Hypoiodous Acid as Guest Molecule in Protonated Water Clusters: A Combined FT-ICR/DFT Study of $I(H_2O)_n^+$

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Supporting Information on all calculated species: Cartesian coordinates of optimized geometries, calculated harmonic frequencies and infrared intensities, thermochemical values.

HCl:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1	0.000000	0.000000	0.109860
2	17	0.000000	0.000000	1.390140

Harmonic frequencies and intensities (cm^{-1},km/mol):

2956.2,45.2;

Sum of electronic and zero-point Energies=	-460.831816
Sum of electronic and thermal Energies=	-460.829456
Sum of electronic and thermal Enthalpies=	-460.828512
Sum of electronic and thermal Free Energies=	-460.849696

ICl:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	0.000000	0.000000	-0.190288
2	17	0.000000	0.000000	2.190288

Harmonic frequencies and intensities (cm^{-1},km/mol):

367.5,6.1;

Sum of electronic and zero-point Energies=	-471.639398
Sum of electronic and thermal Energies=	-471.636696
Sum of electronic and thermal Enthalpies=	-471.635752
Sum of electronic and thermal Free Energies=	-471.663900

H_2O:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.001821	0.000000	-0.001412
2	1	-0.006191	0.000000	0.959878
3	1	0.927752	0.000000	-0.246327

Harmonic frequencies and intensities (cm^{-1},km/mol):

1628.8,72.1;3808.6,4.6;3907.4,59.9;

Sum of electronic and zero-point Energies=	-76.442839
Sum of electronic and thermal Energies=	-76.440003
Sum of electronic and thermal Enthalpies=	-76.439059
Sum of electronic and thermal Free Energies=	-76.461134

HOI:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	1	0.002200	0.000000	-0.018049
2	8	-0.069721	0.000000	0.944603
3	53	1.849432	0.000000	1.603439

Harmonic frequencies and intensities (cm^{-1},km/mol):

570.2,19.0;1104.2,44.2;3797.9,99.7;

Sum of electronic and zero-point Energies=	-87.227453
Sum of electronic and thermal Energies=	-87.224419
Sum of electronic and thermal Enthalpies=	-87.223474
Sum of electronic and thermal Free Energies=	-87.252457

H_2IO^+, 1:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.037327	0.243789	-0.327929
2	53	-0.049122	-0.047611	1.787795
3	1	0.870732	-0.094398	-0.707648
4	1	-0.711425	-0.180257	-0.788597

Harmonic frequencies and intensities (cm^{-1},km/mol):

457.0,15.0;682.0,195.1;844.9,5.8;1605.2,83.6;3617.8,332.5;
3698.9,312.9;

Sum of electronic and zero-point Energies=	-87.500682
Sum of electronic and thermal Energies=	-87.497402
Sum of electronic and thermal Enthalpies=	-87.496458
Sum of electronic and thermal Free Energies=	-87.526284

$I(H_2O)_2^+$, 2:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.033265	0.044198	-0.128779
2	53	0.310293	-0.084621	2.129300
3	8	0.608795	-0.253264	4.391996
4	1	0.197003	-0.772131	-0.599117
5	1	0.445278	0.772732	-0.553731
6	1	-0.161481	0.041847	4.901987
7	1	1.381484	0.232599	4.719182

Harmonic frequencies and intensities (cm^{-1},km/mol):

74.1,66.7;133.9,17.7;140.6,20.6;319.8,78.3;359.3,1.5;557.5,183.7;
559.5,191.6;708.5,17.5;727.9,17.5;1615.0,71.5;1616.8,73.2;
3697.3,497.9;3705.0,20.8;3790.1,211.5;3791.5,230.5;

Sum of electronic and zero-point Energies=	-163.995951
Sum of electronic and thermal Energies=	-163.989669
Sum of electronic and thermal Enthalpies=	-163.988724
Sum of electronic and thermal Free Energies=	-164.025879

$I(H_2O)_2^+$, 3:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.275353	0.109727	0.982688
2	53	-0.345557	2.143203	0.492202
3	1	0.376166	-0.338356	0.419248
4	1	-0.087723	-0.094234	2.030591
5	8	0.016645	-0.364303	3.364719
6	1	0.859682	-0.360506	3.835301
7	1	-0.548581	-1.042534	3.756866

Harmonic frequencies and intensities (cm^{-1},km/mol):

93.5,2.9;125.1,25.7;299.0,238.3;368.8,98.8;442.9,116.9;
524.3,35.1;560.9,29.1;957.2,29.1;1337.0,163.3;1538.7,131.7;
1643.6,94.0;1916.4,3613.9;3724.8,236.8;3758.6,112.5;3844.8,209.4;

Sum of electronic and zero-point Energies=	-163.986847
Sum of electronic and thermal Energies=	-163.981097
Sum of electronic and thermal Enthalpies=	-163.980153
Sum of electronic and thermal Free Energies=	-164.017370

$I(H_2O)_3^+$, 4:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.319967	-0.201771	0.890136
2	53	-0.800557	-0.110323	2.796399
3	8	2.825697	0.206253	1.133403
4	1	-0.067830	0.384508	0.225360
5	1	1.311355	0.016350	0.985919
6	1	3.283871	1.044714	1.256246
7	1	3.447405	-0.401405	0.717229
8	8	-1.977272	-0.030564	4.834960
9	1	-2.910414	0.205889	4.732831
10	1	-1.947424	-0.864812	5.325244

Harmonic frequencies and intensities (cm^{-1},km/mol):

44.8,50.7;58.3,3.2;93.0,31.8;133.5,7.3;142.9,9.1;218.4,246.5;
274.8,107.0;314.1,11.7;370.1,76.5;441.8,26.0;470.7,15.6;
535.9,216.5;660.9,5.1;823.6,52.5;1138.7,73.8;1610.2,60.5;
1619.9,66.3;1655.0,15.0;2798.4,2791.4;3723.7,215.6;3774.0,193.2;
3786.7,68.7;3814.4,190.4;3875.3,160.8;

Sum of electronic and zero-point Energies=	-240.467503
Sum of electronic and thermal Energies=	-240.458256
Sum of electronic and thermal Enthalpies=	-240.457312
Sum of electronic and thermal Free Energies=	-240.503165

$I(H_2O)_3^+$, 5:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.061831	-0.007381	0.101951
2	53	0.282531	-0.079209	2.159460
3	8	2.280818	-0.074452	-1.081315
4	1	-0.531904	0.792882	-0.168440
5	1	0.977497	0.018015	-0.379365
6	1	2.813959	0.681693	-1.351502
7	1	2.455267	-0.790285	-1.703494
8	8	-1.401389	1.903227	-0.657375
9	1	-2.221233	1.694061	-1.120830
10	1	-1.556982	2.712032	-0.155961

Harmonic frequencies and intensities (cm^{-1},km/mol):

65.2,5.7;73.0,14.9;90.5,0.7;98.6,0.8;122.0,31.2;236.6,185.2;
276.5,11.7;315.3,243.5;367.6,166.6;414.3,15.0;454.1,37.2;
572.8,8.5;978.2,30.3;1218.4,107.1;1283.3,50.6;1594.8,30.9;
1638.2,15.3;1658.4,29.6;2528.3,3175.3;2626.1,2466.3;3775.8,77.6;
3780.2,70.1;3861.8,155.7;3868.2,181.5;

Sum of electronic and zero-point Energies=	-240.461339
Sum of electronic and thermal Energies=	-240.452224
Sum of electronic and thermal Enthalpies=	-240.451280
Sum of electronic and thermal Free Energies=	-240.497317

$I(H_2O)_4^+$, 6:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.259872	1.715329	-1.289295
2	53	-0.590053	-0.280014	2.246657
3	8	1.153381	-1.173790	5.823888
4	1	0.027617	2.588398	-1.576794
5	1	-0.267912	1.149052	-2.067727
6	1	2.030962	-1.421594	6.133844
7	1	0.646064	-0.904631	6.596531
8	8	-1.448841	1.402542	0.992066
9	1	-1.016421	1.483823	0.086950
10	1	-2.401919	1.306219	0.866099
11	8	0.307043	-1.944105	3.498492
12	1	-0.300370	-2.689584	3.592100
13	1	0.588577	-1.648049	4.418454

Harmonic frequencies and intensities (cm^{-1},km/mol):

13.4,6.5;48.6,2.7;58.6,5.2;87.0,68.8;91.0,40.9;137.8,31.1;
140.3,11.3;165.4,169.6;174.0,208.7;256.0,135.1;279.0,24.6;
346.7,110.6;348.4,4.5;401.3,63.6;407.9,7.8;447.8,48.4;452.7,22.2;
742.2,67.3;779.7,57.9;1064.1,57.2;1070.5,83.1;1617.8,104.6;
1618.6,27.9;1649.5,30.9;1650.2,5.3;3000.5,4055.5;3036.3,630.8;
3791.7,113.7;3792.8,184.8;3795.3,132.5;3796.6,35.6;3885.0,145.8;
3885.7,148.6;

Sum of electronic and zero-point Energies=	-316.934605
Sum of electronic and thermal Energies=	-316.922107
Sum of electronic and thermal Enthalpies=	-316.921163
Sum of electronic and thermal Free Energies=	-316.976001

$I(H_2O)_4^+$, 7:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.122766	0.227142	0.153954
2	53	0.006440	0.120251	2.310733
3	8	-0.147575	0.047840	4.717823
4	8	1.238527	-1.890490	-0.849827
5	1	-0.773992	0.426709	-0.256364
6	1	0.503205	-0.615233	-0.244964
7	1	2.054206	-1.784947	-1.351742
8	1	0.788813	-2.662095	-1.210352
9	1	0.098959	-0.804014	5.102522
10	1	0.386765	0.720586	5.161178
11	8	-2.134614	0.769046	-1.010794
12	1	-3.011527	0.659617	-0.627665
13	1	-2.181137	1.536726	-1.591425

Harmonic frequencies and intensities (cm^{-1},km/mol):

52.3,4.3;58.7,3.2;61.5,3.1;78.0,33.1;92.1,27.8;109.9,34.9;
131.7,2.4;146.6,2.0;224.6,56.8;250.4,105.9;271.6,318.6;
278.3,11.0;331.5,118.3;364.8,22.5;402.4,47.3;471.6,69.8;
497.6,144.8;608.9,8.1;850.4,47.9;1080.0,102.9;1157.6,29.8;
1616.8,62.3;1620.8,69.0;1639.9,23.6;1663.4,43.3;3005.9,2280.3;
3022.1,2233.1;3741.2,166.6;3788.9,57.7;3789.9,45.0;3833.6,167.1;
3877.2,121.3;3878.9,161.8;

Sum of electronic and zero-point Energies=	-316.934210
Sum of electronic and thermal Energies=	-316.921653
Sum of electronic and thermal Enthalpies=	-316.920708
Sum of electronic and thermal Free Energies=	-316.974725

$I(H_2O)_4^+$, 8:

Input orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	-0.405953	0.326103	0.280436
2	53	0.180805	-0.298755	2.154230
3	8	1.432069	0.248191	-1.294090
4	8	-1.558797	2.624773	0.344938
5	1	-0.850972	1.234546	0.357037
6	1	0.441837	0.332659	-0.445557
7	1	1.883192	1.053783	-1.566568
8	1	1.349958	-0.362862	-2.077376
9	1	-2.486412	2.680262	0.088071
10	1	-1.419596	3.293813	1.024584
11	8	1.238879	-1.451825	-3.284499
12	1	1.868837	-2.172050	-3.392664
13	1	0.800117	-1.337836	-4.133631

Harmonic frequencies and intensities (cm^{-1},km/mol):

11.7,1.4;47.6,0.3;61.3,11.1;84.8,15.7;101.7,2.1;102.8,6.0;
126.8,27.0;186.9,214.5;244.3,185.5;260.5,51.8;283.3,95.9;
319.8,248.2;336.1,8.2;412.2,12.4;445.9,186.4;606.5,49.9;
609.3,31.8;920.5,120.4;1005.1,55.1;1215.1,875.3;1340.8,80.0;
1411.6,2123.1;1633.0,126.8;1640.1,265.8;1659.8,163.4;
1720.3,1104.7;2884.9,2227.1;3189.2,1422.6;3782.8,56.5;
3797.1,43.1;3842.3,131.2;3869.4,148.5;3886.8,139.3;

Sum of electronic and zero-point Energies=	-316.926402
Sum of electronic and thermal Energies=	-316.914324
Sum of electronic and thermal Enthalpies=	-316.913380
Sum of electronic and thermal Free Energies=	-316.968244

$H(H_2O)_4^+$:

Z-Matrix orientation:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	8	0.000000	0.000000	0.000000
2	8	0.000000	0.000000	2.562046
3	8	2.321727	0.000000	-1.083626
4	8	-1.695453	1.587464	-1.081801
5	1	0.046167	0.016671	1.013045
6	1	-0.673619	0.652598	-0.385948
7	1	0.908806	0.043540	-0.448134
8	1	-0.314313	-0.774253	3.042335
9	1	0.626582	0.451955	3.137610
10	1	2.630597	-0.780542	-1.557229
11	1	2.778894	0.757968	-1.463914
12	1	-1.960780	2.454133	-0.755279
13	1	-2.445578	1.229729	-1.569955

Harmonic frequencies and intensities (cm^{-1},km/mol):

66.2,0.9;67.3,1.0;68.7,2.5;101.6,2.6;106.4,13.9;116.8,45.0;
237.8,53.4;260.9,231.5;262.7,227.9;279.5,4.9;339.4,172.3;
339.5,170.0;378.2,53.6;379.9,48.6;416.4,66.5;738.9,0.3;
980.7,60.0;983.6,59.9;1183.4,256.2;1627.6,61.4;1627.7,61.5;
1643.0,0.3;1700.3,13.5;1700.3,13.5;2846.6,2984.3;2847.1,2983.9;
2980.9,146.5;3786.8,74.2;3786.8,74.2;3787.9,0.1;3874.2,23.9;
3874.2,23.9;3874.7,423.2;

Sum of electronic and zero-point Energies=	-306.145410
Sum of electronic and thermal Energies=	-306.134225
Sum of electronic and thermal Enthalpies=	-306.133281
Sum of electronic and thermal Free Energies=	-306.181658