

Supporting Information for “Theoretical Prediction of New Noble-Gas Molecules OBNgF (Ng = Ar, Kr)”

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Table S1. Calculated Transition State Geometries^a for the OBNgF → OB + Ng + F reaction

	MP2/6-311+G*	MP2/aug-cc-pVTZ	CCSD(T)/6-311+G*	CCSD(T)/aug-cc-pVTZ
Ng = Ar				
R(F-Ar)	1.963	1.929	2.103	2.089
R(Ar-B)	2.018	2.119	2.161	2.291
R(B-O)	1.204	1.210	1.208	1.212
A(F-Ar-B)	180.0	180.0	180.0	180.0
A(Ar-B-O)	180.0	180.0	180.0	180.0
Ng = Kr				
R(F-Kr)	2.103	2.097	2.277	
R(Kr-B)	2.382	2.485	2.551	
R(B-O)	1.210	1.213	1.212	
A(F-Kr-B)	179.9	177.2	176.4	
A(Kr-B-O)	179.9	165.2	155.1	

^aBond Length in Å, Angle in degrees**Table S2.** Calculated Transition State Geometries^a for the OBNgF → OBF + Ng reaction

	MP2/6-311+G*	MP2/aug-cc-pVTZ	CCSD(T)/6-311+G*	CCSD(T)/aug-cc-pVTZ
Ng = Ar				
R(F-Ar)	2.292	2.203	2.291	2.207
R(Ar-B)	1.710	1.704	1.718	1.709
R(B-O)	1.205	1.209	1.200	1.204
A(F-Ar-B)	111.5	109.5	110.3	108.9
A(Ar-B-O)	180.0	180.0	180.0	178.6
Ng = Kr				
R(F-Kr)	2.335	2.270	2.337	2.275
R(Kr-B)	1.863	1.840	1.869	1.847
R(B-O)	1.207	1.211	1.203	1.205
A(F-Kr-B)	102.6	102.2	101.9	102.1
A(Kr-B-O)	177.4	178.1	177.6	178.2

^aBond Length in Å, Angle in degrees

Table S3. Calculated Frequencies (in cm^{-1}) of OBNGF

	MP2/6-311+G*	MP2/aug-cc-pVTZ	CCSD(T)/6-311+G*
Ng = Ar			
ν_1	1951.1	1929.9	1943.0
ν_2	418.7	485.7	427.0
ν_3	379.1	403.5	311.6
ν_4	363.7	403.5	311.5
ν_5	363.7	398.0	202.2
ν_6	105.6	117.9	89.8
ν_7	105.6	117.9	89.7
Ng = Kr			
ν_1	1933.2	1921.9	1952.5
ν_2	452.9	462.6	446.8
ν_3	371.3	386.8	351.3
ν_4	371.3	384.0	351.1
ν_5	366.5	384.0	327.6
ν_6	110.6	111.4	105.4
ν_7	110.6	111.4	105.4

Table S4. Calculated Transition State Frequency (in cm^{-1}) of $\text{OBNgF} \rightarrow \text{OB} + \text{Ng} + \text{F}$ reaction

	MP2/6-311+G*	MP2/aug-cc-pVTZ	CCSD(T)/6-311+G*
Ng = Ar			
ν_1	1940.2	1923.2	1908.8
ν_2	499.8	474.1	409.2
ν_3	337.0	299.8	194.0
ν_4	337.0	299.8	193.1
ν_5	93.9	77.8	26.4
ν_6	93.9	77.8	21.5
ν_7	<i>689.9 i</i>	<i>519.3 i</i>	<i>334.3 i</i>
Ng = Kr			
ν_1	1921.0	1899.8	1881.2
ν_2	336.9	290.3	287.3
ν_3	196.3	155.7	122.4
ν_4	178.2	149.8	118.3
ν_5	39.0	32.8	41.4
ν_6	39.0		
ν_7	<i>372.8 i</i>	<i>324.7 i</i>	<i>273.1 i</i>

Table S5. Calculated Transition State Frequency (in cm^{-1}) of $\text{OBNgF} \rightarrow \text{OBF} + \text{Ng}$ reaction

	MP2/6-311+G*	MP2/aug-cc-pVTZ	CCSD(T)/6-311+G*
Ng = Ar			
ν_1	2014.1	1988.6	2036.5
ν_2	621.2	625.7	605.7
ν_3	346.0	378.4	348.3
ν_4	338.5	344.4	328.2
ν_5	252.0	265.5	230.7
ν_6	<i>175.3 i</i>	<i>181.7 i</i>	<i>192.8 i</i>
Ng = Kr			
ν_1	1986.7	1968.9	2010.3
ν_2	521.3	532.7	514.7
ν_3	331.9	354.7	326.8
ν_4	325.4	332.9	325.7
ν_5	251.9	263.0	238.0
ν_6	<i>167.1 i</i>	<i>164.5 i</i>	<i>181.3 i</i>