cc-pVTZ[b]	8.5	30.3	58.0
		R=$CHCH_2$	
MP2/aug-cc-pVDZ	17.0	39.3	65.8
MP2/aug-cc-pVTZ	26.4	47.4	73.9
B3LYP/aug-cc-pVDZ	15.5	31.3	53.3
B3LYP/aug-cc-pVTZ	17.0	33.2	55.5
MPW1PW91/aug-cc-pVDZ	9.0	28.6	51.7
MPW1PW91/aug-cc-pVTZ	12.9	30.3	53.6
CCSD(T)/aug-cc-pVTZ[b]	8.5	32.2	58.8
		R=F	

MP2/aug-cc-pVDZ	15.8	31.3	58.6
MP2/aug-cc-pVTZ	18.7	40.4	67.6
B3LYP/aug-cc-pVDZ	12.7	29.3	52.2
B3LYP/aug-cc-pVTZ	14.5	31.5	54.6
MPW1PW91/aug-cc-pVDZ	13.4	26.8	50.7
MPW1PW91/aug-cc-pVTZ	10.6	28.7	52.9
CCSD(T)/aug-cc-pVTZ[b]	12.2	28.8	56.2
		R=OH	
MP2/aug-cc-pVDZ	14.3	34.3	60.8
MP2/aug-cc-pVTZ	22.4	43.4	69.9
B3LYP/aug-cc-pVDZ	15.4	31.3	53.4
B3LYP/aug-cc-pVTZ	17.2	33.5	55.8
MPW1PW91/aug-cc-pVDZ	11.7	28.8	51.9
MPW1PW91/aug-cc-pVTZ	13.2	30.6	54.1
CCSD(T)/aug-cc-pVTZ[b]	10.1	31.0	57.7

[a]Single-point energies using the CCSD(T)/aptz geometry.

[b]Single-point energies using the MPW1PW91/apdz geometry.

Table S5 Calculated reaction energies (in kcal/mol) of FNgBNR → Ng + FBNR

	Ar	Kr	Xe
		R=H	
MPW1PW91/apdz	–142.3	–125.3	–102.2
MP2/apdz	–146.1	–126.3	–100.0
CCSD(T)/aptz SP[a]	–148.9	–128.2	–101.8
		R=CH_3	
MPW1PW91/apdz	–139.1	–122.6	–100.0
MP2/apdz	–142.4	–123.1	–97.2
CCSD(T)/aptz SP[a]	–145.4	–125.1	–99.1
		R=CCH	
MPW1PW91/apdz	–144.1	–126.2	–102.0
MP2/apdz	–147.6	–126.6	–99.1
CCSD(T)/aptz SP[a]	–150.7	–128.9	–101.2
		R=$CHCH_2$	
MPW1PW91/apdz	–141.3	–124.3	–101.2
MP2/apdz	–144.6	–124.6	–98.1
CCSD(T)/aptz SP[a]	–147.6	–126.7	–100.0
		R=F	
MPW1PW91/apdz	–140.4	–122.6	–98.7
MP2/apdz	–144.7	–123.8	–96.5
CCSD(T)/aptz SP[a]	–147.4	–125.8	–98.3
		R=OH	
MPW1PW91/apdz	–138.2	–121.1	–98.0
MP2/apdz	–142.2	–122.1	–95.6
CCSD(T)/aptz SP[a]	–145.0	–124.0	–97.3

[a]Single-point energies using the MPW1PW91/apdz geometry.

Table S6 Calculated barrier heights (in kcal/mol) of FNgBNR → Ng + FBNR

	Ar	Kr	Xe
		R=H	
MP2/apdz	15.0	23.7	33.3
MP2/aptz	15.4	23.3	31.5
B3LYP/apdz	20.4	27.9	35.8
B3LYP/aptz	19.5	26.8	33.8
MPW1PW91/apdz	20.7	28.5	36.6
MPW1PW91/aptz	19.9	27.5	34.7
CCSD(T)/aptz	15.9	23.9	32.5
CCSD(T)/apqz[a]	16.0	24.1	32.3
CCSD(T)/ap5z[a]	16.1	24.1	32.7
		R=CH_3	
MP2/apdz	13.9	22.4	32.0
MP2/aptz	14.5	22.2	30.3
B3LYP/apdz	19.1	26.6	34.5
B3LYP/aptz	18.4	25.6	32.7
MPW1PW91/apdz	19.5	27.2	35.4
MPW1PW91/aptz	18.9	26.4	33.7
CCSD(T)/aptz[b]	14.8	22.7	31.2
		R=CCH	
MP2/apdz	16.0	25.0	34.7
MP2/aptz	16.5	24.6	32.6
B3LYP/apdz	21.0	28.9	36.9
B3LYP/aptz	20.2	27.7	34.9
MPW1PW91/apdz	21.4	29.5	37.8
MPW1PW91/aptz	20.7	28.5	35.9
CCSD(T)/aptz[b]	16.0	25.1	33.5
		R=$CHCH_2$	
MP2/apdz	14.4	23.0	32.8
MP2/aptz	14.9	22.8	30.9
B3LYP/apdz	19.6	27.3	35.2
B3LYP/aptz	18.9	26.2	33.4
MPW1PW91/apdz	20.2	27.9	36.2
MPW1PW91/aptz	19.4	27.0	34.4
CCSD(T)/aptz[b]	15.3	23.4	41.3
		R=F	

MP2/apdz	16.3	25.4	35.2
MP2/aptz	16.7	24.8	33.2
B3LYP/apdz	21.8	29.6	37.5
B3LYP/aptz	20.9	28.4	35.6
MPW1PW91/apdz	22.1	30.1	38.3
MPW1PW91/aptz	21.3	29.0	36.4
CCSD(T)/aptz[b]	17.0	25.5	34.2
		R=OH	
MP2/apdz	19.4	27.2	35.5
MP2/aptz	14.5	22.3	30.7
B3LYP/apdz	19.1	26.7	34.7
B3LYP/aptz	18.3	25.6	32.9
MPW1PW91/apdz	14.0	22.6	32.4
MPW1PW91/aptz	18.7	26.3	33.8
CCSD(T)/aptz[b]	14.8	22.9	31.6

[a]Single-point energies using the CCSD(T)/aptz geometry.

[b]Single-point energies using the MPW1PW91/apdz geometry.

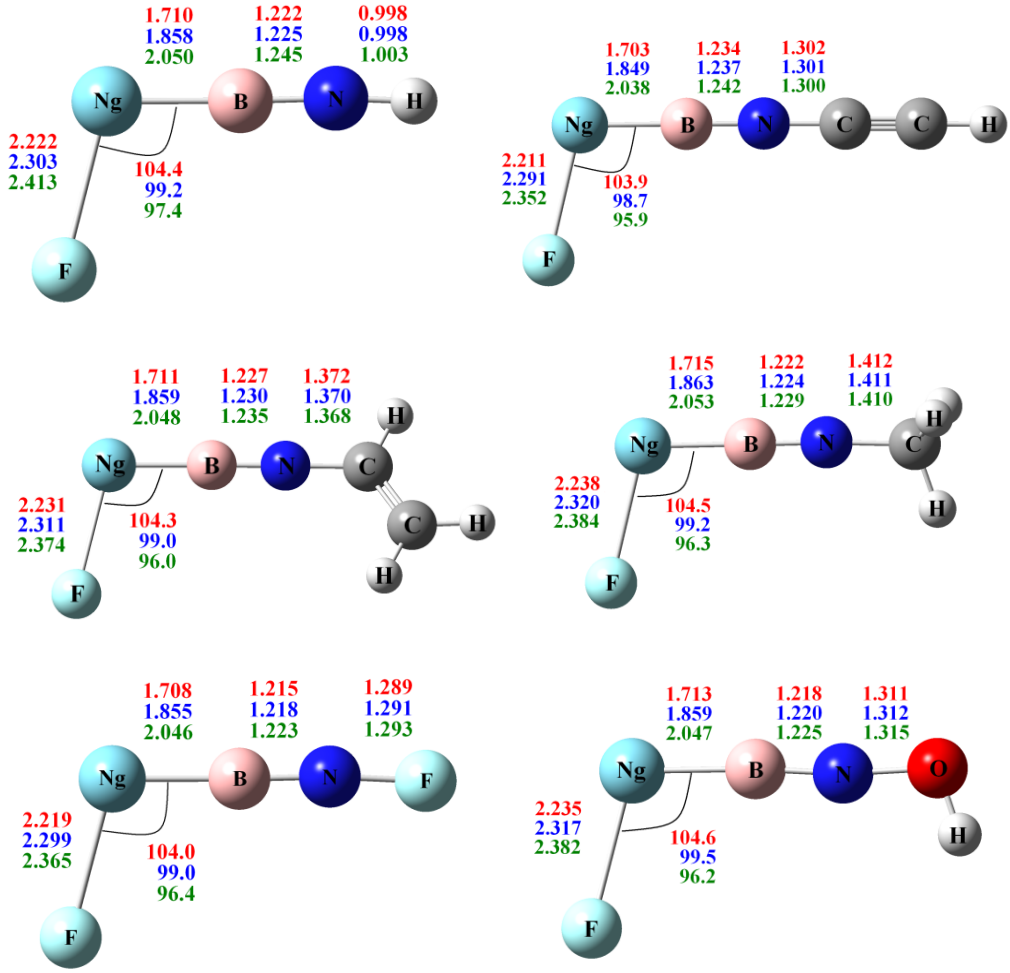

Figure S1 Calculated geometry of the transition states of the two-body dissociation of FNgBNR at the MPW1PW91/aug-cc-pVDZ level. The values in red, blue, and green colors are for Ng = Ar, Kr, and Xe, respectively. The bond lengths are in angstroms, and the bond angles in degrees.