Table 2. Calculated relative energies[a] (in kcal/mol) of $FNgO^-$

	S–T gap[b]	Relative to F^-+Ng+O(S)	Relative to F^-+NgO	Relative to F+Ng+O^-	Relative to F^-+Ng+O(T)	Relative to FO^-+Ng	Barrier[c]
Ng = He							
MP2/aug-cc-pVTZ	117.8	–39.4	NA[d]	-24.7	26.6	48.7	29.0 [25.0][e]
MP2/aug-cc-pVQZ	121.4	–32.9	NA	-19.1	32.2	55.8	29.9 [26.0]
CCSD(T)/aug-cc-pVTZ	90.9	–23.6	NA	-18.4	27.3	50.9	22.1 [18.7]
CCSD(T)/aug-cc-pVQZ	91.1	–20.5	NA	-15.9	29.8	54.7	18.9
CCSD(T)/CBS[f]	91.4	–24.0	NA	-16.4	29.6	54.7	19.2
Ng = Ar							
MP2/aug-cc-pVTZ	61.0	–51.4	-31.1	-36.6	14.7	36.8	44.6 [43.0]
MP2/aug-cc-pVQZ	65.6	–53.7	-31.8	-39.9	11.3	35.0	46.6 [45.0]
CCSD(T)/aug-cc-pVTZ	38.0	–37.1	-29.7	-32.0	13.7	37.4	31.9 [30.6]
CCSD(T)/aug-cc-pVQZ	42.2	–38.7	-30.2	-34.1	11.6	36.5	33.2[g]
CCSD(T)/CBS	42.0	–38.9	-30.3	-34.9	11.2	36.2	33.4
Ng = Kr							
MP2/aug-cc-pVTZ	72.2	–76.0	-39.5	-61.2	-9.9	12.2	65.5 [64.0]
MP2/aug-cc-pVQZ	74.3	–77.8	-39.9	-64.0	-12.7	10.9	66.9 [65.4]
CCSD(T)/aug-cc-pVTZ	52.7	–58.1	-37.4	-52.9	-7.3	16.4	49.4[h]
CCSD(T)/aug-cc-pVQZ[g]	52.8	–59.3	-37.7	-54.7	-9.0	15.9	50.4[h]
CCSD(T)/CBS	52.4	–56.3	-37.6	-52.3	-6.3	18.7	49.7

[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 $FNgO^- \rightarrow FO^- + Ng$ reactions. [d]Not applicable
[e]Values in parentheses including vibrational zero-point energies.
[f]Extrapolated results to the complete basis set limit, see text.
[g]Single-point energy at CCSD(T)/aug-cc-pVTZ structure except for the barrier.
[h]Single-point energy at CCSD(T)/aug-cc-pVDZ structure.

Table 4. Calculated Atomic Charges[a]

	F	Ng	O
$FHeO^-$	–0.83 (–0.94)	0.43 (0.86)	–0.60 (–0.92)
$FArO^-$	–0.83 (–0.90)	0.49 (0.73)	–0.66 (–0.83)
$FKrO^-$	–0.78 (–0.85)	0.52 (0.86)	–0.75 (–1.01)

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