

Table S1. MP2 calculated values of the harmonic vibrational frequencies (in cm^{-1}) and their respective intensity values [Numbers given in parentheses are the respective calculated IR intensities (in $\text{km}\cdot\text{mol}^{-1}$)] of TS1 ($\text{HKrOX} \rightarrow \text{Kr} + \text{HOX}$, X = F, Cl, Br and I).

Normal modes	HKrOF	HKrOCl	HKrOBr	HKrOI
ν_1	-438.0(2)	-458.0(0)	-466.7(0)	-480.2(42)
ν_2	147.5(19)	103.9(11)	92.7(14)	83.2(77)
ν_3	190.9(29)	136.0(25)	119.3(28)	104.0(54)
ν_4	270.3(72)	228.4(51)	188.8(33)	169.2(17)
ν_5	1000.2(2)	818.7(110)	741.4(178)	696.4(162)
ν_6	2650.0(218)	2638.0(216)	2640.4(211)	2638.1(388)

Table S2. MP2 calculated values of the harmonic vibrational frequencies (in cm^{-1}) and their respective harmonic zero point energy (ZPE, in $\text{kJ}\cdot\text{mol}^{-1}$) of TS2 ($\text{HKrOX} \rightarrow \text{H} + \text{Kr} + \text{OX}$, X = F, Cl, Br and I).

Normal modes	HKrOF	HKrOCl	HKrOBr	HKrOI
ν_1	-908.5(6705)	-945.7(8777)	-875.9(9043)	-928.0(8913)
ν_2	190.6(27)	148.4(9)	127.6(12)	94.1(9)
ν_3	395.1(131)	391.7(196)	396.8(246)	347.7(64)
ν_4	495.7(83)	457.0(83)	553.2(81)	351.6(124)
ν_5	535.1(54)	509.3(76)	581.4(89)	474.6(25)
ν_6	1058.0(19)	842.6(33)	675.1(85)	628.6(63)