Table S1: Molecular surface properties[a] of the studied halomethanes, including, from left to right, the minimum, maximum, average positive and average negative electrostatic potentials in kcal/mol, the variances of positive and negative electrostatic potentials[b] in $(kcal/mol)^2$, the electrostatically positive and negative surface areas[c] in $Å^2$, and the minimum, maximum and average average local ionization energy (ALIE) in eV.

Halomethane	V_{min}	V_{max}	V^+_{avg}	V^-_{avg}	A^+	A^-	Var^+	Var^-	$ALIE_{min}$	$ALIE_{max}$	$ALIE_{avg}$
CCl_3Br	−4.47	27.50	7.82	−3.10	54.95	86.15	41.78	1.46	12.98	18.61	14.76
CCl_4	−4.22	21.69	7.36	−2.97	53.13	82.58	35.56	1.36	14.40	18.65	15.22
CF_2Br_2	−7.72	29.62	7.72	−3.12	58.16	64.33	54.26	5.93	13.16	23.05	16.03
CF_2Cl_2	−7.20	24.44	6.41	−3.12	57.44	53.29	36.90	5.94	14.70	23.12	17.44
CF_2ClBr	−7.49	30.08	7.08	−3.11	57.88	58.75	46.39	6.04	13.23	23.08	16.69
CF_3Br	−5.44	32.25	6.48	−3.67	62.00	40.65	49.28	1.83	13.47	23.46	18.28
CF_3Cl	−5.04	26.40	6.28	−3.39	56.82	39.70	37.22	1.54	14.99	23.51	19.28
CF_3I	−7.03	38.66	7.25	−4.63	69.83	43.47	67.06	3.23	11.95	23.25	16.95
CF_4	−2.28	32.95	7.51	−1.47	38.75	42.52	49.51	0.38	21.40	23.96	22.05
$CFCl_3$	−8.46	22.95	7.06	−2.94	53.80	69.97	36.56	5.21	14.54	22.74	16.15
CH_2Br_2	−12.56	31.35	14.39	−6.69	50.13	64.11	93.44	10.26	12.37	18.95	14.09
CH_2Cl_2	−14.27	31.13	15.74	−7.44	42.59	59.58	103.95	13.13	13.67	19.50	15.36
CH_2ClBr	−13.58	31.27	15.03	−7.02	46.28	61.97	99.03	11.53	12.35	19.23	14.68
CH_2F_2	−21.86	30.77	21.37	−14.58	33.32	37.21	73.53	30.11	17.22	22.16	19.67
CH_2FCl	−21.29	31.13	18.15	−10.15	38.16	48.73	98.66	31.02	13.70	21.52	17.00
CH_2I_2	−10.52	30.58	13.23	−5.84	61.90	72.68	78.00	7.18	11.04	18.53	12.68
CH_3Br	−15.33	22.82	14.00	−10.47	45.03	43.07	33.86	18.93	11.83	18.22	14.71
CH_3Cl	−16.82	22.03	14.51	−11.63	42.00	39.71	25.95	22.21	13.07	18.69	15.60
CH_3F	−27.65	24.01	13.87	−19.99	42.11	23.00	25.30	65.74	16.27	21.01	18.07
CH_3I	−13.46	23.16	13.15	−9.08	50.80	48.02	35.35	14.87	10.63	18.06	13.60
CH_4	−2.08	9.30	4.04	−1.40	33.06	26.64	7.28	0.35	15.45	16.76	16.01
$CHBr_3$	−7.79	36.53	11.41	−4.63	58.76	78.46	90.62	5.06	12.71	18.52	13.78
$CHCl_3$	−8.41	37.50	11.55	−4.83	49.80	70.44	108.72	6.16	14.08	19.28	15.24
CHF_2Cl	−13.28	39.88	15.88	−7.01	37.81	53.97	165.50	14.31	14.34	22.62	18.19
CHF_3	−12.33	41.69	21.98	−8.16	27.32	48.56	191.50	9.35	18.49	23.03	20.92
$CHFCl_2$	−14.12	38.55	13.11	−5.85	45.06	61.49	131.86	13.48	14.21	22.27	16.44

[a] The molecular surface properties where calculated on a molecular surface of an isovalue of 0.001 au.

[b] For the studied halomethanes, the total surface area $A = A^+ + A^-$, for all practical purposes

[c] The total variance $Var^{tot} = Var^+ + Var^-$

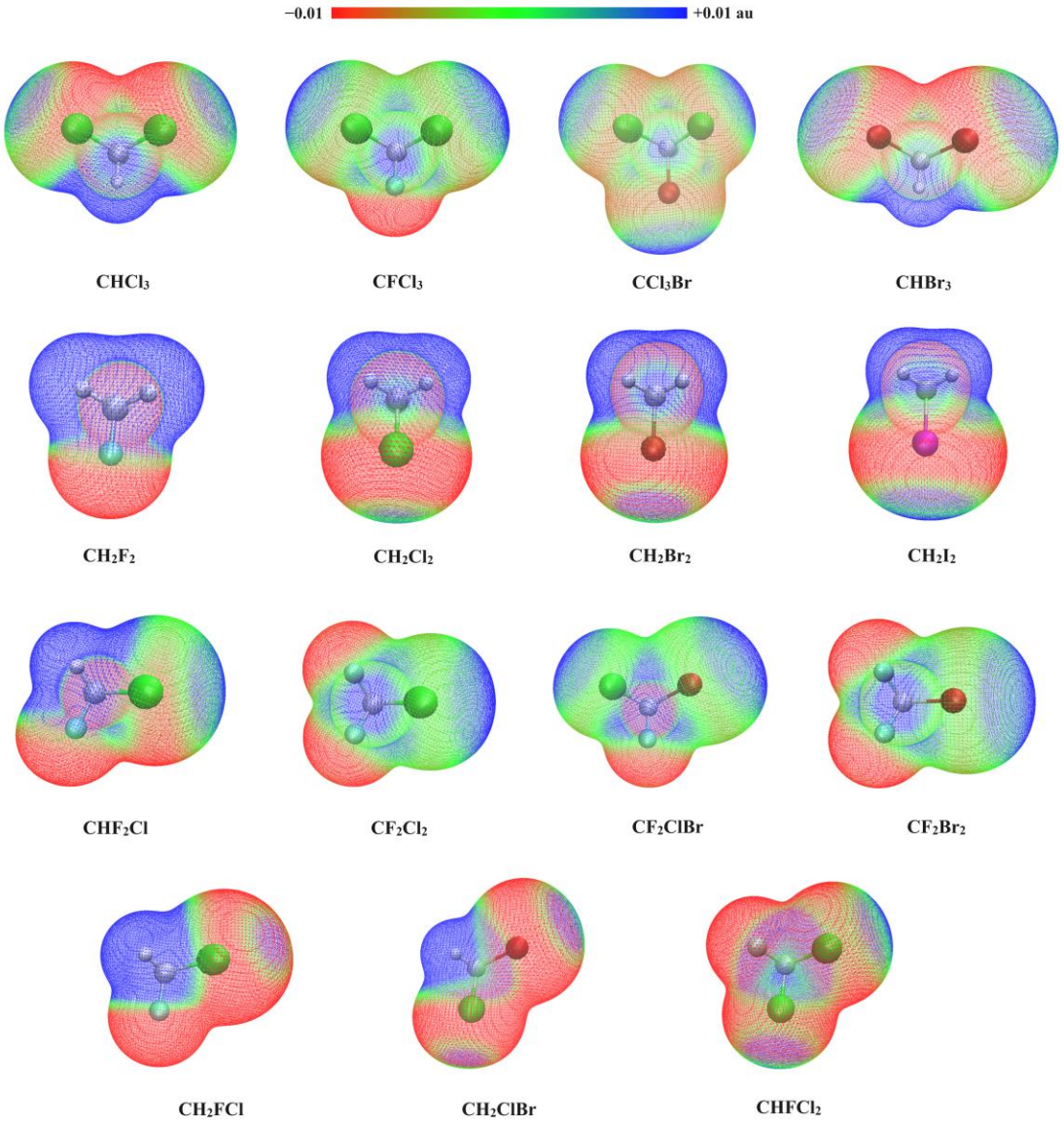

Figure S1: Molecular electrostatic potentials (MEPs) of some halomethanes mapped onto molecular surfaces of electron isodensity values of 0.01 au. The RGB color scale ranges from −0.01 au (red) to +0.01 au (blue)

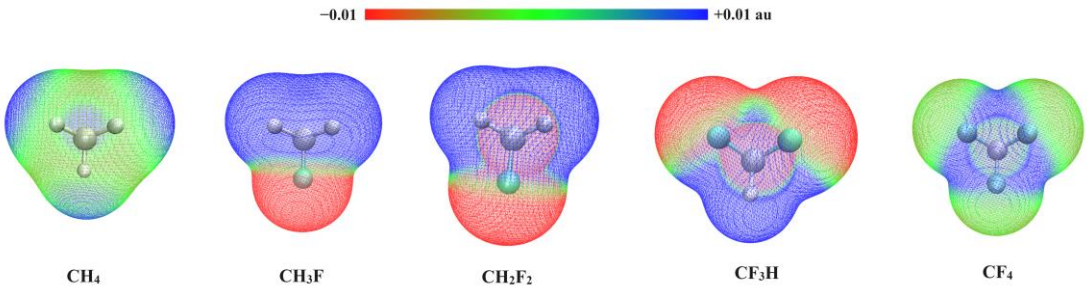

Figure S2: Molecular electrostatic potentials (MEPs) of CH_nF_{4-n}(where $0 \leq n \leq 4$) mapped onto molecular surfaces of electron isodensity values of 0.01 au. The RGB color scale ranges from −0.01 au (red) to +0.01 au (blue)

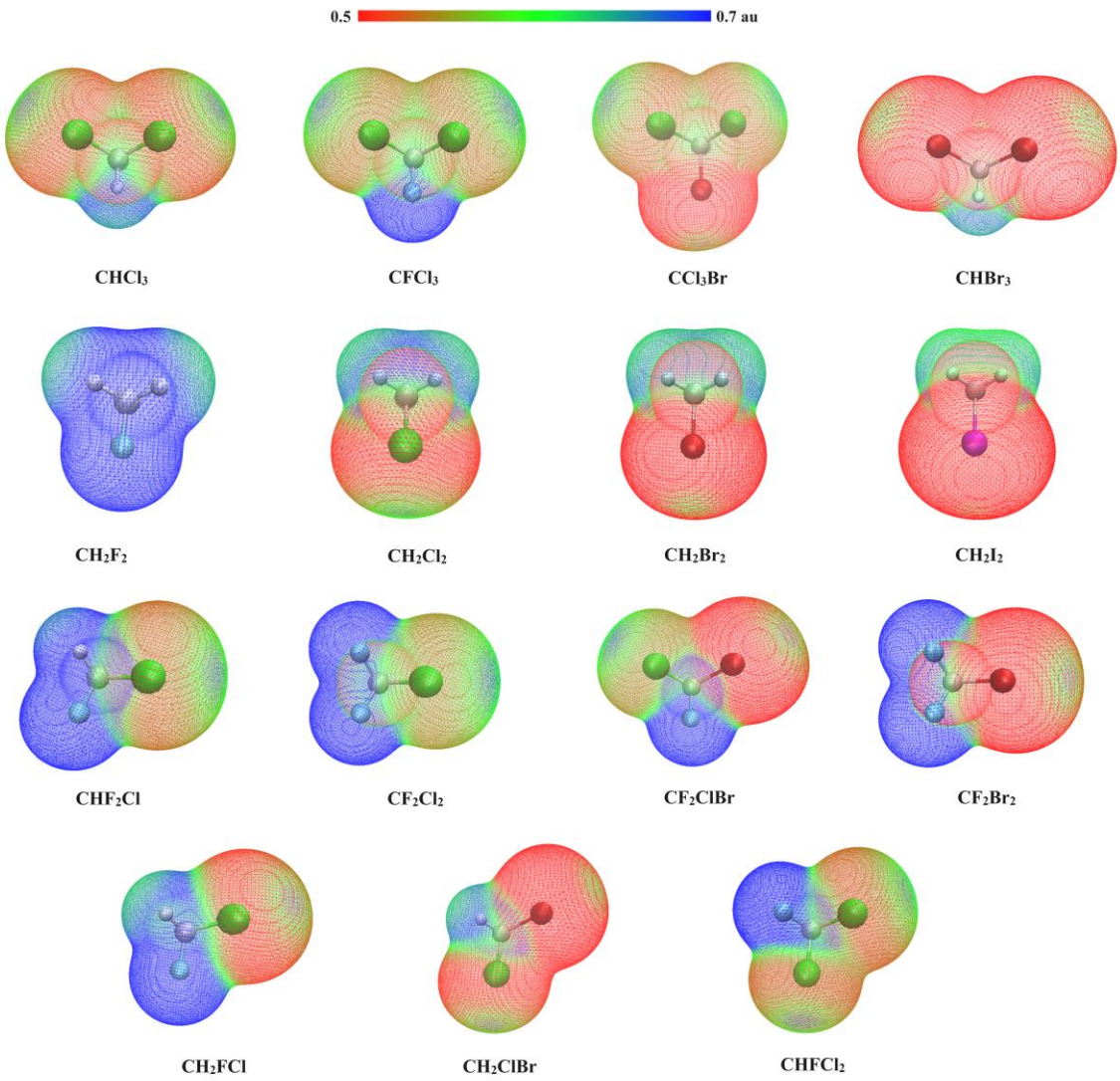

Figure S3: The average local ionization energy (ALIE) maps of some halomethanes onto molecular surfaces of electron isodensity values of 0.01 au. The RGB color scale ranges from 0.5 au (red) to 0.7 au (blue)