Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 Calculated heats of formation and Gibbs free energies of formation (in kcal/mol) at standard condition with Aug-CC-PVTZ basis set

	CCSD		CCSD(T)[a]		CAM-B3LYP		WB97XD	
X	ΔH^O_f	ΔG^O_f	ΔH^O_f	ΔG^O_f	ΔH^O_f	ΔG^O_f	ΔH^O_f	ΔG^O_f
F	39.4	62.6	20.9	44.2	22.6	45.9	25.7	49.0
Cl	65.2	87.8	45.3	67.8	52.8	74.6	52.7	75.5
Br	66.3	88.7	45.5	67.9	56.0	77.8	57.6	80.1
I	397.3	419.3	382.4	404.3	397.6	442.3	399.8	422.1

[a]The single point energies were obtained from the CCSD(T) calculations and used to correct the results of CCSD calculations

Table S2 NBO atomic charges (in atomic units) and atomic hybridizations (in percent) obtained from CCSD/Aug-CC-PVTZ calculations

X	Atomic Charges		Hybridization Bond	atom	%s	%p	%d
F	F	-0.683	Kr-O	Kr	1.10	97.15	1.61
	Kr	1.069		O	8.59	90.95	0.42
	O	-0.852	O-H	O	24.39	75.39	0.20
	H	0.467		H	99.71	0.27	0.02
Cl	Cl	-0.458	Kr-O	Kr	0.65	97.93	1.27
	Kr	0.845		O	6.86	92.95	0.17
	O	-0.850	O-H	O	24.12	75.72	0.15
	H	0.463		H	99.76	0.23	0.01
Br	Br	-0.374	Kr-Br	Kr	0.31	98.28	1.12
	Kr	0.784		Br	3.17	96.05	0.69
	O	-0.869	O-H	O	24.93	74.88	0.18
	H	0.458		H	99.74	0.25	0.01
I	I	-0.179	Kr-I	Kr	0.05	98.37	1.11
	Kr	0.654		I	2.62	97.38	0.00
	O	-0.922	O-H	O	24.75	75.06	0.17
	H	0.447		H	99.75	0.24	0.01

Table S3 The results of AIM analyses, electron densities (ρ), Laplacian of the electron densities ($\nabla^2\rho$) and bond elipticities (ε) obtained from AIM calculations using CCSD/Aug-CC-PVTZ method

	Bond	ρ (e/a_0^3)	$\nabla^2\rho$ (e/a_0^5)	ε
F	Kr-O	0.098	0.116	0.035
	Kr-X	0.085	0.244	0.003
	O-H	0.366	-2.715	0.020
Cl	Kr-O	0.078	0.082	0.032
	Kr-X	0.053	0.068	0.002
	O-H	0.361	-2.665	0.022
Br	Kr-O	0.066	0.079	0.031
	Kr-X	0.045	0.046	0.001
	O-H	0.359	-2.633	0.022
I	Kr-O	0.141	0.288	0.050
	Kr-X	0.037	0.043	0.002
	O-H	0.372	-2.770	0.018

Table S4 The energies of HOMO, LUMO, band gap (E_g) and reactivity parameters obtained from population analyses at CCSD/Aug-CC-PVTZ level of theory. All values (except S, eV^{-1}) are reported in eV.

X	E_{HOMO}	E_{LUMO}	E_g	μ	η	S	ω
F	-0.400	-0.072	0.328	-0.236	0.164	6.098	0.170
C	-0.369	-0.108	0.261	-0.239	0.131	7.663	0.218
Br	-0.353	-0.118	0.235	-0.236	0.118	8.511	0.236
I	-0.327	-0.120	0.207	-0.224	0.104	9.662	0.241