Supporting Information for "Theoretical Prediction of Nobel-Gas Containing Anions $FNgO^-$ (Ng = He, Ar, and Kr)"

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8 Tables, 3 Figures.

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Table S1. Calculated transition state geometry for the $FNgO^- \rightarrow OF^- + Ng$ reaction at various levels.
The bond lengths are in angstroms and the bond angles in degrees.

Method	$FHeO^-$			$FArO^-$			$FKrO^-$		
	R(F–He)	R(He–O)	A(F–He–O)	R(F–Ar)	R(Ar–O)	A(F–Ar–O)	R(F–Kr)	R(Kr–O)	A(F–Kr–O)
MP2/aug-cc-pVDZ	2.589	2.022	100.5	2.846	2.492	69.2	2.820	2.524	62.0
MP2/aug-cc-pVTZ	2.481	1.912	94.8	2.770	2.408	66.0	2.739	2.446	59.8
MP2/aug-cc-pVQZ	2.467	1.896	93.9	2.754	2.398	65.7	2.728	2.437	59.7
CCSD(T)/aug-cc-pVDZ	2.758	2.306	126.9	2.916	2.560	81.1	2.884	2.549	66.8
CCSD(T)/aug-cc-pVTZ	2.573	2.183	122.2	2.867	2.440	73.8			

Table S2. Calculated harmonic vibrational frequencies (in cm^{-1}) of the transition state for the $FNgO^- \rightarrow OF^- + Ng$ reaction.

	MP2/aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ
Ng = He		
ν_1	230	193 (188)[a]
ν_2	67	25 (51)
ν_3	345 *i*	136 *i* (93 *i*)
Ng = Ar		
ν_1	160	132 (132)
ν_2	119	88 (80)
ν_3	408 *i*	271 *i* (172 *i*)
Ng = Kr		
ν_1	183	(141)
ν_2	156	(118)
ν_3	602 *i*	(378 *i*)

[a]Values in parentheses are calculated at CCSD(T)/aug-cc-pVDZ level.

Table S3. The calculated structures of LiFNgO[a] at various theoretical levels. The bond lengths are in angstroms and the bond angles in degrees.

	R(F–Ng)	R(Ng–O)	R(Li–O)	R(Li–F)	A(Ng–O–Li)	A(O–Li–F)	A(Li–F–Ng)	A(F–Ng–O)
Ng = He								
MP2/aug-cc-pVDZ	1.989	1.103	2.070	1.659	77.9	92.1	71.0	119.0
MP2/aug-cc-pVTZ	1.968	1.084	2.065	1.647	77.8	91.5	71.2	119.5
CCSD(T)/aug-cc-pVDZ	2.036	1.198	2.080	1.649	77.6	95.5	71.2	115.8
CCSD(T)/aug-cc-pVTZ	2.004	1.164	2.071	1.637	77.6	94.2	71.5	116.7
Ng = Ar								
MP2/aug-cc-pVDZ	2.820	1.738	1.986	1.649	96.2	112.8	71.4	79.6
MP2/aug-cc-pVTZ	2.778	1.684	1.973	1.637	97.7	110.6	72.2	79.5
CCSD(T)/aug-cc-pVDZ	2.853	1.829	2.004	1.640	94.0	115.3	71.6	79.1
CCSD(T)/aug-cc-pVTZ	2.798	1.764	1.986	1.628	95.6	112.7	72.5	79.2
Ng = Kr								
MP2/aug-cc-pVDZ	2.624	1.800		1.626				
MP2/aug-cc-pVTZ	2.581	1.759		1.613				
CCSD(T)/aug-cc-pVDZ	2.687	1.880		1.620				
CCSD(T)/aug-cc-pVTZ	2.654	1.830		1.604				

[a]Planar structures for Ng = He and Ar; linear structures for Ng = Kr. See Figure 4 in text for labeling.

Table S4. Calculated relative energies[a] (in kcal/mol) of LiFNgO

	S–T gap[b]	Relative to $Li^+ + FNgO^-$	Relative to LiF + Ng + O (S)	Relative to LiF + NgO (S)	Relative to LiOF + Ng	Barrier[c]
Ng = He						
MP2/aug-cc-pVDZ	62.9	–166.6	–14.9	NA[d]	60.2	7.0 [4.5][e]
MP2/aug-cc-pVTZ	73.1	–166.9	–18.1	NA	60.5	10.4 [7.9]
CCSD(T)/aug-cc-pVDZ	30.5	–168.1	–2.9	NA	58.3	0.7
CCSD(T)/aug-cc-pVTZ	43.9	–164.3	–6.2	NA	58.1	2.4
Ng = Ar						
MP2/aug-cc-pVDZ	26.6	–171.0	–34.4	–21.4	40.6	22.9 [21.8]
MP2/aug-cc-pVTZ	42.2	–170.9	–41.5	–21.3	37.0	29.6 [28.5]
CCSD(T)/aug-cc-pVDZ	10.1	–171.2	–21.9	–19.4	39.2	12.9 [12.0]
CCSD(T)/aug-cc-pVTZ	24.2	–171.7	–27.2	–19.8	37.2	16.9[f]
Ng = Kr						
MP2/aug-cc-pVDZ	42.7	–152.2	–39.7	–11.8	35.3	25.4 [25.2]
MP2/aug-cc-pVTZ	55.1	–153.4	–48.7	–12.2	29.9	33.2 [32.8]
CCSD(T)/aug-cc-pVDZ	25.1	–153.9	–24.7	–10.4	36.4	12.0
CCSD(T)/aug-cc-pVTZ	36.5	–155.2	–31.6	–10.9	32.8	17.0[f]

[a]Born-Oppenheimer energies, not including zero-point vibrational energies.

[b]Energy differences between the singlet and the triplet state at the optimized singlet-state geometry.

[c]Energy barriers for the LiFNgO → LiOF+ Ng reactions. [d]Not applicable

[e]Values in parentheses including vibrational zero-point energies.

[f]Single-point energy at CCSD(T)/aug-cc-pVDZ structure.

Table S5. Calculated harmonic vibrational frequencies (in cm^{-1}) of LiFNgO.

	MP2/aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ
Ng = He		
ν_1	1294	956 (837) [a]
ν_2	780	796 (790)
ν_3	457	410 (402)
ν_4	343	339 (347)
ν_5	314	275 (263)
ν_6	224	204 (188)
Ng = Ar		
ν_1	796	814 (813)
ν_2	682	549 (499)
ν_3	421	406 (420)
ν_4	247	233 (227)
ν_5	168	157 (152)
ν_6	144	141 (129)
Ng = Kr		
ν_1	838	(840)
ν_2	714	(530)
ν_3	153	(138)
ν_4	112	(89)
ν_5	112	(89)
ν_6	46	(24)
ν_7	46	(23)

[a]Values in parentheses are calculated at CCSD(T)/aug-cc-pVDZ level.

Table S6. Calculated Atomic Charges[a] (in a.u.) for LiFNgO

	Li	F	Ng	O
LiFHeO	0.79 (0.95)	–0.80 (–0.95)	0.37 (0.50)	–0.36 (–0.50)
LiFArO	0.80 (0.94)	–0.83 (–0.96)	0.48 (0.71)	–0.45 (–0.69)
LiFKrO	0.88 (0.97)	–0.86 (–0.95)	0.52 (0.83)	–0.54 (–0.85)

[a]By ChelpG and NBO (in parentheses) methods using electron density calculated at MP2/aug-cc-pVTZ level.

Table S7. Calculated transition state geometry for the LiFNgO → LiOF+ Ng reaction at various theoretical levels. The bond lengths are in angstroms and the bond angles in degrees.

	R(F–Ng)	R(Ng–O)	R(Li–O)	R(Li–F)	A(Ng–O–Li)	A(O–Li–F)	A(Li–F–Ng)	A(F–Ng–O)
Ng = He								
MP2/aug-cc-pVDZ	2.679	1.939	2.115	1.619	92.1	106.6	81.6	79.6
MP2/aug-cc-pVTZ	2.564	1.895	2.086	1.606	94.0	101.8	85.4	78.9
CCSD(T)/aug-cc-pVDZ	2.412	1.425	2.117	1.624	81.8	107.7	69.1	101.4
CCSD(T)/aug-cc-pVTZ	2.565	1.555	2.129	1.603	83.9	112.0	69.3	94.8
Ng = Ar								
MP2/aug-cc-pVDZ	2.875	2.453	1.997	1.627	107.8	91.4	102.9	57.9
MP2/aug-cc-pVTZ	2.812	2.407	1.965	1.616	109.3	89.1	104.4	57.2
CCSD(T)/aug-cc-pVDZ	2.920	2.414	1.993	1.629	105.1	97.4	96.8	60.7
Ng = Kr								
MP2/aug-cc-pVDZ	2.875	2.511	1.939	1.635	113.0	85.5	108.2	53.3
MP2/aug-cc-pVTZ	2.813	2.464	1.905	1.626	114.5	83.4	109.5	52.6
CCSD(T)/aug-cc-pVDZ	2.904	2.467	1.920	1.641	112.4	89.1	103.6	54.9

Table S8. Calculated harmonic vibrational frequencies (in cm^{-1}) of the transition state for the LiFNgO → LiOF + Ng reaction.

	MP2/aug-cc-pVTZ	CCSD(T)/aug-cc-pVTZ
Ng = He		
ν_1	850	859 (837) [a]
ν_2	317	297 (331)
ν_3	257	257 (295)
ν_4	127	127 (176)
ν_5	90	121 (156)
ν_6	274 *i*	300 *i* (303 *i*)
Ng = Ar		
ν_1	826	(803)
ν_2	409	(388)
ν_3	216	(188)
ν_4	145	(122)
ν_5	76	(91)
ν_6	373 *i*	(332 *i*)
Ng = Kr		
ν_1	808	(778)
ν_2	463	(450)
ν_3	242	(230)
ν_4	155	(144)
ν_5	78	(71)
ν_6	505 *i*	(477 *i*)

[a]Values in parentheses are calculated at CCSD(T)/aug-cc-pVDZ level.

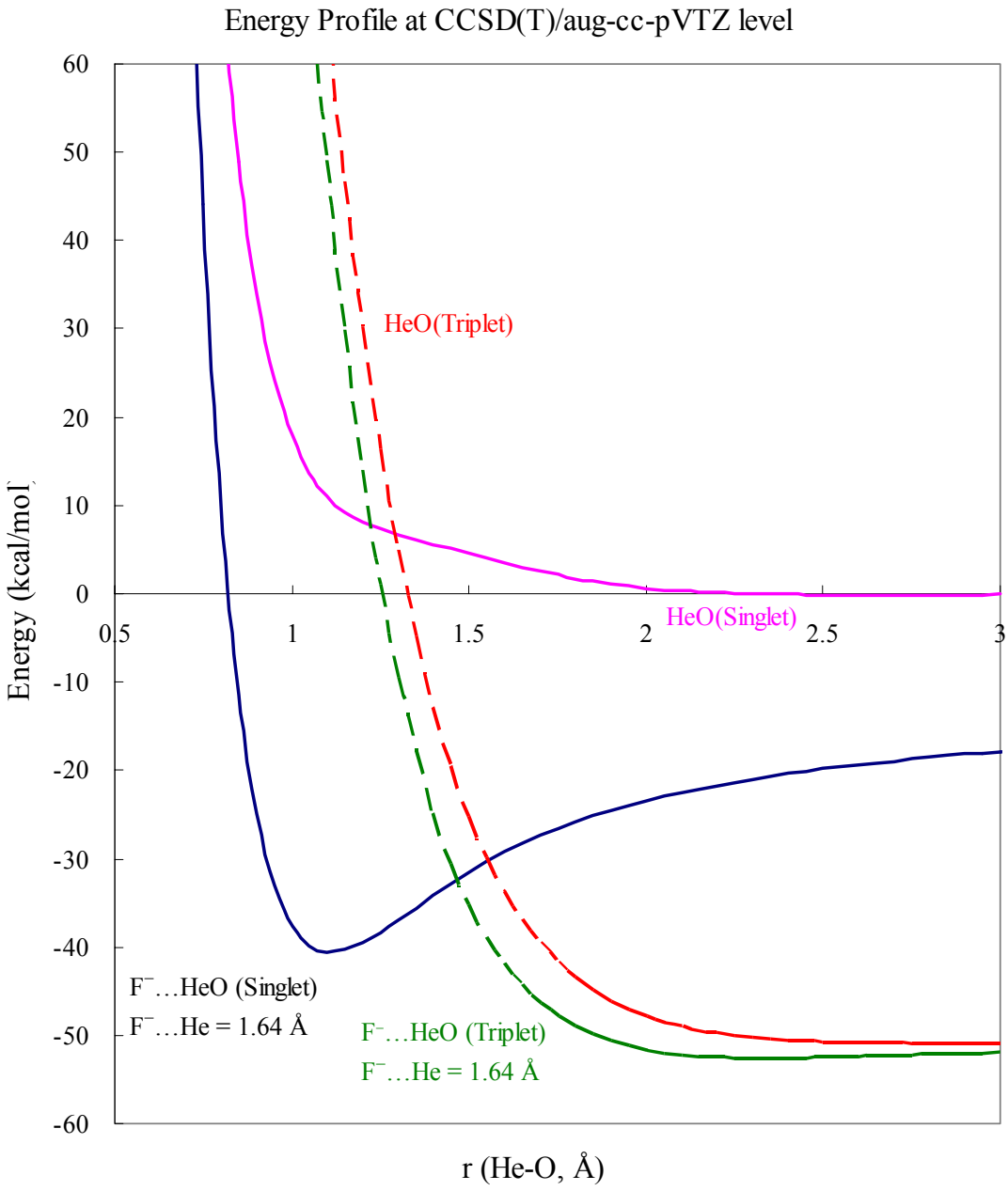

Figure S1. Potential energy profile of HeO and FHeO⁻. The energies were calculated at CCSD(T)/aug-cc-pVTZ level. The HeO energies are relative to He + O (S) and the FHeO⁻ energies are relative to F⁻…He + O (S) with F–He distance fixed at 1.64 Å.

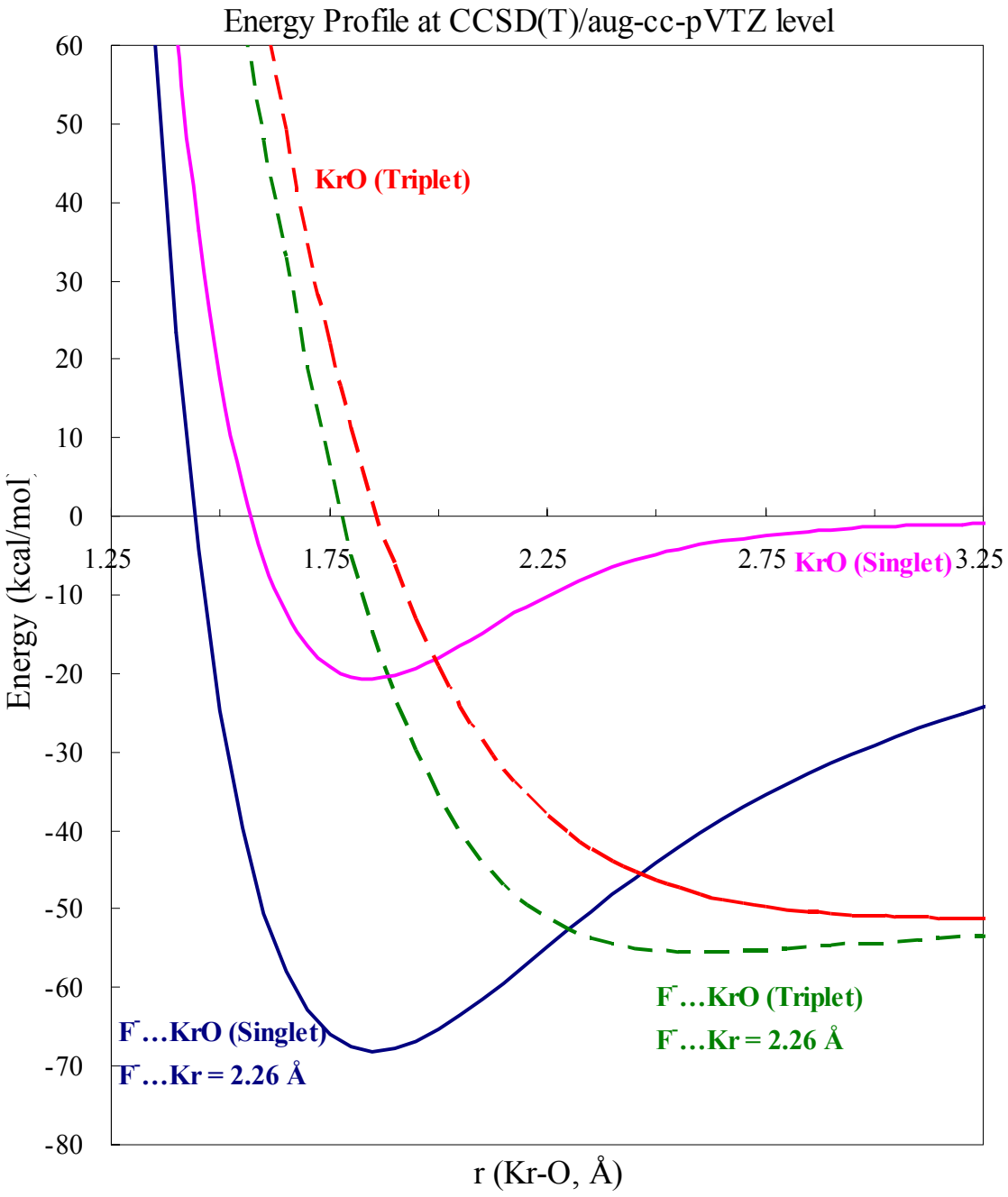

Figure S2. Potential energy profile of KrO and $FKrO^-$. The energies were calculated at CCSD(T)/aug-cc-pVTZ level. The KrO energies are relative to Kr + O (S) and the $FKrO^-$ energies are relative to F^-…Kr + O (S) with F–Kr distance fixed at 2.26 Å.

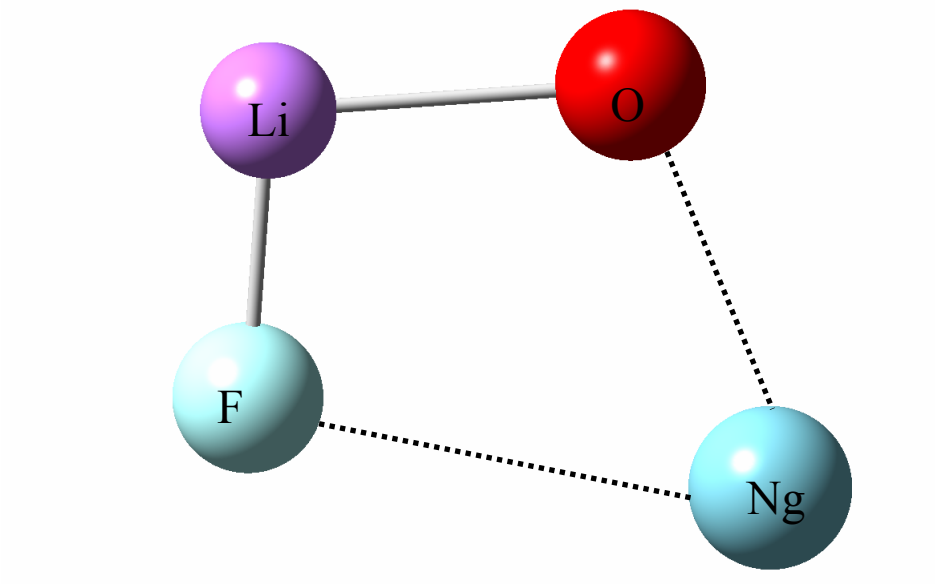

Figure S3. Schematic plot of the transition state structure for the LiFNgO → LiOF+ Ng reaction.