ARTICLE

Computational insights into the formation and nature of the sulfilimine bond in collagen-IV

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Supporting Information

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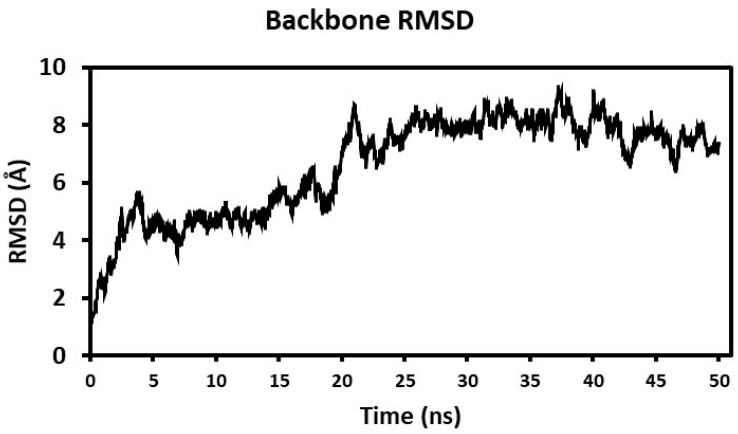

Figure S1. The backbone RMSD of collagen IV over 50 ns MD simulations.

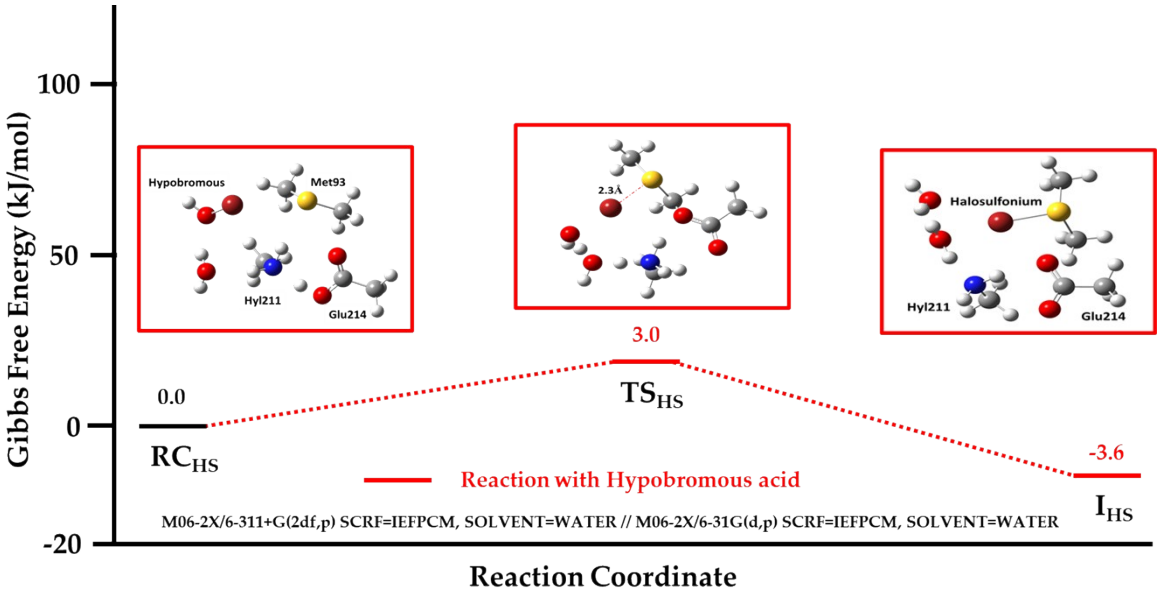

Figure S2. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed bromo halosulfonium intermediate with the reaction of hypobromous acid.

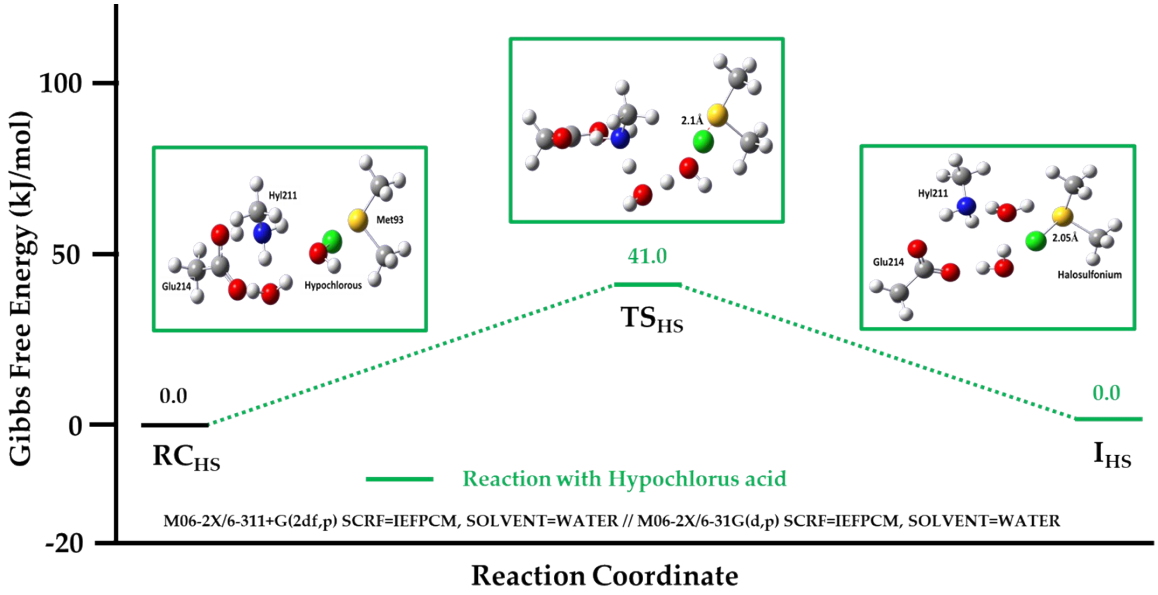

Figure S3. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed chloro halosulfonium intermediate with the reaction of hypochlorous acid.

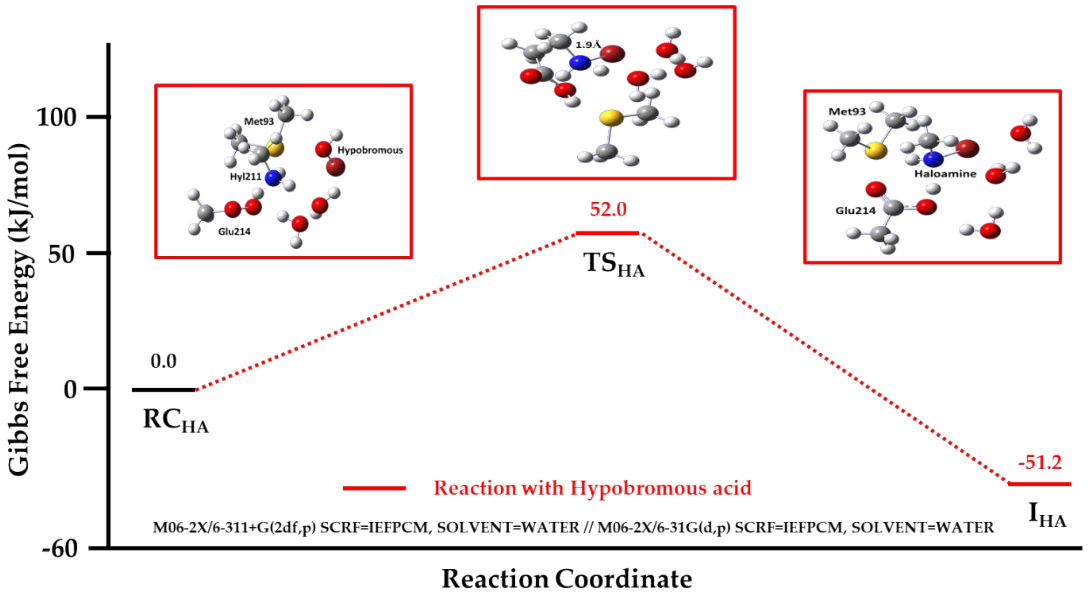

Figure S4. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed bromo haloamine intermediate with the reaction of hypobromous acid.

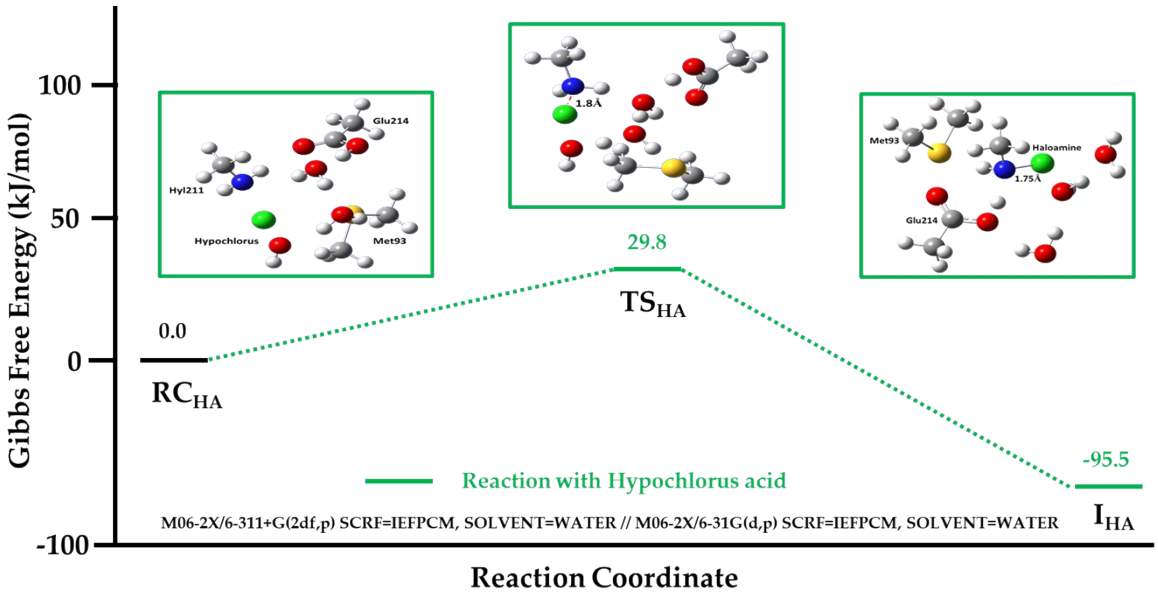

Figure S5. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed chloro haloamine intermediate with the reaction of hypochlorous acid.

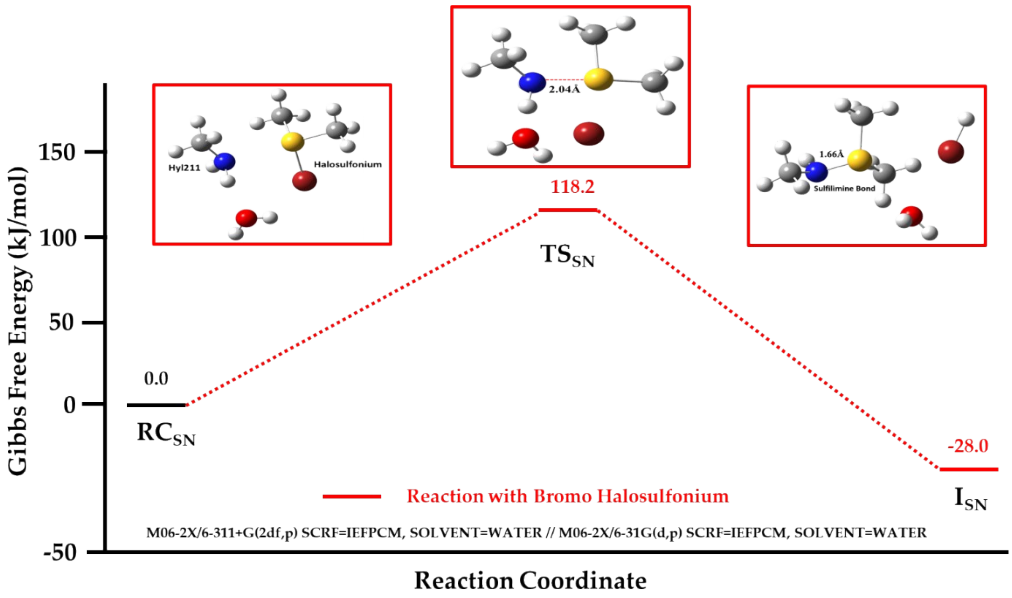

Figure S6. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed sulfilimine bond with the reaction of bromo halosulfonium.

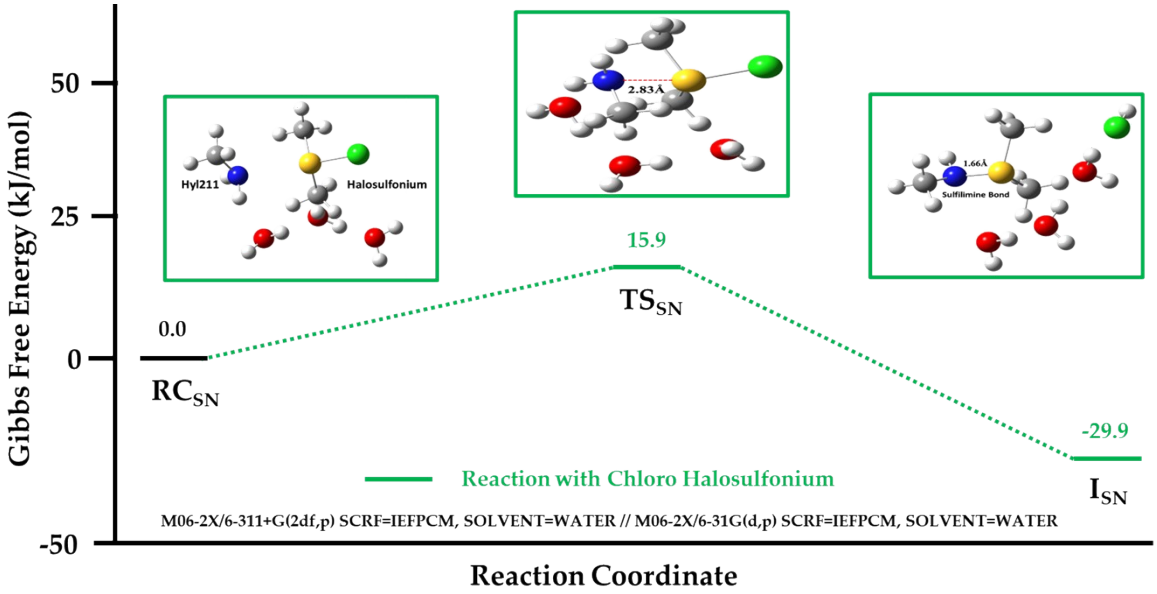

Figure S7. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed sulfilimine bond with the reaction of chloro halosulfonium.

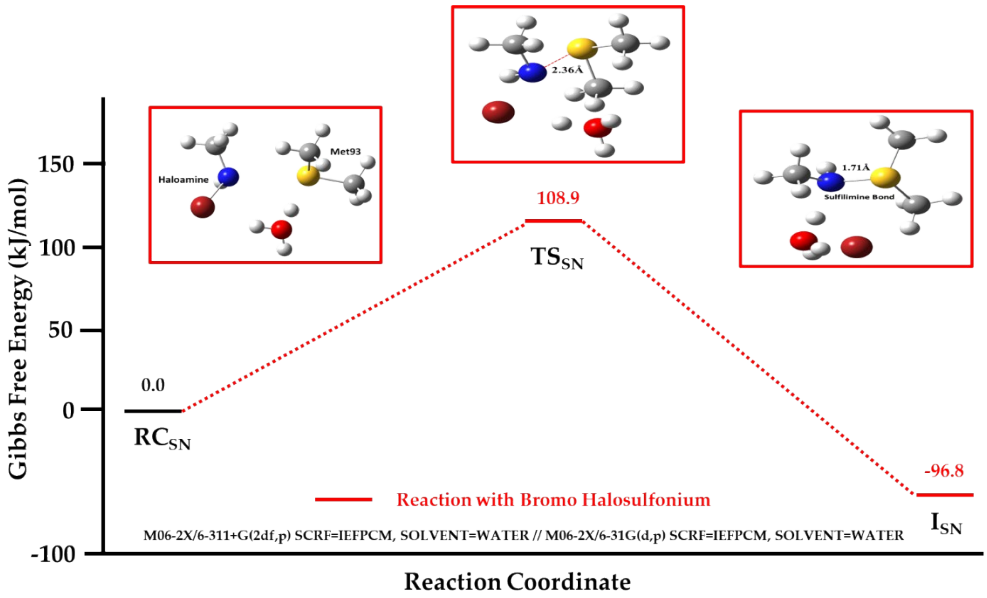

Figure S8. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed sulfilimine bond with the reaction of bromo haloamine.

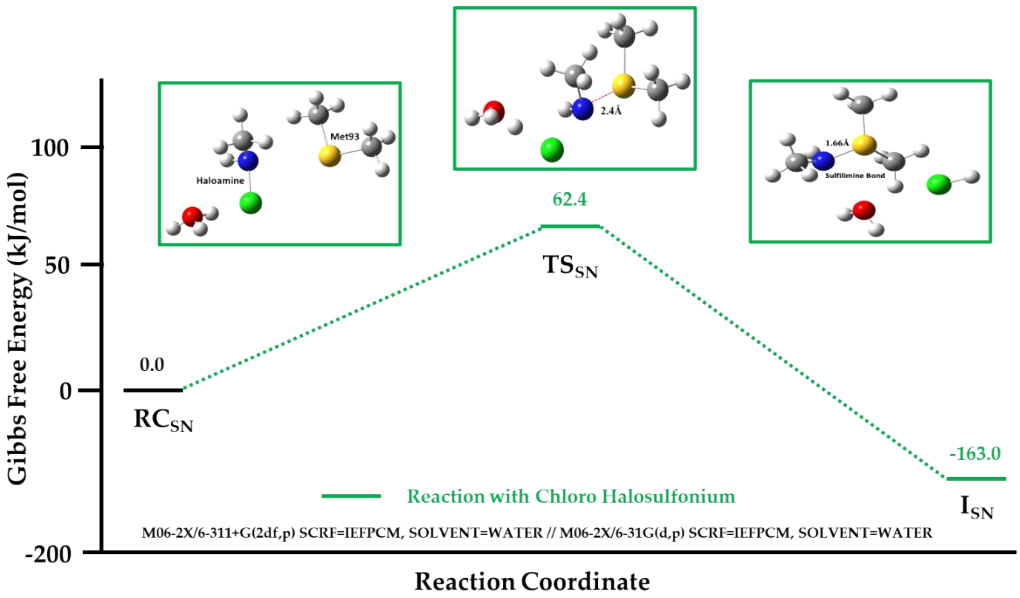

Figure S9. Gibbs free energy (kJ/mol) obtained from QM-cluster approach for the formation of the proposed sulfilimine bond with the reaction of chloro haloamine.

Table S1. Proton affinities (kJ/mol) of neutral, single protonated N of sulfilimine, and water molecules. Calculated S-N bond length of neutral, single, and double protonated sulfilimine complexes. Proton affinities are calculated using IEFPCM(water)-Method/6-311+G(2df,p)// IEFPCM(water)-M06-2X/6-311+G(2df,p) level of theory.

Methods	Compounds	Proton affinity (kJ/mol)	S-N Bond Length (Å)
M06-2X	$(H_3C)_2$-S-NH_2-CH_3		1.775
	$(H_3C)_2$-S=NH-CH_3	974.5	1.645
	$(H_3C)_2$-S=N-CH_3	1210.5	1.594
	H_2O	989.0	
QCISD	$(H_3C)_2$-S-NH_2-CH_3		1.778
	$(H_3C)_2$-S=NH-CH_3	986.2	1.650
	$(H_3C)_2$-S=N-CH_3	1218.4	1.599
	H_2O	993.8	

Table S2. Natural atomic charges were obtained from the present QTAIM analyses for all conformer 1 and 2 sulfilimine species considered in this present study. P(N) indicates the protonation state of N in sulfilimine complex while 1^1 and 1^2 denote isomer 1 and 2 of the single-protonated sulfilimine species, respectively.

P(N)	Atoms & Charges
	Conformer 1
2	S = 0.72334, N = -1.13995
1^1	S = 0.76594, N = -1.14754
1^2	S = 0.92374, N = -1.30361
0	S = 1.02013, N = -1.40706
	Conformer 2
2	S = 0.71789, N = -1.13467
1^1	S = 0.93361, N = -1.31682
1^2	S = 0.93309, N = -1.31613
0	S = 1.05962, N = -1.41681

Table S3. QTAIM analysis of the S-N bond critical points (BCPs) of conformer 1 and 2. P(N) indicates the protonation state of N in sulfilimine complex while 1^1 and 1^2 denote isomer 1 and 2 of the single-protonated sulfilimine species, respectively.

P(N)	$\nabla^2\rho(r)$	$\rho(r)$	ε
		Conformer 1	
2	-0.30607	0.17891	0.10917
1^1	-0.47860	0.21349	0.15101
1^2	-0.25625	0.22366	0.06243
0	-0.18123	0.24780	0.13700
		Conformer 2	
2	-0.29469	0.17661	0.10122
1^1	-0.22805	0.22363	0.03427
1^2	-0.22809	0.22363	0.03426
0	-0.08710	0.25016	0.09462

Table S4. Potential Gibbs free energies (kJ/mol) obtained under protein environment (ε = 4.0) using the QM-cluster approach for the formation of the proposed halosulfonium intermediated from hypobromous and hypochlorous acid.

Reactions	Reactants	$\Delta G^{‡}$ (kJ/mol)	ΔG^{0} (kJ/mol)
Halosulfonium by HOBr	$S(CH_3)_2 + CH_3NH_2 + CH_3COOH + H_2O + HOBr$	4.3	-15.1
Halosulfonium by HOCl	$S(CH_3)_2 + CH_3NH_2 + CH_3COOH + H_2O + HOCl$	41.1	0.0
Haloamine by HOBr	$S(CH_3)_2 + CH_3NH_3 + CH_3COO^- + 2H_2O + HOBr$	49.7	-59.5
Haloamine by HOCl	$S(CH_3)_2 + CH_3NH_3 + CH_3COO^- + 2H_2O + HOCl$	29.7	-95.5

Table S5. Gibbs free energies (kJ/mol) obtained under protein environment (ε = 4.0) using the QM-cluster approach for the formation of the proposed sulfilimine bond from halosulfonium and haloamine.

Reactions	Reactants	$\Delta G^{‡}$ (kJ/mol)	ΔG^{0} (kJ/mol)
Sulfilimine via Bromo Halosulfonium	$BrS(CH_3)_2 + CH_3NH_2 + H_2O$	128.2	-15.3
Sulfilimine via Chloro Halosulfonium	$ClS(CH_3)_2 + CH_3NH_2 + 3H_2O$	21.1	-31.7
Sulfilimine via Bromo Haloamine	$S(CH_3)_2 + CH_3N(H)Br + H_3O^+$	105.1	-98.5
Sulfilimine via Chloro Haloamine	$S(CH_3)_2 + CH_3N(H)Cl + H_3O^+$	69.1	-157.5

Cartesian Coordinates

Table S6. Cartesian coordinates of all single point calculations obtained at the IEFPCM(solvent = water)M06-2X/6-311+G(2df,p) // IEFPCM(water)-M06-2X/6-31G(d,p) level of theory.

Formation of Halosulfonium with the Reaction of Hypobromous acid (HOBr)
Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - Halo sulfonium - HOBr\\0,1\S,0,-0.533068,1.982222,-0.17872\C,0,-2.180201,2.363688,0.473065\H,0,-2.897825,2.008695,-0.26695\H,0,-2.34797,1.831148,1.412912\H,0,-2.302166,3.436952,0.630863\C,0,0.0124,-0.987711,1.609956\H,0,0.096583,-1.827543,2.303143\H,0,-0.765949,-0.31341,1.978388\H,0,0.964913,-0.444457,1.599251\N,0,-0.369603,-1.487359,0.28445\H,0,-0.363217,-0.700732,-0.366305\H,0,0.343484,-2.151416,-0.021835\H,0,-1.836157,-1.803606,0.288115\C,0,0.481223,2.562896,1.207709\H,0,0.408461,3.645556,1.326145\H,0,0.175247,2.068374,2.13295\H,0,1.514125,2.288236,0.985046\O,0,3.268334,-0.25009,0.753627\H,0,4.206579,-0.049393,0.600197\Br,0,2.44678,0.20963,-0.822113\C,0,-3.403978,-0.93543,-0.465535\O,0,-2.900991,-1.825196,0.36166\O,0,-2.738384,-0.290859,-1.264272\C,0,-4.897132,-0.762543,-0.3179\H,0,-5.10645,-0.312672,0.656573\H,0,-5.28069,-0.118041,-1.107127\H,0,-5.393521,-1.734498,-0.346302\O,0,2.256612,-2.917753,0.288764\H,0,2.739617,-2.145044,0.618805\H,0,2.165506,-3.493464,1.056449\\

TS Complex

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Intermediate Complex

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655072\H,0,0.429943,1.240911,2.014519\N,0,0.046713,2.583276,0.461823\H
,0,0.494232,1.975387,-0.236969\H,0,-1.555093,2.124664,0.642009\H,0,0.2
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-4.375328,0.016956\H,0,-1.274642,-3.379835,1.090965\H,0,-1.66944,-3.55
6284,-0.650425\O,0,-2.420326,1.610594,0.791683\H,0,-2.902781,1.666848,
-0.057388\Br,0,-1.223954,-0.384551,0.216756\C,0,2.738439,0.828877,-0.7
30703\O,0,3.066073,2.029606,-0.648311\O,0,1.551163,0.382659,-0.779093\
C,0,3.861305,-0.220183,-0.723834\H,0,4.115514,-0.459922,0.314965\H,0,3
.546957,-1.143811,-1.214951\H,0,4.761713,0.171676,-1.200659\O,0,-3.542
131,1.421804,-1.734527\H,0,-3.402847,2.206813,-2.277292\H,0,-4.498581,
1.297422,-1.729851\\

Formation of Halosulfonium with the Reaction of Hypochlorus acid (HOCl)

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Optimi
zation and Frequency - REACTANT - Formation of Halosulfonium with 1H
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,0,4.639635,-2.348798,-1.165361\C,-1,-0.976411,1.641305,-1.759367\H,0,
-1.79798,2.360982,-1.759917\H,0,-0.892339,1.221722,-2.763307\H,0,-0.04
9812,2.175575,-1.522206\N,0,-1.281045,0.570876,-0.798053\H,0,-0.532517
,-0.119401,-0.810897\H,0,-1.269249,0.984168,0.138239\H,0,-2.659139,-0.
136416,-0.920974\C,-1,3.439804,-1.805912,1.470285\H,0,4.153443,-2.6309
43,1.492247\H,0,3.960105,-0.856757,1.614097\H,0,2.707365,-1.939788,2.2
66696\O,0,1.748457,2.775901,0.227547\H,0,2.458261,3.090523,0.810965\C,
0,-3.981299,-0.968021,0.233556\O,0,-3.592835,-0.619257,-0.976547\O,0,-
3.33911,-0.738542,1.245709\C,-1,-5.311054,-1.68916,0.244036\H,0,-5.239
336,-2.59598,-0.36087\H,0,-5.590211,-1.943585,1.264772\H,0,-6.076586,-
1.053323,-0.206338\O,0,-0.882558,2.601155,1.329562\H,0,0.01045,2.82112
8,1.017316\H,0,-1.441192,3.303689,0.978325\Cl,0,1.995569,1.078091,0.11
9222\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Optimi
zation and Frequency - TS - Formation of Halosulfonium with 1 H2O\\0,1
\S,0,-2.493201,-1.456766,0.016419\C,0,-3.550193,-1.444036,1.476394\H,0
,-2.910054,-1.250227,2.33617\H,0,-4.309767,-0.669481,1.369726\H,0,-4.0
01854,-2.433378,1.560602\C,-1,1.003436,1.630522,1.719562\H,0,1.522145,
2.580157,1.85953\H,0,1.166193,1.005749,2.599302\H,0,-0.062494,1.833854
,1.603302\N,0,1.518575,0.98818,0.49727\H,0,1.158,0.040733,0.375011\H,0
,1.185407,1.670915,-0.422175\H,0,2.557049,0.816464,0.520851\C,-1,-3.71
4435,-1.600134,-1.300512\H,0,-4.14194,-2.601746,-1.242341\H,0,-4.48032
1,-0.835187,-1.173919\H,0,-3.184512,-1.473176,-2.24365\O,0,-1.491035,2
.761248,-0.259834\H,0,-2.13819,3.090261,-0.896996\C,0,3.855241,-1.0427
92,-0.101475\O,0,4.114015,0.114412,0.34881\O,0,2.71644,-1.535839,-0.26
0443\C,-1,5.077671,-1.896141,-0.474225\H,0,5.682746,-2.076554,0.418884
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Intermediate Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Optimi
zation and Frequency - INTERMEDIATE - Formation of Halosulfonium with
1 H2O\\0,1\S,0,-3.081387,-0.38711,0.829917\C,0,-3.650511,1.14956,0.080
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,0,-4.620047,1.375006,0.526908\C,-1,0.794792,2.654516,1.287817\H,0,1.0
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\C,-1,-4.211325,-1.587541,0.104869\H,0,-5.192195,-1.392574,0.541843\H,
0,-4.226814,-1.471944,-0.978735\H,0,-3.859267,-2.575891,0.396955\O,0,0
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66,-0.624523,0.268745\O,0,3.862581,0.533438,-0.144226\O,0,2.49816,-1.1
76113,0.37839\C,-1,4.833454,-1.494549,0.671359\H,0,5.750229,-0.907207,
0.730456\H,0,4.638203,-1.98022,1.630308\H,0,4.964705,-2.28686,-0.07175
\O,0,0.211342,1.652723,-2.158853\H,0,0.629819,-0.115886,-1.911271\H,0,
-0.752045,1.662865,-2.123023\Cl,0,-1.357604,-0.733314,-0.236262\\

Formation of Haloamine with the Reaction of Hypobromous acid (HOBr)

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - Halo
amine - HOBr\\0,1\S,0,0.306329,-1.968383,-0.475584\C,0,1.929967,-2.637
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.047504\H,0,2.047292,-3.65636,-0.408869\C,0,0.448112,0.099558,2.602007
\H,0,0.678119,0.785974,3.415806\H,0,1.247884,-0.636249,2.511203\H,0,-0
.498824,-0.404282,2.792636\N,0,0.35797,0.855277,1.337045\H,0,0.140114,
0.197612,0.574924\H,0,-0.377517,1.584164,1.352584\H,0,1.325931,1.27797
4,1.083872\C,0,-0.769689,-3.104246,0.441856\H,0,-0.689092,-4.12144,0.0
547\H,0,-0.521115,-3.090788,1.505344\H,0,-1.79228,-2.745472,0.309391\O
,0,-2.38452,-0.020824,1.105572\H,0,-3.238027,-0.410167,1.356826\Br,0,-
2.440991,0.031491,-0.726444\C,0,3.013113,0.847177,-0.324271\O,0,2.8063
94,1.497461,0.74161\O,0,2.128127,0.533565,-1.163276\C,0,4.440084,0.383
001,-0.575765\H,0,4.691889,-0.393005,0.153573\H,0,4.551584,-0.02002,-1
.5821\H,0,5.135057,1.211087,-0.42202\O,0,-1.543158,2.850487,0.726644\H
,0,-2.381419,2.374163,0.695222\H,0,-1.107601,2.667133,-0.13556\O,0,0.0
4672,2.183153,-1.388781\H,0,0.786024,1.529412,-1.26065\H,0,0.49123,2.9
85368,-1.686144\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - TS
Haloamine - HOBr\\0,1\C,0,1.511819,-2.003375,2.094557\H,0,1.565502,-1.
878229,3.177267\H,0,2.49585,-1.849304,1.652157\H,0,1.141885,-2.999297,
1.853406\N,0,0.576542,-1.008186,1.547869\H,0,-0.480084,-1.140002,1.830
7\H,0,0.927801,-0.054616,1.691508\O,0,-0.961485,-1.472302,-2.387421\H,
0,-0.751007,-2.365134,-2.686643\Br,0,0.266437,-1.190091,-0.36344\O,0,-
1.980192,-1.376376,1.673157\H,0,-2.385576,-0.542108,1.940635\H,0,-2.28
0619,-1.487423,0.631742\O,0,-2.707319,-1.576822,-0.690352\H,0,-3.26782
,-2.355284,-0.782173\H,0,-1.814789,-1.572053,-1.650486\S,0,-1.247915,1
.779515,0.526067\C,0,-1.840463,3.447912,0.922608\C,0,-1.85762,1.637236
,-1.177793\H,0,-1.418275,4.179742,0.232032\H,0,-2.930082,3.481376,0.87

7672\H,0,-1.515075,3.678726,1.937348\H,0,-1.501449,0.682332,-1.565727\
H,0,-2.948342,1.649005,-1.187639\H,0,-1.466629,2.458116,-1.782729\C,0,
2.520671,1.180441,-0.252212\O,0,2.450844,0.951826,0.942999\O,0,1.61481
8,1.902258,-0.901815\C,0,3.590173,0.636996,-1.151376\H,0,4.474517,0.38
6351,-0.568691\H,0,3.18583,-0.27657,-1.599562\H,0,3.829856,1.337932,-1
.950328\H,0,0.863249,2.08076,-0.289496\\

Intermediate Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - Inte
rmediate Haloamine - HOBr\\0,1\S,0,-1.684416,-2.464652,-0.777373\C,0,-
1.21673,-3.392801,0.710729\H,0,-0.217995,-3.793423,0.53682\H,0,-1.1814
71,-2.730237,1.579551\H,0,-1.920927,-4.20525,0.89672\C,0,0.062642,-0.0
23323,2.051401\H,0,0.428672,0.922189,2.453116\H,0,0.761057,-0.824614,2
.311041\H,0,-0.925157,-0.249447,2.465616\N,0,0.065069,0.055472,0.58708
6\H,0,-0.250848,-0.836757,0.187444\H,0,-2.420141,3.834404,-1.38531\H,0
,1.563049,0.113249,-0.00034\C,0,-3.253472,-1.751752,-0.20832\H,0,-3.96
6679,-2.541684,0.032724\H,0,-3.093513,-1.11106,0.661941\H,0,-3.6469,-1
.143141,-1.023487\O,0,-3.053436,3.258249,-0.941455\H,0,-3.19337,3.6792
71,-0.085015\Br,0,-1.225994,1.296185,-0.049579\C,0,2.659373,-1.436232,
-0.235762\O,0,2.50204,-0.122086,-0.340816\O,0,1.802755,-2.171403,0.223
898\C,0,3.994434,-1.90852,-0.744213\H,0,4.794026,-1.376161,-0.224732\H
,0,4.093313,-2.980991,-0.589548\H,0,4.078372,-1.675203,-1.808305\O,0,1
.610934,2.704183,1.097124\H,0,1.588487,3.440346,1.719743\H,0,0.754997,
2.733067,0.647657\O,0,3.653377,2.486909,-0.871054\H,0,3.002276,2.72728
2,-0.191693\H,0,3.554869,1.526767,-0.904887\\

Formation of Haloamine with the Reaction of Hypochlorus acid (HOCl)

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Optim
ization and Frequency - REACTANT - Formation of Haloamine with 2 H2O\\
0,1\S,0,0.966243,2.286917,0.114158\C,0,-0.14197,3.649088,0.562219\H,0,
-1.146741,3.366448,0.24352\H,0,-0.139337,3.805884,1.642174\H,0,0.15102
2,4.568406,0.052489\C,-1,-2.095754,-3.170204,0.511378\H,0,-1.571649,-2
.83699,-0.386183\H,0,-3.065482,-3.576296,0.21635\H,0,-1.510046,-3.9659
31,0.984425\N,0,-2.297447,-2.013391,1.381292\H,0,-2.78162,-2.261049,2.
238607\H,0,-1.397774,-1.594054,1.602109\H,0,1.143997,-1.81304,-0.39878
7\C,-1,2.539499,2.934798,0.731618\H,0,2.834636,3.829598,0.181518\H,0,2
.463893,3.160248,1.796865\H,0,3.277112,2.145534,0.580892\O,0,-3.624671
,1.022203,-0.958253\H,0,-3.755281,1.781715,-0.371528\C,0,3.014208,-1.5
95944,-0.188019\O,0,1.993195,-2.332444,-0.593765\O,0,2.888712,-0.48356
4,0.300337\C,-1,4.337085,-2.285707,-0.384797\H,0,4.459412,-2.548099,-1
.43774\H,0,5.149588,-1.637716,-0.062444\H,0,4.348075,-3.214187,0.19041
\O,0,-1.023722,0.676032,-1.925794\H,0,-0.456986,1.456857,-1.965689\H,0
,-1.918662,0.995008,-1.698241\O,0,0.032938,-0.847018,0.106209\H,0,0.63
1387,-0.189749,0.500217\H,0,-0.426305,-0.353353,-0.614843\Cl,0,-3.1598
25,-0.299413,0.140355\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Optimi
zation and Frequency - TS - Formation of Haloamine with 2 H2O\\0,1\S,0

,-0.803185,2.672338,0.151799\C,0,0.53103,2.237095,-0.997114\H,0,1.3472
91,1.852484,-0.384177\H,0,0.2083,1.455121,-1.689794\H,0,0.859546,3.113
175,-1.558926\C,-1,2.113565,-3.249726,-0.774762\H,0,2.02313,-3.347608,
0.305642\H,0,3.133287,-3.462712,-1.089676\H,0,1.413425,-3.919501,-1.27
4169\N,0,1.775982,-1.858078,-1.137943\H,0,1.81855,-1.70501,-2.146712\H
,0,0.841866,-1.561021,-0.75901\H,0,-1.280258,-1.483771,0.893562\C,-1,-
2.083656,3.16201,-1.035099\H,0,-1.727417,3.969717,-1.676896\H,0,-2.384
001,2.304608,-1.640366\H,0,-2.942852,3.512607,-0.462259\O,0,3.546175,1
.017351,1.010932\H,0,3.610112,1.793628,0.440646\C,0,-3.04952,-1.404495
,0.20055\O,0,-2.1755,-1.958386,1.023324\O,0,-2.778462,-0.477218,-0.547
356\C,-1,-4.412531,-2.0392,0.279921\H,0,-4.789551,-1.966336,1.302368\H
,0,-5.095803,-1.544333,-0.407195\H,0,-4.334258,-3.100081,0.032096\O,0,
1.309008,0.770047,1.867996\H,0,0.885429,1.569552,2.198\H,0,2.433508,0.
986304,1.476639\O,0,-0.10921,-0.618458,0.392183\H,0,-0.718249,-0.01999
2,-0.072655\H,0,0.485981,0.001085,1.05048\Cl,0,2.805978,-0.605857,-0.2
952\\

Intermediate Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Optimi
zation and Frequency - INTERMEDIATE - Formation of Haloamine wit h 2 H
2O\\0,1\S,0,-0.224513,2.316981,-0.210205\C,0,1.453649,2.911476,-0.5515
58\H,0,2.150257,2.187244,-0.123826\H,0,1.620406,2.986192,-1.627683\H,0
,1.612886,3.885835,-0.08523\C,-1,1.805074,-3.7147,-0.556366\H,0,1.7729
55,-3.727182,0.533526\H,0,2.790404,-4.041724,-0.899783\H,0,1.038367,-4
.388676,-0.944009\N,0,1.456356,-2.367424,-1.024583\H,0,1.480987,-2.344
265,-2.043228\H,0,0.103054,-1.560379,-0.217293\H,0,-1.938584,-1.609652
,0.746259\C,-1,-1.183605,3.678756,-0.928803\H,0,-0.97465,4.612558,-0.4
04386\H,0,-0.952848,3.78864,-1.989788\H,0,-2.238674,3.427367,-0.814667
\O,0,3.797356,0.891979,1.065434\H,0,4.075176,1.768788,1.351832\C,0,-3.
548338,-0.825513,0.144488\O,0,-2.920917,-1.783751,0.814735\O,0,-2.9670
21,0.086451,-0.418559\C,-1,-5.042516,-0.996151,0.155447\H,0,-5.399825,
-1.01891,1.187088\H,0,-5.51405,-0.180007,-0.387734\H,0,-5.300523,-1.95
2273,-0.305213\O,0,1.219592,0.549619,2.044013\H,0,0.692311,1.358712,2.
058939\H,0,2.906942,0.773466,1.454098\O,0,-0.453832,-0.993448,0.379898
\H,0,-0.827272,-0.281861,-0.170427\H,0,0.691348,-0.064797,1.497034\Cl,
0,2.664826,-1.202871,-0.526093\\

Formation of Sulfilimine Bond with the Reaction of Brominated Halosulfonium

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Reactant of Sulfilimine bond from H a
losulfonium with Bromine and 1 H2O\\1,1\S,0,0.644546,0.763474,0.531183
\C,0,2.285846,0.759861,1.290137\H,0,2.297736,-0.038152,2.031365\H,0,3.
057897,0.616796,0.535522\H,0,2.386492,1.729731,1.782083\C,0,-2.639259,
1.860815,0.057239\H,0,-2.319702,1.980731,1.096579\H,0,-3.734002,1.7907
06,0.045674\H,0,-2.352826,2.767589,-0.482726\N,0,-1.954589,0.703887,-0
.523478\H,0,-2.241413,0.584393,-1.491573\H,0,-2.235265,-0.146902,-0.03
2994\C,0,0.915335,1.926862,-0.820327\H,0,1.019448,2.907109,-0.349465\H
,0,1.817709,1.65024,-1.364293\H,0,0.020147,1.880162,-1.435881\O,0,-2.3
23783,-1.919562,1.027742\H,0,-1.408433,-2.200306,0.909954\H,0,-2.82219

,-2.495244,0.435659\Br,0,0.717215,-1.145668,-0.511392\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_TS
(SN Bond) of Sulfilimine bond from H alosulfonium with Bromine and 1
H2O. From Reactant to TS.\\1,1\S,0,0.670409,-0.738922,0.528138\C,0,-0.
181803,-2.374989,0.642464\H,0,-1.13291,-2.196266,1.136047\H,0,-0.32797
5,-2.798157,-0.350436\H,0,0.480937,-2.998228,1.246999\C,0,2.410031,1.5
0866,-0.503055\H,0,2.769412,1.433003,0.525531\H,0,2.334908,2.567652,-0
.764289\H,0,3.091887,1.014911,-1.191051\N,0,1.059808,0.929137,-0.58714
4\H,0,0.748442,0.746039,-1.54346\H,0,0.393931,1.579368,-0.115489\C,0,2
.174141,-1.476281,-0.189631\H,0,2.363233,-2.392091,0.368569\H,0,1.9998
21,-1.715905,-1.240234\H,0,3.015163,-0.801115,-0.073639\O,0,-0.321605,
2.534644,1.15652\H,0,-1.238128,2.227337,1.132704\H,0,-0.364411,3.48268
2,0.980561\Br,0,-1.603454,-0.030055,-0.382939\\

Product Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Intermediate of Sulfilimine Bond fr o
m Halosulfonium with Br and 1 H2O\\1,1\S,0,-1.185739,-0.138494,0.08656
3\C,0,-0.69888,0.302909,1.756022\H,0,-0.815458,1.38224,1.826013\H,0,-1
.323349,-0.23322,2.471207\H,0,0.352364,0.032719,1.859334\C,0,-3.482805
,0.28468,-1.167957\H,0,-3.5794,-0.691064,-1.652688\H,0,-2.927743,0.962
822,-1.817431\H,0,-4.476075,0.69999,-0.99942\N,0,-2.811492,0.223634,0.
1393\C,0,-1.028854,-1.936178,0.130563\H,0,0.040125,-2.153704,0.1152\H,
0,-1.502886,-2.33887,1.025819\H,0,-1.496616,-2.324342,-0.7745\H,0,-3.3
19699,-0.323954,0.832123\O,0,0.628049,2.244359,-0.02218\H,0,0.568403,2
.486531,-0.953597\H,0,1.179624,2.930088,0.371871\Br,0,2.265313,-0.2326
42,-0.243659\H,0,2.905853,-1.499637,-0.270288\\

Formation of Sulfilimine Bond with the Reaction of Chlorinated Halosulfonium

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Reactant of Sulfilimine bond from H a
losulfonium with Cl and 3 H2O\\1,1\S,0,-1.718082,-0.611766,0.575733\C,
0,-2.191757,1.013373,1.189647\H,0,-1.397928,1.703235,0.902913\H,0,-3.1
54843,1.293616,0.764338\H,0,-2.250409,0.907582,2.275294\C,0,4.238649,0
.449063,0.517717\H,0,4.359655,0.923887,-0.458432\H,0,5.017295,0.830007
,1.187259\H,0,3.258431,0.733077,0.907988\N,0,4.270225,-1.010061,0.3422
17\H,0,4.230326,-1.465955,1.249778\H,0,5.151435,-1.292599,-0.077191\C,
0,-3.310963,-1.454751,0.586838\H,0,-3.567583,-1.58351,1.641089\H,0,-4.
064453,-0.863369,0.067832\H,0,-3.169105,-2.428008,0.118804\Cl,0,-1.508
135,-0.257365,-1.404827\O,0,0.763727,0.58167,0.634572\H,0,0.692076,1.4
09708,0.129981\H,0,1.18901,-0.065532,0.027553\O,0,-0.16529,2.928697,-0
.53885\H,0,-0.322668,2.939329,-1.490032\H,0,0.239921,3.780889,-0.34039
3\O,0,1.933555,-1.285383,-0.983124\H,0,1.515367,-2.121586,-0.748427\H,
0,2.837996,-1.312867,-0.549535\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the TS of Sulfilimine bond from Halosulfo
nium with Cl and 3H2O\\1,1\S,0,-0.799108,-0.312859,-0.044084\C,0,-0.99
5605,-2.015338,-0.591246\H,0,-1.151149,-2.62435,0.297279\H,0,-1.820946
,-2.086171,-1.298992\H,0,-0.035052,-2.258596,-1.050041\C,0,1.895554,-0
.536437,1.957765\H,0,2.047898,0.327377,1.304229\H,0,2.83944,-0.735967,
2.481069\H,0,1.145588,-0.262256,2.706233\N,0,1.401466,-1.650522,1.1514
63\H,0,1.340592,-2.49448,1.713419\H,0,2.042959,-1.828475,0.382669\C,0,
-0.58906,0.495933,-1.643836\H,0,0.391858,0.162839,-1.99328\H,0,-1.3872
18,0.183035,-2.316143\H,0,-0.602335,1.56769,-1.457265\Cl,0,-2.748793,0
.190198,0.335122\O,0,2.159752,1.82161,-0.687597\H,0,1.418979,2.100422,
-0.114895\H,0,2.952029,2.192169,-0.282004\O,0,-0.126156,2.348017,0.800
294\H,0,-0.5082,3.228966,0.697638\H,0,-0.027751,2.224241,1.753004\O,0,
2.229929,-0.824018,-1.458563\H,0,2.73069,-0.902597,-2.278315\H,0,2.354
012,0.102366,-1.165756\\

Product Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Intermediate of Sulfilimine Bond fro
m Halosulfonium with Cl and 3 H2O\\1,1\S,0,-0.691226,-0.548352,-0.1421
37\C,0,0.118184,-0.393672,1.450382\H,0,-0.558394,0.211977,2.051082\H,0
,0.269905,-1.385499,1.877222\H,0,1.067683,0.113291,1.281306\C,0,-3.157
896,-1.420925,-0.572077\H,0,-3.02658,-1.647359,-1.634824\H,0,-3.49637,
-0.393028,-0.438947\H,0,-3.906068,-2.096058,-0.155957\N,0,-1.934362,-1
.596862,0.223164\C,0,0.503486,-1.534453,-1.062338\H,0,1.372393,-0.8975
71,-1.23023\H,0,0.778436,-2.423336,-0.493263\H,0,0.038271,-1.802798,-2
.011112\H,0,-1.622356,-2.561679,0.30582\Cl,0,3.768614,-0.31338,0.25851
1\H,0,4.651484,-1.105272,0.74893\O,0,1.404338,1.523645,-0.715614\H,0,1
.755297,1.614819,-1.611671\H,0,1.996285,2.05267,-0.163962\O,0,-2.54510
7,1.28705,1.023212\H,0,-2.086441,1.9596,0.477614\H,0,-2.723309,1.71479
4,1.867394\O,0,-1.069743,2.913178,-0.6225\H,0,-0.212451,2.454006,-0.68
7568\H,0,-0.86261,3.773892,-0.241067\\

Formation of Sulfilimine Bond with the Reaction of Brominated Haloamine

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Reactant of Sulfilimine bond from Hal
oamine with Br and H3O\\1,1\S,0,2.272374,0.199917,-0.4522\C,0,2.13236,
1.032941,1.153362\H,0,1.111762,1.406651,1.231895\H,0,2.329236,0.325919
,1.96008\H,0,2.836728,1.86352,1.195283\C,0,-1.1381,2.145156,-0.126165\
H,0,-1.159613,2.217973,0.962364\H,0,-2.078866,2.525446,-0.534093\H,0,-
0.307645,2.747039,-0.5079\N,0,-0.846605,0.757177,-0.508094\H,0,-0.9029
19,0.681471,-1.524792\C,0,3.934723,-0.508314,-0.28913\H,0,4.660625,0.2
99975,-0.199014\H,0,3.984457,-1.161876,0.582127\H,0,4.136965,-1.080015
,-1.194426\O,0,0.504704,-1.948851,0.334311\H,0,0.572088,-2.757851,-0.2
02922\H,0,-0.432146,-1.637113,0.338809\H,0,1.167281,-1.170027,-0.04049

6\Br,0,-2.284607,-0.376797,0.046344\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the TS of Sulfilimine bond from Haloami n
e with Br and H3O+\\1,1\S,0,-2.461144,-0.474275,-0.364107\C,0,-2.55649
1,0.30394,1.262216\H,0,-1.630448,0.853068,1.444115\H,0,-3.417127,0.972
362,1.301412\H,0,-2.675082,-0.484972,2.005582\C,0,-0.030924,-1.846201,
0.882069\H,0,0.27566,-1.433798,1.843407\H,0,0.679458,-2.609544,0.56515
7\H,0,-1.009391,-2.316687,0.988766\N,0,-0.125725,-0.718846,-0.09195\H,
0,-0.095724,-1.119819,-1.036186\C,0,-2.164197,0.987706,-1.378173\H,0,-
2.99216,1.689403,-1.272472\H,0,-1.225477,1.445549,-1.058703\H,0,-2.088
346,0.663128,-2.416098\O,0,0.862499,2.304082,0.756213\H,0,1.1826,3.105
172,0.301181\H,0,0.980899,2.410574,1.718511\H,0,1.362199,1.439511,0.40
3789\Br,0,2.072029,-0.202827,-0.256157\\

Product Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Intermediate of Sulfilimine Bond from
Haloamine with Br and H3O+\\1,1\S,0,-1.458849,-0.50582,-0.25805\C,0,-
1.116169,-1.342762,1.295526\H,0,-0.029857,-1.408854,1.36307\H,0,-1.558
737,-0.792044,2.125413\H,0,-1.551022,-2.340231,1.211854\C,0,-0.744736,
1.922934,-1.062537\H,0,-1.512749,1.914946,-1.838263\H,0,0.190726,1.505
807,-1.438445\H,0,-0.581993,2.946027,-0.723327\N,0,-1.139463,1.132554,
0.136837\C,0,-3.259152,-0.560925,-0.329926\H,0,-3.530805,-1.592847,-0.
55724\H,0,-3.693531,-0.244168,0.618667\H,0,-3.569119,0.086407,-1.15064
5\H,0,-1.959677,1.540767,0.593349\O,0,1.082994,1.569994,1.489354\H,0,1
.147903,1.409828,2.446133\H,0,0.128134,1.408276,1.150065\Br,0,1.950505
,-0.508324,-0.36842\H,0,1.627272,0.847222,0.93182\\

Formation of Sulfilimine Bond with the Reaction of Chlorinated Haloamine

Reactant Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Reactant of Sulfilimine bond from H a
loamine with Cl and H3O+\\1,1\S,0,2.030842,-0.474491,-0.137894\C,0,2.4
6268,1.286312,-0.126906\H,0,2.541168,1.660406,0.896318\H,0,3.405214,1.
45158,-0.652782\H,0,1.660095,1.810763,-0.646151\C,0,-0.858209,1.441542
,0.763158\H,0,-0.206655,0.789063,1.34673\H,0,-1.85975,1.472203,1.20657
5\H,0,-0.43896,2.451309,0.761364\N,0,-0.83713,0.999139,-0.632979\H,0,-
1.457791,1.591315,-1.185346\C,0,3.535012,-1.132492,0.636081\H,0,4.4139
59,-0.89663,0.03286\H,0,3.660509,-0.725666,1.641416\H,0,3.425961,-2.21
5737,0.701056\Cl,0,-1.568704,-0.59204,-0.779257\O,0,-4.173162,-0.50503
7,0.789332\H,0,-4.249999,-1.285304,1.373014\H,0,-4.971565,-0.418383,0.
232148\H,0,-3.339381,-0.554235,0.228667\\

TS Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the TS of Sulfilimine bond from Haloamine
with Cl and H3O+\\1,1\S,0,2.204215,-0.211296,-0.584781\C,0,3.036026,1
.366656,-0.294241\H,0,2.570578,1.910279,0.532117\H,0,4.086268,1.183431
,-0.060109\H,0,2.960196,1.953453,-1.209121\C,0,-0.391483,0.855813,0.75
7147\H,0,-0.746218,0.456427,1.706876\H,0,-1.098978,1.588043,0.365065\H
,0,0.556802,1.36706,0.932484\N,0,-0.161665,-0.284889,-0.163689\H,0,-0.
253328,0.053635,-1.126752\C,0,2.47101,-1.000496,1.017001\H,0,3.537794,
-1.157132,1.179698\H,0,2.055841,-0.381566,1.816093\H,0,1.952001,-1.958
054,0.990227\Cl,0,-2.153241,-1.079779,-0.250486\O,0,-3.942425,1.104198
,0.09194\H,0,-4.597889,0.943064,0.795265\H,0,-4.40244,1.334453,-0.7360
73\H,0,-3.305227,0.272692,-0.040147\\

Product Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\SPE_Op
timization and Frequency for the Intermediate of Sulfilimine Bond from
Haloamine with Cl and H3O+\\1,1\S,0,-0.701078,-0.528801,-0.132171\C,0
,0.005093,-1.001078,1.448627\H,0,0.59729,-0.143599,1.764096\H,0,-0.793
965,-1.234941,2.152908\H,0,0.643395,-1.867738,1.2722\C,0,-2.092218,1.6
38349,-0.750242\H,0,-2.670064,1.187509,-1.561875\H,0,-1.166639,2.06464
4,-1.138892\H,0,-2.679842,2.433494,-0.291255\N,0,-1.746491,0.69024,0.3
22702\C,0,-1.72338,-1.965047,-0.512013\H,0,-1.048123,-2.7839,-0.765303
\H,0,-2.343394,-2.227189,0.345702\H,0,-2.332742,-1.709251,-1.378795\H,
0,-2.553892,0.345371,0.838929\Cl,0,2.858982,-0.17651,-0.440158\H,0,3.8
18271,-0.956019,-0.783985\O,0,0.816492,1.873113,0.487908\H,0,1.604311,
2.327938,0.807322\H,0,0.096488,2.175238,1.055959\\

Sulfilimine Complexes

Double Protonated Sulfilimine Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - doubl
e protonated SN\\2,1\S,0,-0.463868,0.014548,-0.515413\C,0,-1.820328,-0
.86009,0.245201\H,0,-1.721161,-1.912209,-0.013229\H,0,-1.849904,-0.680
174,1.31672\H,0,-2.700432,-0.445137,-0.248866\C,0,2.230365,-0.030034,-
0.02956\H,0,2.233999,0.933171,0.468157\H,0,2.312581,0.065963,-1.107724
\H,0,3.019219,-0.66313,0.365071\N,0,0.932242,-0.72981,0.288202\H,0,0.9
78883,-1.703592,-0.044513\C,0,-0.503252,1.608464,0.281915\H,0,-1.43894
8,2.047253,-0.069018\H,0,-0.504727,1.499651,1.363884\H,0,0.332458,2.19
2679,-0.093822\H,0,0.793517,-0.768607,1.307196\\

Single Protonated Sulfilimine Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - singl
e protonated SN\\1,1\S,0,-0.342163,-0.011601,-0.451315\C,0,-1.587871,-
1.141722,0.141837\H,0,-1.294914,-2.13425,-0.189504\H,0,-1.647362,-1.08
2654,1.226449\H,0,-2.528932,-0.84483,-0.316756\C,0,2.277912,-0.023008,
-0.075718\H,0,2.435482,1.047085,0.065293\H,0,2.357962,-0.26914,-1.1325
02\H,0,3.040531,-0.573425,0.469852\N,0,0.972142,-0.480184,0.420311\C,0
,-0.928427,1.543325,0.222599\H,0,-1.82209,1.815292,-0.337\H,0,-1.14671
3,1.430238,1.282272\H,0,-0.146698,2.280127,0.052353\H,0,0.852659,-0.39
3105,1.4261\\

Neutral Sulfilimine Complex

m062x/6-311+g(2df,p) scrf=(iefpcm,solvent=water)\\spe - neutral SN
\\0,1\S,0,-0.252137,-0.031262,-0.411472\C,0,-1.511067,-1.179239,0.1291
8\H,0,-1.213386,-2.169482,-0.205697\H,0,-1.552388,-1.139153,1.217162\H
,0,-2.464995,-0.89599,-0.311274\C,0,2.258707,-0.003617,-0.033702\H,0,2
.490821,1.064001,0.076969\H,0,2.347677,-0.24827,-1.10108\H,0,3.039743,
-0.555506,0.492679\N,0,0.970042,-0.383078,0.549606\C,0,-1.052567,1.483
077,0.184412\H,0,-1.96985,1.659692,-0.37624\H,0,-1.254318,1.368475,1.2
49206\H,0,-0.349852,2.296637,0.015245\\

Cartesian coordinates

Table S7. Cartesian coordinates of all single point calculations obtained at the IEFPCM(ε = 4.0)M06-2X/6-311+G(2df,p) // IEFPCM(ε = 4.0)-M06-2X/6-31G(d,p) level of theory.

Formation of Halosulfonium with the Reaction of Hypobromous acid (HOBr)

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-hs-br-1h2o-eps4\
\0,1\S,0,-0.541543,1.995349,-0.188211\C,0,-2.199135,2.318492,0.468581\
H,0,-2.906482,1.968302,-0.283507\H,0,-2.357949,1.755656,1.392301\H,0,-
2.345725,3.383764,0.655669\C,0,0.038208,-0.946534,1.621162\H,0,0.15305
8,-1.786033,2.310048\H,0,-0.737957,-0.283213,2.013225\H,0,0.982822,-0.
390483,1.5846\N,0,-0.373813,-1.449539,0.306149\H,0,-0.381248,-0.666058
,-0.348788\H,0,0.33013,-2.117884,-0.012142\H,0,-1.838705,-1.763716,0.3
29976\C,0,0.458747,2.584506,1.204675\H,0,0.361272,3.66391,1.333076\H,0
,0.164408,2.074372,2.12502\H,0,1.497317,2.334971,0.979017\O,0,3.331268
,-0.308161,0.717953\H,0,4.270925,-0.159369,0.5197\Br,0,2.459169,0.2164
34,-0.809004\C,0,-3.412701,-0.943884,-0.46543\O,0,-2.904109,-1.788246,
0.404333\O,0,-2.749822,-0.326059,-1.287598\C,0,-4.90908,-0.783289,-0.3
35766\H,0,-5.128063,-0.262992,0.600843\H,0,-5.298634,-0.204886,-1.1718
17\H,0,-5.39198,-1.761096,-0.291038\O,0,2.213301,-2.931688,0.272457\H,
0,2.728706,-2.174613,0.589876\H,0,2.127244,-3.50717,1.040927\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-hs-br-1h2o-eps4\\
0,1\S,0,-0.259671,2.069898,-0.312456\C,0,-1.007634,1.847729,1.316043\H
,0,-1.425975,0.843316,1.301426\H,0,-0.240416,1.956403,2.083252\H,0,-1.
791527,2.597081,1.433641\C,0,-0.290509,-2.324635,1.466061\H,0,0.080104
,-3.187447,2.022312\H,0,-1.317599,-2.105224,1.767953\H,0,0.341248,-1.4
6163,1.687667\N,0,-0.229187,-2.581737,0.018009\H,0,-0.653668,-1.740601
,-0.435688\H,0,0.973722,-2.790606,-0.347921\H,0,-0.864679,-3.343155,-0
.212684\C,0,0.701002,3.571992,-0.005347\H,0,0.000956,4.389906,0.169415
\H,0,1.355214,3.427479,0.854838\H,0,1.288638,3.772143,-0.900693\O,0,3.
176748,-0.839445,0.071507\H,0,3.30543,-0.870509,1.029061\Br,0,1.460473
,0.540374,-0.150333\C,0,-2.805883,-0.74286,-0.410886\O,0,-3.13552,-1.9
2676,-0.207322\O,0,-1.628471,-0.336594,-0.68147\C,0,-3.878653,0.343127
,-0.2793\H,0,-4.852179,-0.036116,-0.594687\H,0,-3.960771,0.631,0.77458
6\H,0,-3.614503,1.232735,-0.854297\O,0,2.145169,-2.891415,-0.648155\H,
0,2.515655,-3.65431,-0.188963\H,0,2.729475,-1.838168,-0.250239\\

Intermediate Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-hs-br-1h2o-eps4\\
0,1\S,0,1.895906,1.20224,-0.475721\C,0,1.220374,1.966343,1.011921\H,0,
0.138458,1.913724,0.876297\H,0,1.565572,1.427227,1.893678\H,0,1.570446
,3.000042,1.015491\C,0,-0.858929,-0.727871,2.68075\H,0,-1.023803,-1.38
9729,3.533584\H,0,-1.193762,0.280145,2.957755\H,0,0.21704,-0.691392,2.
489805\N,0,-1.524497,-1.272221,1.494724\H,0,-1.439792,-0.606549,0.7241
79\H,0,-0.643171,-2.60624,0.654169\H,0,-2.52325,-1.356817,1.663625\C,0
,3.64589,1.05799,-0.05377\H,0,4.046603,2.072366,-0.019196\H,0,3.751911
,0.555091,0.906852\H,0,4.123953,0.490864,-0.851268\O,0,-0.12842,-3.023
79,-0.08851\H,0,-0.662132,-2.705176,-0.847528\Br,0,1.194268,-0.877828,
-0.256355\C,0,-2.40327,1.248005,-0.465009\O,0,-3.272468,0.345747,-0.55
4899\O,0,-1.161947,1.089482,-0.668273\C,0,-2.855303,2.637304,-0.020097
\H,0,-2.619429,2.757538,1.042571\H,0,-2.308756,3.40774,-0.567142\H,0,-
3.929524,2.766963,-0.153694\O,0,-1.633002,-1.445334,-1.81886\H,0,-1.04
7162,-0.674788,-1.722874\H,0,-2.411465,-1.066774,-1.353847\\

Formation of Halosulfonium with the Reaction of Hypochlorus acid (HOCl)

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-hs-cl-1h2o-eps4\
\0,1\S,0,-2.538646,-1.793772,0.102367\C,0,-3.931115,-1.521597,1.230429
\H,0,-3.528047,-1.46936,2.242115\H,0,-4.430825,-0.580504,0.991843\H,0,
-4.639635,-2.348798,1.165361\C,-1,0.976411,1.641305,1.759367\H,0,1.797
98,2.360982,1.759917\H,0,0.892339,1.221722,2.763307\H,0,0.049812,2.175
575,1.522206\N,0,1.281045,0.570876,0.798053\H,0,0.532517,-0.119401,0.8
10897\H,0,1.269249,0.984168,-0.138239\H,0,2.659139,-0.136416,0.920974\
C,-1,-3.439804,-1.805912,-1.470285\H,0,-4.153443,-2.630943,-1.492247\H
,0,-3.960105,-0.856757,-1.614097\H,0,-2.707365,-1.939788,-2.266696\O,0
,-1.748457,2.775901,-0.227547\H,0,-2.458261,3.090523,-0.810965\C,0,3.9
81299,-0.968021,-0.233556\O,0,3.592835,-0.619257,0.976547\O,0,3.33911,
-0.738542,-1.245709\C,-1,5.311054,-1.68916,-0.244036\H,0,5.239336,-2.5
9598,0.36087\H,0,5.590211,-1.943585,-1.264772\H,0,6.076586,-1.053323,0
.206338\O,0,0.882558,2.601155,-1.329562\H,0,-0.01045,2.821128,-1.01731
6\H,0,1.441192,3.303689,-0.978325\Cl,0,-1.995569,1.078091,-0.119222\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-hs-cl-1h2o-eps4\
\0,1\S,0,-2.493201,-1.456766,0.016419\C,0,-3.550193,-1.444036,1.476394
\H,0,-2.910054,-1.250227,2.33617\H,0,-4.309767,-0.669481,1.369726\H,0,
-4.001854,-2.433378,1.560602\C,-1,1.003436,1.630522,1.719562\H,0,1.522
145,2.580157,1.85953\H,0,1.166193,1.005749,2.599302\H,0,-0.062494,1.83
3854,1.603302\N,0,1.518575,0.98818,0.49727\H,0,1.158,0.040733,0.375011
\H,0,1.185407,1.670915,-0.422175\H,0,2.557049,0.816464,0.520851\C,-1,-
3.714435,-1.600134,-1.300512\H,0,-4.14194,-2.601746,-1.242341\H,0,-4.4
80321,-0.835187,-1.173919\H,0,-3.184512,-1.473176,-2.24365\O,0,-1.4910
35,2.761248,-0.259834\H,0,-2.13819,3.090261,-0.896996\C,0,3.855241,-1.
042792,-0.101475\O,0,4.114015,0.114412,0.34881\O,0,2.71644,-1.535839,-
0.260443\C,-1,5.077671,-1.896141,-0.474225\H,0,5.682746,-2.076554,0.41

8884\H,0,4.779084,-2.851286,-0.907431\H,0,5.705554,-1.350116,-1.183238
\O,0,0.657621,2.482681,-1.31425\H,0,-0.485386,2.689598,-0.797885\H,0,1
.151873,3.310441,-1.286148\Cl,0,-1.996411,0.613496,-0.13329\\

Intermediate Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-hs-cl-1h2o-eps4\
\0,1\S,0,3.081387,-0.38711,-0.829917\C,0,3.650511,1.14956,-0.080052\H,
0,2.927031,1.921089,-0.341445\H,0,3.727875,1.024838,0.999693\H,0,4.620
047,1.375006,-0.526908\C,-1,-0.794792,2.654516,-1.287817\H,0,-1.037928
,3.624533,-0.847653\H,0,-1.301363,2.585055,-2.258181\H,0,0.283338,2.63
3441,-1.467791\N,0,-1.158261,1.58929,-0.351481\H,0,-0.941215,0.674552,
-0.742986\H,0,-0.507184,1.720577,1.194561\H,0,-2.171206,1.531455,-0.20
1146\C,-1,4.211325,-1.587541,-0.104869\H,0,5.192195,-1.392574,-0.54184
3\H,0,4.226814,-1.471944,0.978735\H,0,3.859267,-2.575891,-0.396955\O,0
,-0.691769,-1.020746,1.546016\H,0,-1.39473,-0.986948,0.840622\C,0,-3.6
36066,-0.624523,-0.268745\O,0,-3.862581,0.533438,0.144226\O,0,-2.49816
,-1.176113,-0.37839\C,-1,-4.833454,-1.494549,-0.671359\H,0,-5.750229,-
0.907207,-0.730456\H,0,-4.638203,-1.98022,-1.630308\H,0,-4.964705,-2.2
8686,0.07175\O,0,-0.211342,1.652723,2.158853\H,0,-0.629819,-0.115886,1
.911271\H,0,0.752045,1.662865,2.123023\Cl,0,1.357604,-0.733314,0.23626
2\\

Formation of Haloamine with the Reaction of Hypobromous acid (HOBr)

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-ha-br-2h2o-eps4\\
0,1\S,0,-0.154814,1.918987,-0.511145\C,0,-1.717229,2.707316,-0.04403\H
,0,-2.504293,2.102232,-0.495081\H,0,-1.837039,2.716234,1.041568\H,0,-1
.765004,3.727937,-0.427943\C,0,-0.532667,-0.25156,2.615381\H,0,-0.7531
91,-1.013649,3.36158\H,0,-1.342448,0.478316,2.594822\H,0,0.408143,0.24
331,2.852161\N,0,-0.437132,-0.884587,1.285067\H,0,-0.200176,-0.162412,
0.587125\H,0,0.285816,-1.623233,1.23411\H,0,-1.406815,-1.272348,0.9980
72\C,0,1.009078,3.000021,0.364831\H,0,0.952055,4.020575,-0.017527\H,0,
0.803716,2.991981,1.437215\H,0,2.009185,2.600386,0.190902\O,0,2.253693
,0.049226,1.203044\H,0,3.133709,0.196495,1.586044\Br,0,2.578404,-0.153
179,-0.587119\C,0,-3.152899,-0.698425,-0.300038\O,0,-2.910323,-1.44900
3,0.687954\O,0,-2.299232,-0.313093,-1.143028\C,0,-4.57704,-0.182479,-0
.442408\H,0,-4.709696,0.662399,0.24104\H,0,-4.76976,0.158604,-1.459364
\H,0,-5.292842,-0.95456,-0.156224\O,0,1.241282,-2.97317,0.422018\H,0,2
.154899,-2.687897,0.304859\H,0,0.780639,-2.659127,-0.390496\O,0,-0.196
596,-1.856596,-1.591476\H,0,-0.96376,-1.259111,-1.367991\H,0,-0.576385
,-2.52471,-2.173382\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-ha-br-2h2o-eps4\\
0,1\C,0,1.531483,-1.9934,2.0958\H,0,1.571386,-1.876858,3.179961\H,0,2.
517328,-1.818857,1.665356\H,0,1.180989,-2.993096,1.842248\N,0,0.585421
,-1.009107,1.547918\H,0,-0.472066,-1.153312,1.826461\H,0,0.923557,-0.0
5152,1.694371\O,0,-0.936757,-1.481478,-2.391963\H,0,-0.718675,-2.37468
3,-2.684791\Br,0,0.283633,-1.189816,-0.364556\O,0,-1.96551,-1.402901,1

.664975\H,0,-2.378655,-0.573225,1.935257\H,0,-2.264252,-1.511625,0.621
14\O,0,-2.686787,-1.595783,-0.699303\H,0,-3.247098,-2.373901,-0.795474
\H,0,-1.791429,-1.584385,-1.65795\S,0,-1.276593,1.760857,0.529996\C,0,
-1.90217,3.416026,0.929103\C,0,-1.843505,1.627819,-1.189103\H,0,-1.472
522,4.161697,0.258311\H,0,-2.990616,3.43506,0.856669\H,0,-1.606353,3.6
39521,1.954384\H,0,-1.466388,0.6811,-1.577506\H,0,-2.93363,1.626881,-1
.225386\H,0,-1.448075,2.459033,-1.776567\C,0,2.503378,1.213134,-0.2451
81\O,0,2.438818,0.978713,0.949037\O,0,1.591021,1.933717,-0.887947\C,0,
3.574543,0.683112,-1.15043\H,0,4.459338,0.429317,-0.569945\H,0,3.17435
1,-0.22622,-1.610307\H,0,3.812448,1.394741,-1.940407\H,0,0.842077,2.10
5628,-0.271277\\

Intermediate Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-ha-br-2h2o-eps4\\
0,1\S,0,1.660583,2.48814,-0.772296\C,0,1.145346,3.422679,0.696086\H,0,
0.133839,3.781745,0.506698\H,0,1.126232,2.772192,1.574366\H,0,1.816912
,4.263424,0.8761\C,0,-0.075055,0.014575,2.03068\H,0,-0.422795,-0.93883
9,2.429784\H,0,-0.791546,0.800595,2.286933\H,0,0.905108,0.261751,2.450
421\N,0,-0.066294,-0.064705,0.565756\H,0,0.238344,0.832859,0.169518\H,
0,2.495231,-3.79191,-1.390292\H,0,-1.571039,-0.135278,-0.020499\C,0,3.
231887,1.812356,-0.165849\H,0,3.924002,2.618354,0.082746\H,0,3.066838,
1.176081,0.706565\H,0,3.654068,1.205208,-0.967482\O,0,3.121232,-3.2237
32,-0.926036\H,0,3.233316,-3.650837,-0.068564\Br,0,1.256591,-1.278918,
-0.056092\C,0,-2.687995,1.402704,-0.237287\O,0,-2.516437,0.090152,-0.3
45931\O,0,-1.83207,2.147234,0.207836\C,0,-4.038689,1.857744,-0.719062\
H,0,-4.819504,1.335911,-0.161477\H,0,-4.13765,2.933151,-0.587551\H,0,-
4.154082,1.596355,-1.773398\O,0,-1.561229,-2.746841,1.084006\H,0,-1.51
3879,-3.516669,1.663166\H,0,-0.713378,-2.735186,0.61843\O,0,-3.645373,
-2.53278,-0.845254\H,0,-2.977295,-2.765324,-0.179687\H,0,-3.560638,-1.
571379,-0.880477\\

Formation of Haloamine with the Reaction of Hypochlorus acid (HOCl)

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-ha-cl-2h2o-eps4\
\0,1\S,0,-0.966243,2.286917,-0.114158\C,0,0.14197,3.649088,-0.562219\H
,0,1.146741,3.366448,-0.24352\H,0,0.139337,3.805884,-1.642174\H,0,-0.1
51022,4.568406,-0.052489\C,-1,2.095754,-3.170204,-0.511378\H,0,1.57164
9,-2.83699,0.386183\H,0,3.065482,-3.576296,-0.21635\H,0,1.510046,-3.96
5931,-0.984425\N,0,2.297447,-2.013391,-1.381292\H,0,2.78162,-2.261049,
-2.238607\H,0,1.397774,-1.594054,-1.602109\H,0,-1.143997,-1.81304,0.39
8787\C,-1,-2.539499,2.934798,-0.731618\H,0,-2.834636,3.829598,-0.18151
8\H,0,-2.463893,3.160248,-1.796865\H,0,-3.277112,2.145534,-0.580892\O,
0,3.624671,1.022203,0.958253\H,0,3.755281,1.781715,0.371528\C,0,-3.014
208,-1.595944,0.188019\O,0,-1.993195,-2.332444,0.593765\O,0,-2.888712,
-0.483564,-0.300337\C,-1,-4.337085,-2.285707,0.384797\H,0,-4.459412,-2
.548099,1.43774\H,0,-5.149588,-1.637716,0.062444\H,0,-4.348075,-3.2141
87,-0.19041\O,0,1.023722,0.676032,1.925794\H,0,0.456986,1.456857,1.965
689\H,0,1.918662,0.995008,1.698241\O,0,-0.032938,-0.847018,-0.106209\H
,0,-0.631387,-0.189749,-0.500217\H,0,0.426305,-0.353353,0.614843\Cl,0,
3.159825,-0.299413,-0.140355\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-ha-cl-2h2o-eps4\\
0,1\S,0,-0.803185,2.672338,0.151799\C,0,0.53103,2.237095,-0.997114\H,0
,1.347291,1.852484,-0.384177\H,0,0.2083,1.455121,-1.689794\H,0,0.85954
6,3.113175,-1.558926\C,-1,2.113565,-3.249726,-0.774762\H,0,2.02313,-3.
347608,0.305642\H,0,3.133287,-3.462712,-1.089676\H,0,1.413425,-3.91950
1,-1.274169\N,0,1.775982,-1.858078,-1.137943\H,0,1.81855,-1.70501,-2.1
46712\H,0,0.841866,-1.561021,-0.75901\H,0,-1.280258,-1.483771,0.893562
\C,-1,-2.083656,3.16201,-1.035099\H,0,-1.727417,3.969717,-1.676896\H,0
,-2.384001,2.304608,-1.640366\H,0,-2.942852,3.512607,-0.462259\O,0,3.5
46175,1.017351,1.010932\H,0,3.610112,1.793628,0.440646\C,0,-3.04952,-1
.404495,0.20055\O,0,-2.1755,-1.958386,1.023324\O,0,-2.778462,-0.477218
,-0.547356\C,-1,-4.412531,-2.0392,0.279921\H,0,-4.789551,-1.966336,1.3
02368\H,0,-5.095803,-1.544333,-0.407195\H,0,-4.334258,-3.100081,0.0320
96\O,0,1.309008,0.770047,1.867996\H,0,0.885429,1.569552,2.198\H,0,2.43
3508,0.986304,1.476639\O,0,-0.10921,-0.618458,0.392183\H,0,-0.718249,-
0.019992,-0.072655\H,0,0.485981,0.001085,1.05048\Cl,0,2.805978,-0.6058
57,-0.2952\\

Intermediate Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-ha-cl-2h2o-eps4\
\0,1\S,0,-0.224569,2.316888,-0.210424\C,0,1.453555,2.911851,-0.551163\
H,0,2.150217,2.187623,-0.123513\H,0,1.620556,2.986971,-1.627222\H,0,1.
612471,3.886085,-0.084465\C,-1,1.805082,-3.714753,-0.556485\H,0,1.7727
84,-3.727394,0.533401\H,0,2.790444,-4.041807,-0.89979\H,0,1.038384,-4.
388611,-0.944354\N,0,1.456553,-2.367385,-1.02456\H,0,1.481356,-2.34408
3,-2.043198\H,0,0.103175,-1.560334,-0.217383\H,0,-1.938542,-1.60966,0.
746024\C,-1,-1.18376,3.678638,-0.928922\H,0,-0.975184,4.61234,-0.40417
2\H,0,-0.952705,3.788883,-1.989806\H,0,-2.238805,3.426968,-0.815181\O,
0,3.797317,0.892254,1.065555\H,0,4.075058,1.769004,1.352211\C,0,-3.548
407,-0.825556,0.144347\O,0,-2.920871,-1.783807,0.814471\O,0,-2.967208,
0.086535,-0.418616\C,-1,-5.042568,-0.996354,0.155328\H,0,-5.399848,-1.
019262,1.186976\H,0,-5.514205,-0.180203,-0.387754\H,0,-5.300485,-1.952
454,-0.305428\O,0,1.219529,0.549674,2.04399\H,0,0.692228,1.358755,2.05
8906\H,0,2.906884,0.773574,1.454126\O,0,-0.453763,-0.993408,0.37976\H,
0,-0.827157,-0.281822,-0.170594\H,0,0.691316,-0.064748,1.496988\Cl,0,2
.66505,-1.203016,-0.525705\\

Formation of Sulfilimine Bond with the Reaction of Brominated Halosulfonium

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-sn-hs-br-1h2o
-eps4\\1,1\S,0,0.16494,0.783746,0.516234\C,0,1.609476,1.311451,1.46699
6\H,0,1.870052,0.483537,2.125598\H,0,2.436252,1.573635,0.808646\H,0,1.
284712,2.17052,2.058065\C,0,-3.238492,0.429625,-0.083951\H,0,-2.963449
,0.745286,0.927216\H,0,-4.155677,-0.168036,-0.012835\H,0,-3.462964,1.3
29709,-0.662078\N,0,-2.103575,-0.270661,-0.686793\H,0,-2.342231,-0.584
248,-1.623292\H,0,-1.887496,-1.101773,-0.137014\C,0,0.025676,2.128127,
-0.677139\H,0,-0.330087,2.995702,-0.117146\H,0,0.991117,2.32407,-1.141
635\H,0,-0.724585,1.798036,-1.393597\O,0,-0.701484,-1.80894,1.590779\H
,0,-0.209723,-2.622981,1.432366\H,0,-1.194308,-1.971322,2.403426\Br,0,

1.085894,-0.753175,-0.716616\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-sn-hs-br-1h2o-eps4\\1,1\S,0,0.667986,-0.739478,0.527853\C,0,-0.193432,-2.370832,0.648707\H,0,-1.141162,-2.184367,1.145724\H,0,-0.346017,-2.796297,-0.342182\H,0,0.468514,-2.995383,1.25275\C,0,2.416581,1.497815,-0.506701\H,0,2.776686,1.421465,0.521422\H,0,2.346132,2.556625,-0.769321\H,0,3.094596,0.999732,-1.195104\N,0,1.063354,0.925074,-0.588091\H,0,0.748658,0.744583,-1.543711\H,0,0.401584,1.577976,-0.113841\C,0,2.166446,-1.485868,-0.192621\H,0,2.349761,-2.403881,0.363637\H,0,1.989533,-1.722148,-1.243416\H,0,3.01233,-0.8169,-0.075987\O,0,-0.306176,2.523532,1.164998\H,0,-1.223954,2.220081,1.141195\H,0,-0.34571,3.474597,1.005168\Br,0,-1.604296,-0.021569,-0.385475\\

Product Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-sn-hs-br-1h2o-eps4\\1,1\S,0,-1.193055,-0.136311,0.084155\C,0,-0.698275,0.321018,1.747171\H,0,-0.811521,1.40132,1.806748\H,0,-1.321557,-0.205504,2.470231\H,0,0.352644,0.048889,1.84862\C,0,-3.4922,0.281533,-1.167586\H,0,-3.574053,-0.695575,-1.652177\H,0,-2.950464,0.968981,-1.818215\H,0,-4.491782,0.679753,-0.996009\N,0,-2.817512,0.231748,0.138705\C,0,-1.042696,-1.934009,0.144307\H,0,0.025389,-2.155885,0.130595\H,0,-1.518511,-2.327358,1.042585\H,0,-1.51226,-2.327781,-0.757266\H,0,-3.324929,-0.309579,0.837114\O,0,0.64117,2.248212,-0.029854\H,0,0.656839,2.509298,-0.957992\H,0,1.2594,2.849484,0.401716\Br,0,2.266482,-0.239989,-0.243642\H,0,2.965082,-1.474617,-0.25041\\

Formation of Sulfilimine Bond with the Reaction of Chlorinated Halosulfonium

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm geom=modredundant\\spe - rc-sn-hs-cl-3h2o-eps4\\1,1\S,0,-0.089605,-0.830836,-0.078983\C,0,-0.909358,-2.28582,0.602072\H,0,-1.111485,-2.961544,-0.228183\H,0,-0.278219,-2.754809,1.355994\H,0,-1.838847,-1.900055,1.022157\C,0,-3.614165,0.020464,-0.782597\H,0,-3.000906,0.077164,-1.685609\H,0,-4.493827,0.660086,-0.92882\H,0,-3.959582,-1.011985,-0.682454\N,0,-2.795955,0.381682,0.374308\H,0,-3.352815,0.359198,1.223612\H,0,-2.420022,1.326085,0.278354\C,0,0.331492,0.085539,1.419446\H,0,-0.517765,0.74746,1.593759\H,0,0.486794,-0.618289,2.236193\H,0,1.235443,0.656674,1.201773\Cl,0,1.726366,-1.648895,-0.52788\O,0,1.062773,1.520115,-1.124613\H,0,1.9606,1.604385,-0.743179\H,0,1.154709,1.561813,-2.082701\O,0,3.249064,1.374933,0.442023\H,0,3.934699,0.746446,0.186139\H,0,3.720007,2.162589,0.739276\O,0,-0.959966,2.739025,0.313231\H,0,-0.250485,2.435219,-0.285672\H,0,-1.27393,3.568673,-0.061755\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-sn-hs-cl-3h2o-eps4\\1,1\S,0,-0.799108,-0.312859,-0.044084\C,0,-0.995604,-2.015338,-0.591246\H,0,-1.151148,-2.62435,0.297279\H,0,-1.820945,-2.086171,-1.298992\H,0,-0.035051,-2.258596,-1.050041\C,0,1.895554,-0.536437,1.957765\H,0,2.047898,0.327378,1.304229\H,0,2.83944,-0.735966,2.481069\H,0,1.145588,-0.262256,2.706233\N,0,1.401467,-1.650522,1.151463\H,0,1.340593,-2.49448,1.713419\H,0,2.04296,-1.828474,0.382669\C,0,-0.58906,0.495933

,-1.643836\H,0,0.391858,0.162839,-1.99328\H,0,-1.387218,0.183035,-2.31
6143\H,0,-0.602335,1.56769,-1.457265\Cl,0,-2.748793,0.190197,0.335122\
O,0,2.159752,1.821611,-0.687597\H,0,1.418979,2.100422,-0.114895\H,0,2.
952029,2.19217,-0.282004\O,0,-0.126156,2.348017,0.800294\H,0,-0.508201
,3.228966,0.697638\H,0,-0.027751,2.224241,1.753004\O,0,2.229929,-0.824
017,-1.458563\H,0,2.73069,-0.902596,-2.278315\H,0,2.354012,0.102367,-1
.165756\\

Product Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-sn-hs-cl-3h2
o-eps4\\1,1\S,0,-0.685018,-0.552706,-0.145701\C,0,0.138631,-0.426595,1
.442568\H,0,-0.540537,0.154627,2.06384\H,0,0.309617,-1.425962,1.843893
\H,0,1.078684,0.098537,1.275995\C,0,-3.166328,-1.386564,-0.563166\H,0,
-3.051915,-1.597054,-1.630842\H,0,-3.486911,-0.356097,-0.408565\H,0,-3
.920143,-2.056028,-0.148254\N,0,-1.93541,-1.5952,0.212716\C,0,0.495868
,-1.537313,-1.085098\H,0,1.377443,-0.913263,-1.232845\H,0,0.750971,-2.
444258,-0.535579\H,0,0.03157,-1.774438,-2.042361\H,0,-1.635154,-2.5656
36,0.269789\Cl,0,3.768843,-0.294865,0.259306\H,0,4.611828,-1.089225,0.
812078\O,0,1.386236,1.520941,-0.723457\H,0,1.738969,1.615786,-1.618451
\H,0,1.979612,2.043455,-0.167299\O,0,-2.509131,1.282671,1.080631\H,0,-
2.068629,1.945684,0.508935\H,0,-2.63654,1.718255,1.930086\O,0,-1.09836
4,2.890627,-0.640189\H,0,-0.231319,2.449505,-0.700834\H,0,-0.90866,3.7
67436,-0.287308\\

Formation of Sulfilimine Bond with the Reaction of Brominated Haloamine

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-sn-ha-br-h3o
-eps4\\1,1\S,0,2.263563,0.169906,-0.474356\C,0,2.232904,1.112763,1.075
301\H,0,1.225749,1.513192,1.187466\H,0,2.46497,0.4577,1.915753\H,0,2.9
53123,1.928564,1.018511\C,0,-1.162714,2.145124,-0.022244\H,0,-1.212408
,2.175681,1.067162\H,0,-2.09749,2.528359,-0.440976\H,0,-0.332157,2.772
085,-0.360391\N,0,-0.842561,0.776121,-0.447473\H,0,-0.852215,0.740827,
-1.467677\C,0,3.91337,-0.574955,-0.351343\H,0,4.664739,0.214595,-0.365
928\H,0,3.996409,-1.161514,0.563937\H,0,4.045471,-1.220362,-1.219216\O
,0,0.495327,-1.889938,0.521567\H,0,0.607821,-2.759196,0.098481\H,0,-0.
448834,-1.611117,0.450712\H,0,1.152371,-1.145432,0.073488\Br,0,-2.2957
32,-0.387509,-0.005204\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-sn-ha-br-h3o
-eps4\\1,1\S,0,-2.454889,-0.481475,-0.366031\C,0,-2.550358,0.292852,1.
261942\H,0,-1.628996,0.850549,1.440802\H,0,-3.416934,0.953083,1.306914
\H,0,-2.657736,-0.498991,2.003863\C,0,-0.022231,-1.846889,0.877627\H,0
,0.260031,-1.43267,1.845515\H,0,0.705884,-2.597362,0.571333\H,0,-0.994
294,-2.334317,0.96446\N,0,-0.1174,-0.718709,-0.095426\H,0,-0.08499,-1.
119156,-1.039682\C,0,-2.167719,0.983296,-1.377845\H,0,-3.000361,1.6791
42,-1.271138\H,0,-1.232142,1.447525,-1.058662\H,0,-2.089942,0.660725,-
2.416127\O,0,0.823869,2.291234,0.762146\H,0,1.122417,3.098247,0.302839
\H,0,0.947142,2.401747,1.723371\H,0,1.338759,1.436884,0.407187\Br,0,2.
076631,-0.191894,-0.254963\\

Product Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-sn-ha-br-h3o-eps4\\1,1\S,0,-1.460566,-0.50564,-0.262811\C,0,-1.113476,-1.347797,1.287551\H,0,-0.026884,-1.415267,1.35054\H,0,-1.552239,-0.798243,2.120122\H,0,-1.550462,-2.344114,1.202894\C,0,-0.743124,1.925618,-1.058182\H,0,-1.507216,1.920241,-1.837459\H,0,0.194078,1.508726,-1.429929\H,0,-0.581286,2.947395,-0.715202\N,0,-1.144618,1.132066,0.137128\C,0,-3.261161,-0.563571,-0.331197\H,0,-3.531694,-1.593608,-0.567443\H,0,-3.692966,-0.257155,0.621857\H,0,-3.574295,0.091474,-1.144441\H,0,-1.967001,1.539039,0.590796\O,0,1.068716,1.554158,1.50329\H,0,1.127236,1.381443,2.458268\H,0,0.114896,1.398922,1.155307\Br,0,1.956294,-0.502002,-0.368995\H,0,1.615775,0.838229,0.939256\\

Formation of Sulfilimine Bond with the Reaction of Chlorinated Haloamine

Reactant Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - rc-sn-ha-cl-h3o-eps4\\1,1\S,0,2.040992,-0.477722,-0.136979\C,0,2.464919,1.285069,-0.119765\H,0,2.555405,1.651887,0.905003\H,0,3.399111,1.458576,-0.657473\H,0,1.652501,1.808625,-0.624502\C,0,-0.864554,1.450667,0.762697\H,0,-0.212981,0.798412,1.346185\H,0,-1.865746,1.480845,1.206318\H,0,-0.445651,2.460419,0.760607\N,0,-0.84428,1.007068,-0.633243\H,0,-1.467614,1.597221,-1.184749\C,0,3.550769,-1.133933,0.626328\H,0,4.425546,-0.896894,0.017701\H,0,3.68202,-0.72862,1.631446\H,0,3.443534,-2.217353,0.690397\Cl,0,-1.573011,-0.586038,-0.775483\O,0,-4.186327,-0.520063,0.784711\H,0,-4.259508,-1.297585,1.372512\H,0,-4.98014,-0.446701,0.219054\H,0,-3.347381,-0.562421,0.23183\\

TS Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - ts-sn-ha-cl-h3o-eps4\\1,1\S,0,2.204215,-0.211296,-0.584781\C,0,3.036026,1.366656,-0.294241\H,0,2.570578,1.910279,0.532117\H,0,4.086268,1.183431,-0.060109\H,0,2.960196,1.953453,-1.209121\C,0,-0.391483,0.855813,0.757147\H,0,-0.746218,0.456427,1.706876\H,0,-1.098978,1.588043,0.365065\H,0,0.556802,1.36706,0.932484\N,0,-0.161665,-0.284889,-0.163689\H,0,-0.253328,0.053635,-1.126752\C,0,2.47101,-1.000496,1.017001\H,0,3.537794,-1.157132,1.179698\H,0,2.055841,-0.381566,1.816093\H,0,1.952001,-1.958054,0.990227\Cl,0,-2.153241,-1.079779,-0.250486\O,0,-3.942425,1.104198,0.09194\H,0,-4.597889,0.943064,0.795265\H,0,-4.40244,1.334453,-0.736073\H,0,-3.305227,0.272692,-0.040147\\

Product Complex

m062x/6-311+g(2df,p) scrf=iefpcm\\spe - im-sn-ha-cl-h3o-eps4\\1,1\S,0,-0.693602,-0.530295,-0.134592\C,0,0.022417,-0.991627,1.444493\H,0,0.62125,-0.134523,1.749169\H,0,-0.774176,-1.213565,2.155762\H,0,0.654013,-1.864033,1.274174\C,0,-2.111036,1.622554,-0.744179\H,0,-2.67899,1.16289,-1.557711\H,0,-1.193218,2.06813,-1.129413\H,0,-2.715449,2.404273,-0.284301\N,0,-1.748389,0.678903,0.327001\C,0,-1.707162,-1.976363,-0.503478\H,0,-1.027492,-2.791984,-0.754644\H,0,-2.321851,-2.237085,0.358442\H,0,-2.322058,-1.729553,-1.368852\H,0,-2.548209,0.324106,0.848365\Cl,0,2.855803,-0.170112,-0.436195\H,0,3.766705,-1.008378,-0.774518\O,0,0.803818,1.89305,0.471706\H,0,1.582336,2.386344,0.75495\H,0,0.088981,2.185895,1.05107\\

