Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

The effects of gas-liquid interface and gas phase on Cl/ClO radicals' interaction with water molecules

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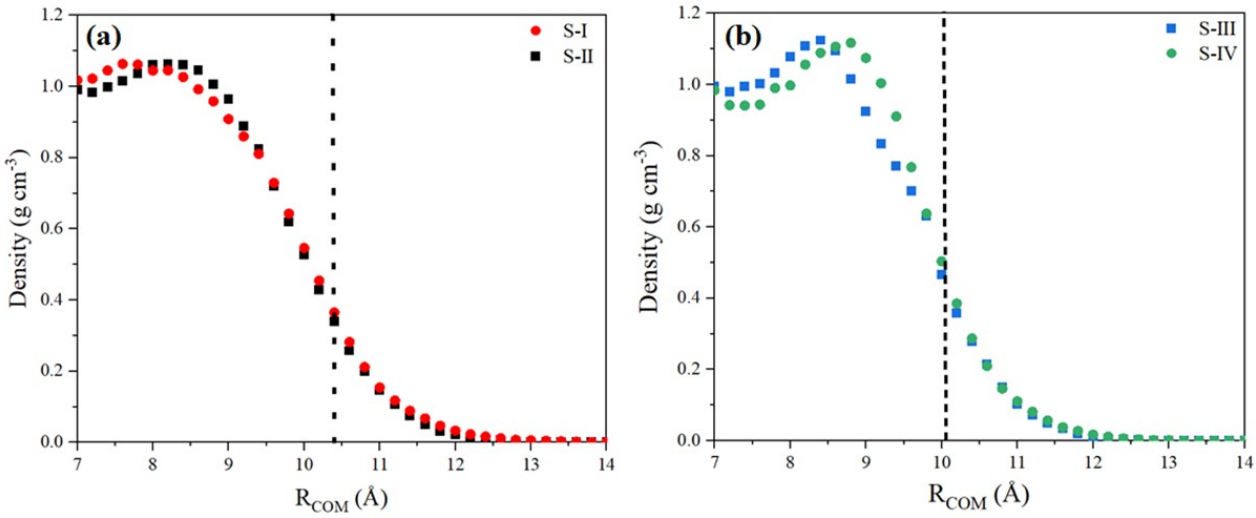

Fig. S1. An illustration of the density profile of water molecules relative to the distance from the center of mass of droplet. Where, a vertical dotted line at (a) 10.4 and (b) 10.1 indicates 50% of bulk water density, which is defined as the gas-liquid interface.

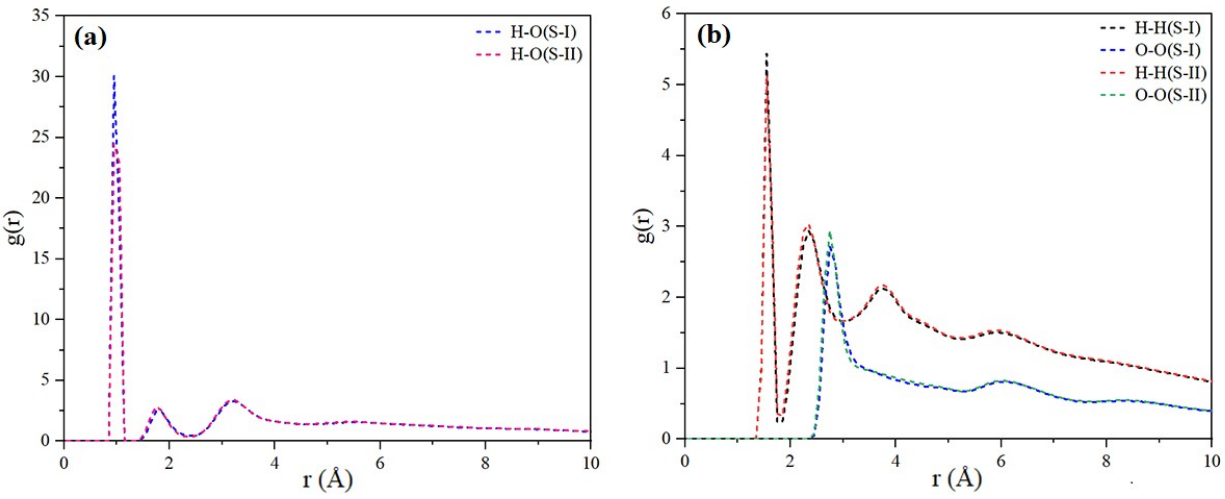

Fig. S2. Radial distribution functions for H-O, O-O, H-H related to water molecules in droplet systems S-I and S-II. Where, the RDFs of H-O, O-O, and H-H bonds for both S-I and S-II is almost same.

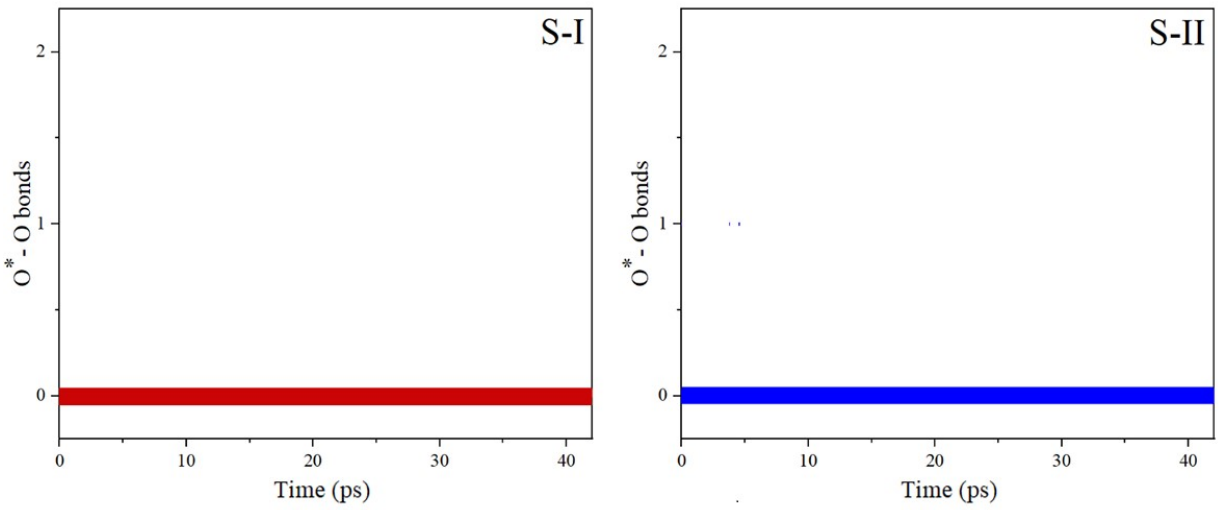

Fig. S3. Coordination analysis confirms the lack of hemibond (O*-O ~ 2.3 Å) between ClO radical and neighboring water molecules.

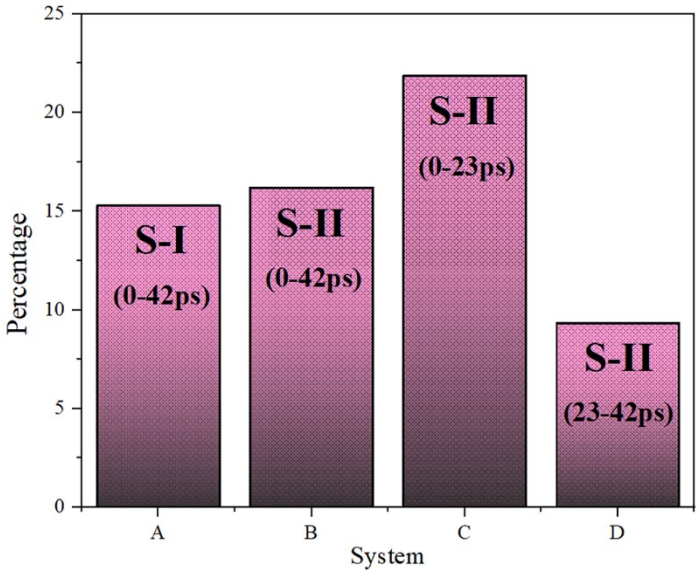

Fig. S4. The distribution analysis of O…Cl-O*…H structures related to S-I and S-II systems within BOMD simulation.

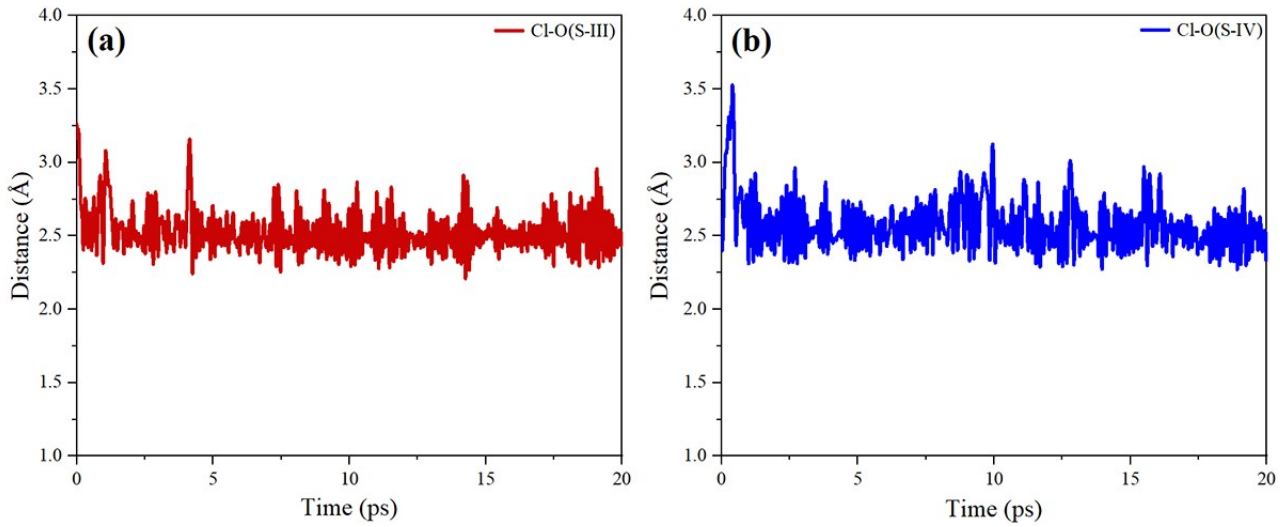

Fig. S5. The distance between Cl and O of water molecules in S-III and S-IV systems.

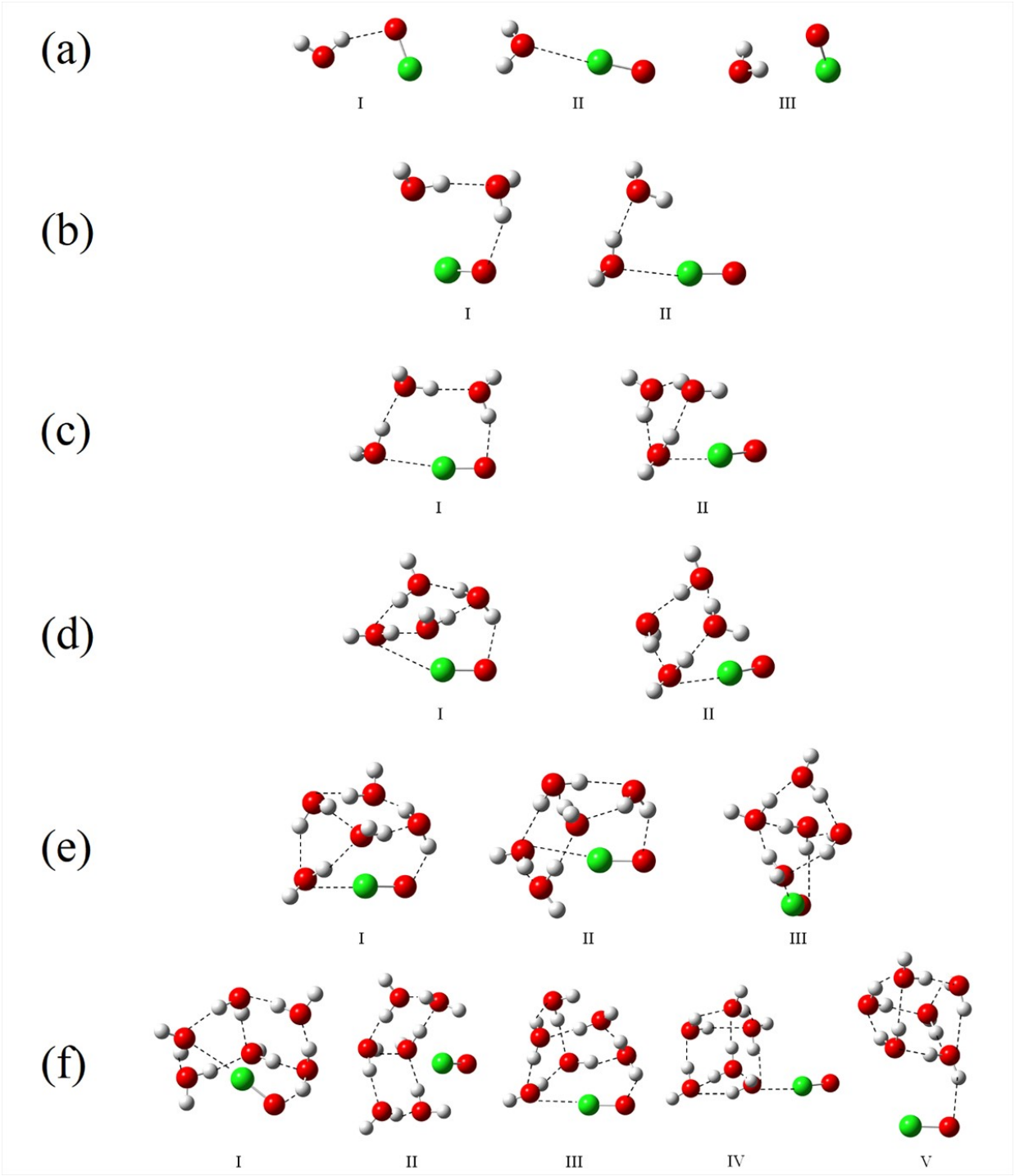

Fig. S6. The low-lying structures after optimization of $ClO(H_2O)_n$. Where (a) to (f) are related to $ClO(H_2O)_1$ to $ClO(H_2O)_6$, respectively.

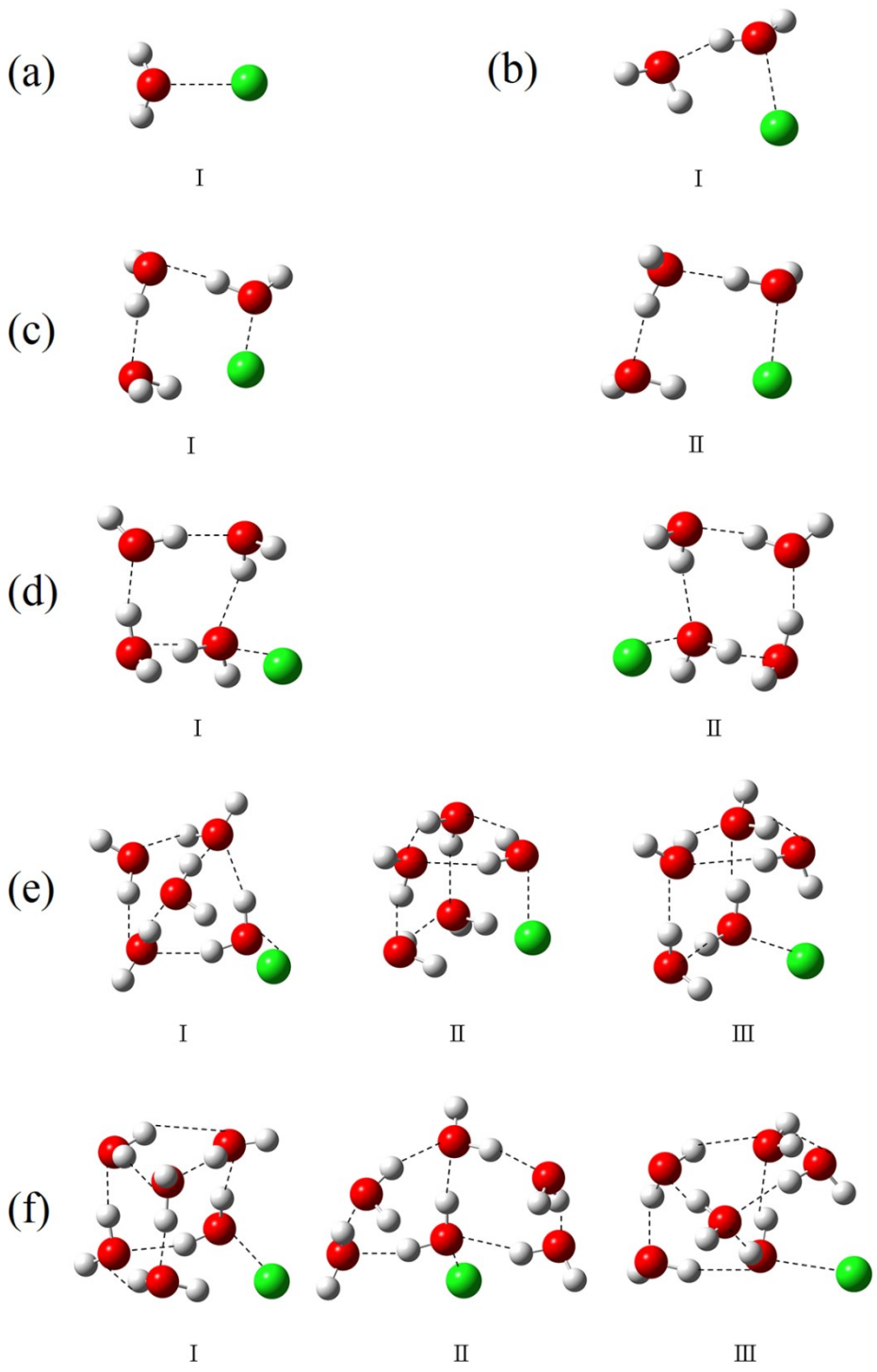

Fig. S7. The low-lying structures after optimization of $Cl(H_2O)_n$. Where (a) to (f) are related to $Cl(H_2O)_1$ to $Cl(H_2O)_6$, respectively.

Table S1. Relative energies of $ClO(H_2O)_n$ clusters (in kcal mol^{-1}) with respect to the total energy of the most stable structures in corresponding $ClO(H_2O)_{1–6}$ clusters.

$ClO(H_2O)_n$	Structure	Relative Energy (kcal mol^{-1})
$ClO(H_2O)_1$	I	0.00
	II	0.08
	III	1.41
$ClO(H_2O)_2$	I	0.00
	II	0.36
$ClO(H_2O)_3$	I	0.00
	II	0.16
$ClO(H_2O)_4$	I	0.00
	II	1.15
$ClO(H_2O)_5$	I	0.00
	II	0.03
	III	1.32
$ClO(H_2O)_6$	I	0.00
	II	1.75
	III	1.91
	IV	2.18
	V	2.92

Table S2. Relative energies of $Cl(H_2O)_n$ clusters (in kcal mol^{-1}) with respect to the total energy of the most stable structures in corresponding $Cl(H_2O)_{3–6}$ clusters.

$Cl(H_2O)_n$	Structure	Relative Energy (kcal mol^{-1})
$Cl(H_2O)_3$	I	0.00
	II	0.30
$Cl(H_2O)_4$	I	0.00
	II	0.16
$Cl(H_2O)_5$	I	0.00
	II	0.92
	III	1.40
$Cl(H_2O)_6$	I	0.00
	II	0.64
	III	1.21

Table S3. Bond length (in Å) in $ClO(H_2O)_{1-6}$ clusters along with their dipole moments.

$ClO(H_2O)_n$	O*-H/O-H/Cl-O*/Cl-O Bond	Bond Length (Å)	Dipole Moment
$ClO(H_2O)_1$	R_{O1Cl}	1.55	0.72
	R_{O1H1}	2.06	
	R_{O2Cl}	3.28	
$ClO(H_2O)_2$	R_{O1Cl}	1.55	1.40
	R_{O1H1}	2.02	
	R_{O2H3}	1.90	
	R_{O3Cl}	3.06	
$ClO(H_2O)_3$	R_{O1Cl}	1.56	1.99
	R_{O1H1}	1.98	
	R_{O2H3}	1.85	
	R_{O3H5}	1.83	
	R_{O4Cl}	2.66	
$ClO(H_2O)_4$	R_{O1Cl}	1.56	3.53
	R_{O1H1}	2.21	
	R_{O3H2}	1.83	
	R_{O4H3}	1.83	
	R_{O5H5}	1.75	
	R_{O2H7}	1.74	
	R_{O4Cl}	2.89	
$ClO(H_2O)_5$	R_{O1Cl}	1.56	2.66
	R_{O1H1}	2.20	
	R_{O3H2}	1.77	
	R_{O4H3}	1.76	
	R_{O5H5}	2.10	
	R_{O6H7}	1.88	
	R_{O6H6}	1.95	
	R_{O2H9}	1.69	
	R_{O5Cl}	2.77	
$ClO(H_2O)_6$	R_{O1Cl}	1.56	1.98
	R_{O1H1}	2.08	
	R_{O3H2}	1.75	
	R_{O4H3}	1.72	
	R_{O5H5}	1.88	
	R_{O6H7}	1.75	
	R_{O7H9}	1.77	
	R_{O7H6}	1.94	
	R_{O2H11}	1.64	
	R_{O5Cl}	2.75	

Table S4. Bond length (in Å) in $Cl(H_2O)_{1-6}$ clusters along with their dipole moments.

$Cl(H_2O)_n$	O-H/Cl-O/Cl-H Bond	Bond Length (Å)	Dipole Moment
$Cl(H_2O)_1$	R_{OCl}	2.57	2.33
$Cl(H_2O)_2$	R_{O1Cl}	2.40	2.23
	R_{O2H1}	1.80	
	R_{H4Cl}	2.53	
$Cl(H_2O)_3$	R_{O1Cl}	2.35	1.07
	R_{O2H2}	1.67	
	R_{O3H3}	1.79	
	R_{H6Cl}	2.32	
$Cl(H_2O)_4$	R_{O4Cl}	2.40	0.98
	R_{O4H2}	1.95	
	R_{O1H3}	1.77	
	R_{O2H5}	1.73	
	R_{O3H8}	1.59	
	R_{H1Cl}	2.89	
$Cl(H_2O)_5$	R_{O1Cl}	2.34	4.42
	R_{O2H2}	1.88	
	R_{O3H4}	1.75	
	R_{O4H5}	1.83	
	R_{O4H1}	1.90	
	R_{O5H8}	1.69	
	R_{O2H9}	1.94	
	R_{H10Cl}	2.35	
$Cl(H_2O)_6$	R_{O1Cl}	2.33	3.10
	R_{O2H2}	1.77	
	R_{O2H5}	2.25	
	R_{O3H7}	1.72	
	R_{O4H9}	1.90	
	R_{O4H1}	1.86	
	R_{O5H12}	1.64	
	R_{O6H6}	1.90	
	R_{O6H3}	1.81	
	R_{H10Cl}	2.30	

Coordinates of the $ClO(H_2O)_{1-6}$ geometries optimized with M06-2X/6-311++G(3df,3pd)

(a)-I

0 2

O	-2.185248	-0.272701	0.000051
H	-3.045316	0.149632	-0.000386
H	-1.545580	0.445960	0.000078
Cl	1.092430	-0.387819	-0.000010
O	0.437697	1.022367	0.000008

(a)-II

0 2

O	2.295718	0.000010	-0.058532
H	2.796894	0.760418	0.242163
H	2.787937	-0.767293	0.239461
Cl	-0.459552	0.000977	-0.011212
O	-2.017275	-0.001226	0.022154

(a)-III

0 2

O	-2.298603	-0.238437	-0.000166
H	-1.929908	0.228768	-0.752699
H	-1.930707	0.225302	0.754890
Cl	1.087824	-0.398697	-0.000168
O	0.469555	1.028910	0.000251

(b)-I

0 2

Cl	1.256445	-0.483613	-0.255529
O	1.252313	0.831191	0.568902
O	-1.499139	1.437910	-0.135042
H	-0.570954	1.561363	0.099258
H	-1.608496	1.841336	-0.997953
O	-1.638370	-1.401892	0.130876
H	-1.737264	-0.444304	0.027508
H	-2.361289	-1.674648	0.697283

(b)-II

0 2

Cl	0.998751	0.239431	0.005122
O	2.327924	-0.57595	-0.008596
O	-2.100307	-1.291121	-0.097603
H	-1.786544	2.038209	-0.560197
H	-1.161073	-1.495109	-0.054636
O	-1.429234	1.437793	0.095534
H	-1.913524	0.606058	-0.005359
H	-2.504693	-1.785269	0.618448

(c)-I

0 2

Cl	-0.432365	-1.159900	-0.016249
O	-1.968882	-0.897526	-0.012939
O	2.222079	-1.010635	-0.034848
H	2.867782	-1.234723	0.636286
H	2.096487	-0.046927	0.019183
O	1.503609	1.682936	0.035678
H	1.794987	2.222191	-0.701450
H	0.533455	1.751167	0.037496
O	-1.307414	1.912520	-0.025326
H	-1.783359	1.070825	-0.040467
H	-1.754287	2.457400	0.624667

(c)-II

0 2

Cl	1.370730	-0.223082	-0.131052
O	2.664786	0.507057	0.334207
O	-1.801521	-0.077287	1.551574
H	-1.791181	0.685480	0.950662
H	-1.068267	0.060276	2.154813
O	-1.094269	-1.338813	-0.772533
H	-1.410362	-1.187946	0.137244
H	-1.431698	-2.188578	-1.058086
O	-1.523309	1.406755	-0.790788
H	-1.447515	0.528282	-1.191710
H	-2.118886	1.913178	-1.344714

(d)-I

0 2

Cl	1.192915	0.918204	-0.105289
O	2.377205	-0.088589	-0.056369
O	0.103752	-2.053710	0.096102
H	1.043619	-1.845191	0.073014
H	-0.248326	-1.556765	0.856695
O	-1.012565	-0.310728	1.954294
H	-1.349007	0.391521	1.369935
H	-1.729422	-0.537937	2.548105
O	-1.641417	1.479781	-0.071615
H	-2.375061	2.067029	-0.257226
H	-1.631142	0.797145	-0.775503
O	-1.248049	-0.598809	-1.753196
H	-0.740474	-1.199004	-1.163688
H	-1.881150	-1.149828	-2.215149

(d)-II

0 2

Cl	-1.537874	-0.151859	0.187916
O	-2.685863	0.251248	-0.783880
O	1.135473	1.833368	0.883550
H	1.021873	0.975903	1.333668
H	0.317474	2.312428	1.030645
O	1.490151	0.770874	-1.605918
H	2.256781	1.143967	-2.043741
H	1.379971	1.271046	-0.772206
O	1.435863	-1.776360	-0.677944
H	1.505694	-0.909998	-1.130746
H	0.731894	-2.249047	-1.126317
O	0.726002	-0.765600	1.700711
H	1.079428	-1.210744	2.472031
H	1.037745	-1.260194	0.909946

(e)-I

0 2

Cl	-0.742555	1.368094	-0.346620
O	-2.241803	1.113733	-0.018439
O	-1.173826	-1.227078	1.443419
H	-1.814495	-0.509586	1.397046
H	-1.171594	-1.591022	0.535427
O	1.711728	-1.196518	-1.110968
H	1.773981	-1.191034	-0.144281
H	1.932048	-0.285709	-1.339965
O	1.377621	-0.459987	1.623472
H	1.743641	-0.802819	2.440123
H	0.414981	-0.690608	1.628688
O	-0.918987	-1.867780	-1.199855
H	0.029246	-1.653662	-1.316652
H	-1.066538	-2.706231	-1.639300
O	2.020730	1.508189	-0.256379
H	1.919784	1.005832	0.569197
H	2.658668	2.202770	-0.087729

(e)-II

0 2

Cl	-1.227608	-1.10933	0.024962
O	-2.472937	-0.496064	-0.679481
O	1.211902	-1.653916	1.137713
H	1.592122	-1.524625	0.245657
H	1.753890	-2.304886	1.585486
O	-1.346117	2.115081	0.187487
H	-0.659023	2.139636	-0.490595

H	-2.019209	1.518872	-0.156332
O	1.950130	-0.937849	-1.376052
H	1.490969	-1.294884	-2.137877
H	1.766559	0.021447	-1.366146
O	0.903325	1.130079	1.619453
H	-0.035281	1.338287	1.495647
H	0.969171	0.163897	1.668361
O	1.342350	1.698620	-0.919277
H	1.976009	2.397995	-1.089452
H	1.324911	1.555269	0.062158

(e)-III

0 2

Cl	2.019753	0.480945	-0.033016
O	2.833282	-0.843765	0.051554
O	-1.234344	0.138503	1.603036
H	-2.068138	-0.059309	1.110855
H	-1.461358	0.195096	2.532799
O	0.040129	-1.982567	0.131074
H	-0.227442	-1.364484	0.826540
H	0.999788	-2.037208	0.185169
O	-0.210096	2.114069	-0.086167
H	-0.674926	2.952452	-0.085478
H	-0.597138	1.578000	0.628129
O	-1.067865	-0.144705	-1.708306
H	-0.559228	-0.835189	-1.249841
H	-0.685386	0.692065	-1.409659
O	-3.214078	-0.274316	-0.108643
H	-3.686820	-1.103204	-0.199833
H	-2.551368	-0.252027	-0.837777

(f)-I

0 2

O	2.211855	-0.612948	-1.420085
H	2.809677	-1.088831	-1.997890
H	1.307150	-0.947278	-1.611211
O	-2.117615	0.627690	-1.345033
H	-2.870323	0.871560	-1.885268
H	-2.462716	0.350151	-0.472336
O	-0.312152	-1.526253	-1.589911
H	-0.426562	-1.820810	-0.674483
H	-0.963835	-0.816647	-1.700376
O	-2.613398	-0.285452	1.155105
H	-1.827970	-0.848605	1.296046
H	-2.643489	0.320129	1.897412

O	2.001261	-0.733603	1.281455
H	2.233810	-0.740304	0.329714
H	1.968029	0.203293	1.505837
O	-0.373215	-1.858574	1.261372
H	0.522929	-1.432864	1.339549
H	-0.333012	-2.684712	1.746001
Cl	0.116409	1.607179	-0.073701
O	1.291683	2.053250	0.842087

(f)-II

0 2

O	-0.164628	-0.413652	2.083482
H	-0.996905	-0.668667	1.610845
H	-0.319600	-0.557914	3.018474
O	2.451918	1.440010	-0.508910
H	2.524168	0.577058	-0.056381
H	3.238618	1.933513	-0.271999
O	-2.353040	-0.931836	0.677431
H	-2.142549	-1.609941	0.029643
H	-2.490995	-0.104045	0.169734
O	2.286075	-0.942531	0.861575
H	1.450104	-0.837562	1.349310
H	2.147400	-1.715936	0.308860
O	-0.037671	2.015978	0.593323
H	-0.011655	1.324089	1.269885
H	0.833391	1.976415	0.161542
O	-2.35864	1.447392	-0.628151
H	-3.005142	2.139869	-0.484237
H	-1.512461	1.772170	-0.247107
Cl	0.094445	-0.558946	-1.476479
O	0.010993	-1.956231	-0.798552

(f)-III

0 2

O	-2.978418	-0.387053	0.154039
H	-2.393581	-0.104607	0.871925
H	-2.603902	-1.223661	-0.143810
O	-1.300773	0.772487	-1.780642
H	-2.098462	0.611983	-1.249390
H	-0.830222	1.464641	-1.293812
O	0.418078	-1.800778	1.297820
H	0.047794	-1.920878	0.401849
H	1.368312	-1.744432	1.152412
O	-0.712663	-1.771020	-1.193751
H	-0.787070	-0.842141	-1.514325

H	-0.503316	-2.317708	-1.952348
O	-0.855577	0.450934	1.936929
H	-1.002689	0.487427	2.883953
H	-0.310504	-0.358254	1.769510
O	-0.057200	2.433359	0.165513
H	-0.363507	1.873496	0.902345
H	-0.319924	3.333492	0.363293
Cl	1.877418	0.544373	-0.282185
O	2.721674	-0.762141	-0.254214

(f)-IV

0 2

O	2.272241	-1.879063	0.901931
H	2.420958	-2.673437	1.417091
H	2.949119	-0.968592	-0.824677
O	2.574140	-0.482116	-1.569518
H	1.693861	-0.872802	-1.659645
H	1.404044	-1.972160	0.469829
O	1.854025	0.791869	1.885295
H	2.270774	1.342061	1.208832
H	2.138855	-0.112733	1.692369
O	2.123121	2.046165	-0.712823
H	2.366129	1.189568	-1.124066
H	2.590333	2.730579	-1.193738
O	-0.325329	0.994873	0.233688
H	0.185998	1.594094	-0.328305
H	0.247008	0.923875	1.023684
O	0.061108	-1.483056	-0.685648
H	-0.758757	-1.933325	-0.896587
H	-0.184253	-0.577173	-0.377955
Cl	-2.971892	0.243427	0.055671
O	-4.409543	-0.339700	-0.097079

(f)-V

0 2

O	1.888950	-0.922462	1.786057
H	1.871970	0.045036	1.768308
H	2.479579	-1.180108	1.065496
O	2.341955	1.137478	-1.343636
H	2.505521	1.567206	-0.494735
H	1.385079	1.237253	-1.451504
O	1.478292	1.878622	1.277079
H	1.320348	2.584539	1.905391
H	0.659190	1.760713	0.759020
O	2.694485	-1.514647	-0.928667

H	2.656513	-0.565236	-1.173514
H	3.399745	-1.906826	-1.445075
O	-0.041933	-1.490815	-0.116164
H	0.435696	-1.393507	0.729592
H	0.664718	-1.786716	-0.705930
O	-0.381019	1.116604	-0.571157
H	-0.341166	0.136624	-0.445209
H	-1.298938	1.326680	-0.769803
Cl	-3.137621	-0.502815	0.312795
O	-3.280567	0.635495	-0.735953

Coordinates of the $Cl(H_2O)_{1-6}$ geometries optimized with M06-2X/6-311++G(3df,3pd)

(a)-I

0 2

Cl	-0.961581	0.000003	0.002302
O	1.612479	-0.000002	-0.118266
H	1.723618	0.764665	0.453512
H	1.723425	-0.764705	0.453491

(b)-I

0 2

Cl	-1.255403	-0.465126	-0.004738
O	0.149484	1.479629	-0.115105
H	0.937268	0.905299	-0.043016
H	-0.044960	1.778376	0.778515
O	1.944249	-0.574821	0.101089
H	2.522836	-0.856280	-0.610463
H	1.176838	-1.158725	0.067641

(c)-I

0 2

Cl	1.526077	-0.465238	-0.325839
O	-1.443500	-1.529771	0.330711
H	-1.620069	-1.745929	1.248496
H	-0.480089	-1.482661	0.251447
O	-1.723296	1.049536	-0.538225
H	-1.824402	0.113906	-0.276386
H	-1.685168	1.049528	-1.496760
O	0.521328	1.313454	0.839115
H	1.122614	1.978039	0.488723
H	-0.292445	1.330418	0.270933

(c)-II

0 2

Cl	-1.470647	-0.698990	-0.027147
O	-0.913355	1.577529	-0.052111
H	-1.206386	1.729986	0.852040
H	0.072987	1.467207	-0.010632
O	1.647411	-1.496041	-0.052514
H	0.679548	-1.491657	-0.097306
H	1.870397	-2.040968	0.704723
O	1.705942	1.216359	0.059878
H	2.218106	1.586522	-0.661403
H	1.846354	0.248973	0.032056

(d)-I

0 2

Cl	-1.938096	0.111637	-0.629926
O	0.693134	1.931040	0.301501
H	0.109575	2.139198	-0.433326
H	0.149738	1.371928	0.874051
O	2.552904	0.098649	-0.516738
H	1.988974	0.847164	-0.236302
H	3.403403	0.219677	-0.092484
O	-0.685152	-0.315460	1.374377
H	-1.379498	-0.761564	1.866655
H	-0.143225	-1.009309	0.892274
O	0.804905	-1.889594	-0.039898
H	1.542935	-1.273302	-0.241842
H	0.349403	-2.028699	-0.874222

(d)-II

0 2

Cl	1.936918	0.111226	-0.630097
O	-2.550177	0.100044	-0.517654
H	-3.400764	0.221944	-0.093788
H	-1.985515	0.847951	-0.236612
O	-0.691985	1.932445	0.302235
H	-0.107393	2.140231	-0.431907
H	-0.150273	1.371199	0.874376
O	0.684457	-0.315818	1.373845
H	0.142969	-1.010157	0.892065
H	1.378063	-0.761293	1.867777
O	-0.806087	-1.890983	-0.039058
H	-1.542830	-1.273313	-0.241772
H	-0.351541	-2.032903	-0.873436

(e)-I

0 2

Cl	-2.532704	-0.054849	-0.104871
O	-0.040867	0.440838	1.852191
H	0.344088	-0.424161	1.645947
H	-0.974254	0.337374	1.620798
O	2.962550	-0.000348	-0.487461
H	2.372347	0.773162	-0.508445
H	3.740049	0.268206	0.004674
O	0.827951	1.730513	-0.299104
H	0.637903	2.668446	-0.353072
H	0.501095	1.405383	0.576492
O	1.081372	-1.712234	0.401101

H	1.275606	-2.649742	0.446313
H	1.892530	-1.253311	0.097126
O	-0.624907	-0.411168	-1.426778
H	-0.218967	0.453405	-1.237784
H	-0.163215	-1.027138	-0.828839

(e)-II

0 2

Cl	1.638237	-0.898867	-0.389970
O	-0.246027	-1.925482	0.460927
H	1.385334	1.081926	0.703524
H	-0.851378	-1.647899	-0.251409
O	-1.174532	0.181274	1.850169
H	-1.823411	0.254389	1.137699
H	-0.433503	-1.244349	1.151494
O	-0.264797	1.478387	-1.657032
H	0.441015	0.835198	-1.794563
H	0.021290	1.954161	-0.865088
O	-2.114503	-0.301521	-0.829193
H	-1.547150	0.395504	-1.224295
H	-2.887217	-0.388941	-1.389330
O	0.910239	1.896976	0.932422
H	1.539249	2.471566	1.373293
H	-0.577299	0.932107	1.729811

(e)-III

0 2

Cl	1.916458	-0.632175	-0.438940
O	-1.047681	-1.734531	-1.056734
H	-0.092917	-1.585327	-1.116529
H	-1.444967	-0.934793	-1.422458
O	-1.366389	-0.840831	1.418492
H	-1.707115	-1.400114	2.118508
H	-1.274536	-1.390535	0.604766
O	0.357457	2.297324	-0.395274
H	0.937539	1.952783	-1.081097
H	-0.521915	1.942163	-0.599097
O	1.114160	0.464424	1.453277
H	0.863790	1.237703	0.896193
H	0.295161	-0.058304	1.546735
O	-2.127630	0.946176	-0.564929
H	-2.115643	0.500924	0.298028
H	-2.958513	1.421981	-0.621743

(f)-I

0 2

Cl	2.502469	-0.215743	-0.184273
O	0.018832	0.816228	-1.945811
H	-0.247755	1.504965	-1.317648
H	0.901107	0.550696	-1.648802
O	-2.485674	0.175296	0.862516
H	-2.103163	-0.439729	1.497506
H	-2.450283	-0.309581	0.022452
O	-0.777806	2.179303	0.373164
H	-1.508761	1.566896	0.616217
H	-1.017268	3.057778	0.672141
O	-1.559015	-1.205689	-1.394052
H	-1.896301	-1.667382	-2.162718
H	-0.971560	-0.470735	-1.713792
O	-0.444188	-1.885470	1.013947
H	-0.728536	-1.851108	0.082037
H	0.174344	-2.615950	1.085297
O	1.031156	0.375351	1.530403
H	0.558257	1.120693	1.116557
H	0.481512	-0.419064	1.362046

(f)-II

0 2

Cl	0.036792	-0.974948	1.322166
O	-2.265448	1.277410	0.663465
H	-1.792342	0.795698	1.350783
H	-1.557988	1.736063	0.186548
O	-2.785782	-0.906294	-0.910570
H	-2.815116	-0.111327	-0.340486
H	-3.236097	-1.603170	-0.429903
O	2.655059	-1.118603	-0.885059
H	2.973580	-1.842440	-0.341937
H	1.707451	-1.281464	-0.997907
O	0.126751	1.945457	-0.773123
H	0.272565	2.554340	-1.499354
H	0.991676	1.837904	-0.300160
O	-0.151923	-0.749482	-1.004143
H	-1.120746	-0.967664	-1.016239
H	-0.100902	0.232391	-1.025598
O	2.351473	1.277588	0.485602
H	2.595636	0.464080	0.002139
H	2.015776	0.951099	1.325919

(f)-III

0 2

Cl	-2.499548	-1.119794	-0.056461
O	2.476083	0.958935	0.082955
H	1.920852	1.110210	0.860557
H	2.748208	0.028473	0.142955
O	-1.433468	2.004791	-0.099541
H	-2.106642	1.317355	-0.170866
H	-0.839371	1.838604	-0.848696
O	0.171704	1.005102	1.777800
H	-0.094427	1.116631	2.691775
H	-0.466923	1.509085	1.219427
O	0.568501	0.928222	-1.743355
H	1.382157	1.025399	-1.185984
H	0.834874	0.963548	-2.663154
O	2.629107	-1.833466	0.012138
H	2.995929	-2.549397	0.532452
H	1.666120	-1.926950	0.046671
O	-0.101847	-1.109307	0.011296
H	-0.045775	-0.498305	0.773192
H	0.016689	-0.532371	-0.768830