# Supplementary Information

## Assessment of Hydrogen Bond Strength and Cooperativity in Self- and Cross-Associating Cyclic $(HF)_m(H_2O)_n$, (m + n) = 2 to 8 Clusters

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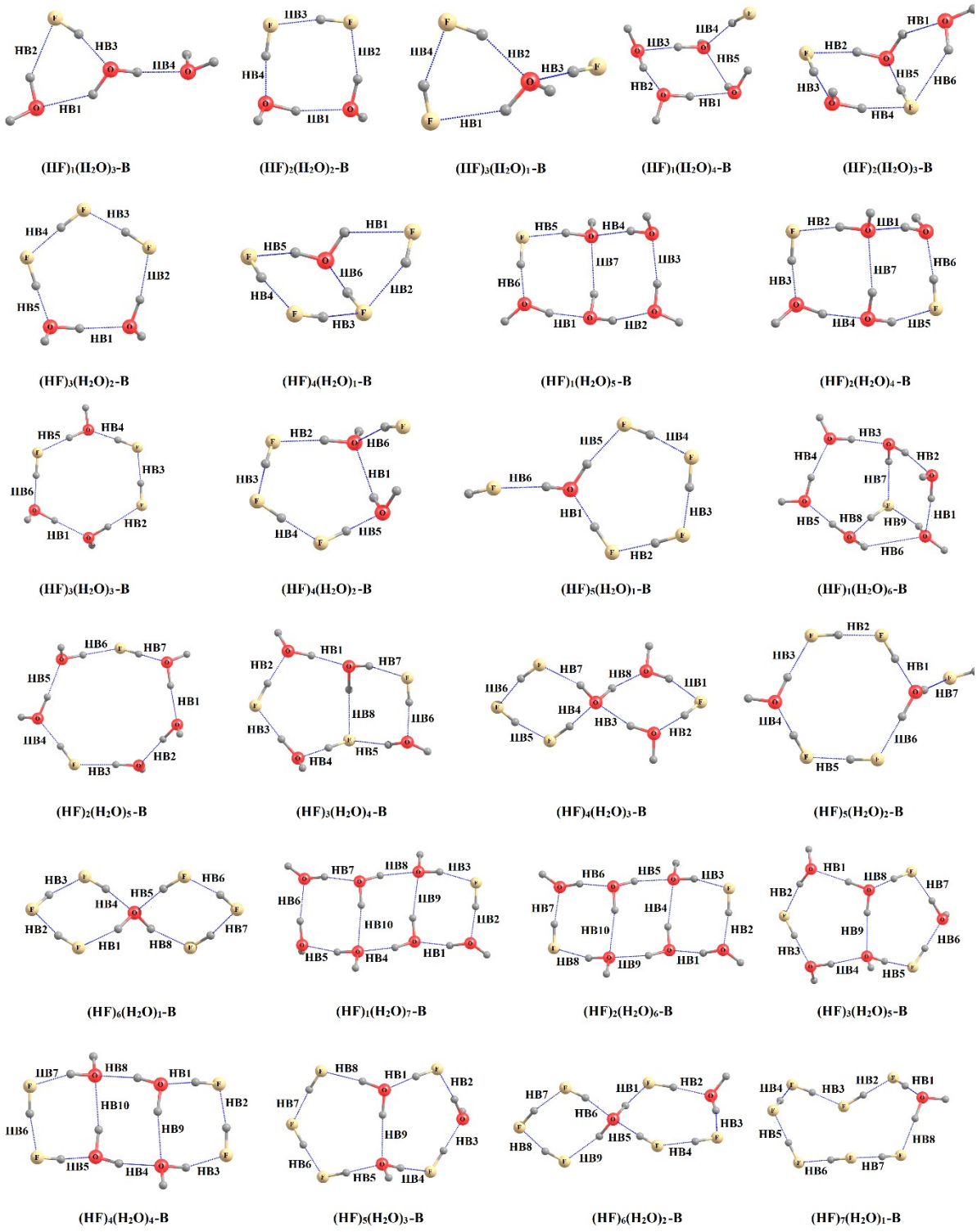


**Figure S1:** The MP2/aVDZ-optimized geometries of cyclic $(HF)_m(H_2O)_n$-B (m + n =4 to 8) clusters.

**Table S1**: Molecular energies (in a.u.) of various species in the estimation of HB energy $E_{HB1}$ in cyclic $(HF)_2(H_2O)_2$-A cluster, calculated at MP2/aug-cc-pvTZ level of theory. See text for details.

| **Species** | **Uncorrected Energy (in a.u.)** | **ZPE Corrected** | **BSSE Corrected** |
|---|---|---|---|
| $(HF)_2$ $(H_2O)_2$-A | $E_M$ = -353.392688 | $E_M$ = -353.317646 | $E_M$ = -353.392688 |
| Fragment F1 | $E_{F1}$ = -277.030417 | $E_{F2}$ = -276.981151 | $E_{F2}$ = -277.031373 |
| Fragment F2 | $E_{F2}$ = -253.021536 | $E_{F1}$ = -252.960427 | $E_{F1}$ = -253.022523 |
| Fragment F3 | $E_{F3}$ = -176.682423 | $E_{F3}$ = -176.646681 | $E_{F3}$ = -176.683281 |
| HF1…W1 dimer | $E_{HF1\ldots W1}$ = -176.682423 | $E_{HF1\ldots W1}$ = -176.646681 | $E_{HF1\ldots W1}$ = -176.683281 |
| HF1 monomer | $E_{HF1}$ = -100.338637 | $E_{HF1}$ = -100.330753 | $E_{HF1}$ = -100.339643 |
| W1 monomer | $E_{W1}$ = -76.328570 | $E_{W1}$ =-76.307814 | $E_{W1}$ = -76.329601 |

**Table S2:** The individual F-H…O HB energies (kcal/mol), distances (in Å) and angles (degrees), in cyclic $(HF)_m(H_2O)_n$-B clusters calculated at MP2/aVTZ level, along with the respective cooperativity contribution (kcal/mol). See Figures S1and text for details.

| Conformer B | HB Label | HB Distances | HB Angles | HB energy by MTA | HB energy in Dimer | Cooperativity |
|---|---|---|---|---|---|---|
| $(HF)_1(H_2O)_3$ | HB3 | 1.57 | 167 | 13.9 | 9.2 | 4.7 |
| $(HF)_2(H_2O)_2$ | HB4 | 1.51 | 172 | 16.7 | 9.6 | 7.0 |
| $(HF)_3(H_2O)_1$ | HB2 | 1.72 | 155 | 10.5 | 8.5 | 2.0 |
| | HB3 | 1.78 | 176 | 8.3 | 9.1 | -0.8 |
| $(HF)_1(H_2O)_4$ | HB4 | 1.63 | 168 | 11.6 | 9.2 | 2.4 |
| $(HF)_2(H_2O)_3$ | HB3 | 1.58 | 172 | 13.9 | 9.6 | 4.3 |
| | HB5 | 1.47 | 171 | 15.5 | 9.6 | 5.9 |
| $(HF)_3(H_2O)_2$ | HB5 | 1.46 | 178 | 19.1 | 9.7 | 9.4 |
| $(HF)_4(H_2O)_1$ | HB6 | 1.40 | 172 | 21.6 | 8.5 | 13.1 |
| $(HF)_1(H_2O)_5$ | HB6 | 1.45 | 171 | 17.5 | 9.3 | 8.2 |
| $(HF)_2(H_2O)_4$ | HB3 | 1.50 | 172 | 17.0 | 9.7 | 7.4 |
| | HB6 | 1.58 | 173 | 13.7 | 9.6 | 4.1 |
| $(HF)_3(H_2O)_3$ | HB4 | 1.48 | 178 | 17.5 | 9.6 | 7.9 |
| | HB6 | 1.49 | 178 | 17.2 | 9.6 | 7.5 |
| $(HF)_4(H_2O)_2$ | HB5 | 1.47 | 177 | 18.5 | 9.6 | 8.9 |
| | HB6 | 1.67 | 163 | 10.4 | 8.8 | 1.5 |
| $(HF)_5(H_2O)_1$ | HB1 | 1.44 | 178 | 19.9 | 9.8 | 10.1 |
| $(HF)_1(H_2O)_6$ | HB8 | 1.45 | 171 | 18.6 | 9.7 | 8.9 |
| $(HF)_2(H_2O)_5$ | HB4 | 1.52 | 178 | 16.2 | 9.5 | 6.6 |
| | HB7 | 1.51 | 178 | 16.2 | 9.6 | 6.6 |
| $(HF)_3(H_2O)_4$ | HB2 | 1.48 | 176 | 18.0 | 9.7 | 8.3 |
| | HB4 | 1.46 | 179 | 18.8 | 9.7 | 9.1 |
| | HB6 | 1.59 | 172 | 13.2 | 9.5 | 3.7 |
| $(HF)_4(H_2O)_3$ | HB2 | 1.57 | 172 | 14.0 | 9.6 | 4.5 |
| | HB4 | 1.50 | 171 | 17.4 | 9.8 | 7.7 |
| $(HF)_5(H_2O)_2$ | HB1 | 1.45 | 179 | 19.4 | 9.6 | 9.8 |
| | HB4 | 1.49 | 178 | 17.3 | 9.6 | 7.7 |
| $(HF)_6(H_2O)_1$ | HB4 | 1.60 | 169 | 14.1 | 9.1 | 5.0 |
| | HB5 | 1.60 | 169 | 14.1 | 9.6 | 4.5 |
| $(HF)_1(H_2O)_7$ | HB2 | 1.52 | 172 | 16.2 | 9.7 | 6.5 |
| $(HF)_2(H_2O)_6$ | HB2 | 1.52 | 172 | 16.2 | 9.7 | 6.6 |
| | HB7 | 1.52 | 172 | 16.2 | 9.7 | 6.6 |
| $(HF)_3(H_2O)_5$ | HB3 | 1.56 | 178 | 14.5 | 9.6 | 5.0 |
| | HB6 | 1.49 | 177 | 17.6 | 9.7 | 7.9 |
| | HB8 | 1.45 | 178 | 19.8 | 9.8 | 10.0 |
| $(HF)_4(H_2O)_4$ | HB1 | 1.46 | 173 | 18.8 | 9.7 | 9.1 |
| | HB5 | 1.46 | 173 | 18.8 | 9.7 | 9.1 |
| $(HF)_5(H_2O)_3$ | HB1 | 1.50 | 177 | 17.2 | 9.6 | 7.6 |
| | HB3 | 1.48 | 178 | 18.3 | 9.7 | 8.6 |
| | HB5 | 1.53 | 177 | 15.1 | 9.6 | 5.4 |
| $(HF)_6(H_2O)_2$ | HB2 | 1.50 | 177 | 16.6 | 9.6 | 7.0 |
| | HB5 | 1.56 | 177 | 15.2 | 9.8 | 5.5 |
| | HB6 | 1.58 | 170 | 14.7 | 9.6 | 5.1 |
| $(HF)_7(H_2O)_1$ | HB1 | 1.46 | 178 | 18.7 | 9.6 | 9.1 |

**Table S3:** The individual F-H…F HB energies (kcal/mol), distances (in Å) and angles (degrees), in cyclic $(HF)_m(H_2O)_n$-B clusters calculated at MP2/aVTZ level, along with the respective cooperativity contribution (kcal/mol). See Figures S1 and text for details.

| Conformers B | HB Label | HB Distance | Bond Angle | HB energy with MTA | HB energy in Dimer | Cooperativity |
|---|---|---|---|---|---|---|
| **$(HF)_2(H_2O)_2$** | HB3 | 1.59 | 169 | 10.4 | 4.5 | 5.9 |
| **$(HF)_3(H_2O)_1$** | HB4 | 1.77 | 149 | 7.4 | 4.3 | 3.1 |
| **$(HF)_3(H_2O)_2$** | HB3 | 1.58 | 175 | 10.0 | 4.3 | 5.7 |
| | HB4 | 1.51 | 177 | 12.7 | 4.0 | 8.8 |
| **$(HF)_4(H_2O)_1$** | HB2 | 1.86 | 146 | 7.1 | 4.6 | 2.5 |
| | HB3 | 1.60 | 165 | 11.2 | 4.7 | 6.5 |
| | HB4 | 1.65 | 165 | 8.9 | 4.6 | 4.4 |
| **$(HF)_3(H_2O)_3$** | HB3 | 1.56 | 178 | 11.0 | 4.2 | 6.8 |
| **$(HF)_4(H_2O)_2$** | HB3 | 1.56 | 176 | 10.7 | 4.2 | 6.5 |
| | HB4 | 1.51 | 176 | 13.0 | 3.9 | 9.1 |
| **$(HF)_5(H_2O)_1$** | HB2 | 1.49 | 176 | 13.6 | 3.8 | 9.8 |
| | HB3 | 1.54 | 176 | 11.3 | 4.1 | 7.3 |
| | HB4 | 1.59 | 174 | 9.8 | 4.4 | 5.4 |
| **$(HF)_4(H_2O)_3$** | HB5 | 1.55 | 167 | 11.6 | 4.2 | 7.4 |
| | HB6 | 1.62 | 166 | 9.4 | 4.5 | 5.0 |
| **$(HF)_5(H_2O)_2$** | HB2 | 1.52 | 178 | 12.2 | 4.0 | 8.3 |
| | HB5 | 1.55 | 177 | 11.1 | 4.2 | 6.9 |
| **$(HF)_6(H_2O)_1$** | HB2 | 1.62 | 165 | 9.4 | 4.4 | 5.0 |
| | HB3 | 1.59 | 165 | 10.3 | 3.9 | 6.5 |
| | HB6 | 1.59 | 165 | 10.3 | 4.4 | 6.0 |
| | HB7 | 1.62 | 165 | 9.4 | 4.4 | 5.0 |
| **$(HF)_4(H_2O)_4$** | HB2 | 1.55 | 169 | 11.6 | 4.3 | 7.4 |
| | HB6 | 1.55 | 169 | 11.6 | 4.3 | 7.4 |
| **$(HF)_5(H_2O)_3$** | HB6 | 1.56 | 176 | 10.9 | 4.2 | 6.7 |
| | HB7 | 1.61 | 174 | 9.1 | 4.5 | 4.7 |
| **$(HF)_6(H_2O)_2$** | HB4 | 1.58 | 174 | 10.2 | 4.4 | 5.8 |
| | HB7 | 1.59 | 166 | 10.5 | 4.3 | 6.2 |
| | HB8 | 1.62 | 165 | 9.4 | 4.4 | 5.0 |
| **$(HF)_7(H_2O)_1$** | HB2 | 1.49 | 179 | 13.0 | 3.6 | 9.4 |
| | HB3 | 1.52 | 177 | 11.2 | 3.7 | 7.5 |
| | HB4 | 1.53 | 179 | 11.2 | 3.9 | 7.3 |
| | HB5 | 1.54 | 178 | 10.7 | 3.9 | 6.8 |
| | HB6 | 1.55 | 178 | 10.3 | 4.0 | 6.3 |
| | HB7 | 1.58 | 178 | 9.6 | 4.2 | 5.4 |

**Table S4:** The individual O-H…O HB energies (kcal/mol), distances (in Å) and angles (degrees), in cyclic $(HF)_m(H_2O)_n$-B clusters calculated at MP2/aVTZ level, along with the respective cooperativity contribution (kcal/mol). See Figures S1 and text for details.

| Conformers B | HB Label | HB Distance | HB Angle | HB energy by MTA | HB energy in Dimer | Cooperativity |
|---|---|---|---|---|---|---|
| **$(HF)_1(H_2O)_3$** | HB1 | 2.00 | 140 | 7.1 | 4.6 | 2.5 |
| | HB4 | 1.86 | 175 | 6.3 | 5.1 | 1.2 |
| **$(HF)_2(H_2O)_2$** | HB1 | 1.74 | 165 | 9.4 | 4.8 | 4.7 |
| **$(HF)_1(H_2O)_4$** | HB1 | 1.78 | 167 | 8.4 | 4.9 | 3.5 |
| | HB2 | 1.74 | 168 | 9.1 | 4.8 | 4.4 |
| | HB3 | 1.69 | 169 | 10.4 | 4.5 | 5.9 |
| | HB5 | 2.10 | 144 | 7.1 | 4.3 | 2.8 |
| **$(HF)_2(H_2O)_3$** | HB1 | 2.00 | 138 | 6.6 | 4.4 | 2.2 |
| **$(HF)_3(H_2O)_2$** | HB1 | 1.69 | 175 | 10.1 | 4.5 | 5.6 |
| **$(HF)_1(H_2O)_5$** | HB1 | 1.64 | 167 | 11.2 | 4.1 | 7.1 |
| | HB2 | 1.80 | 164 | 5.8 | 3.5 | 2.4 |
| | HB3 | 1.80 | 166 | 7.9 | 5.0 | 2.9 |
| | HB4 | 1.85 | 169 | 6.0 | 4.5 | 1.5 |
| | HB7 | 2.05 | 152 | 6.8 | 4.7 | 2.2 |
| **$(HF)_2(H_2O)_4$** | HB1 | 1.80 | 168 | 6.2 | 4.2 | 2.0 |
| | HB4 | 1.68 | 168 | 10.5 | 4.5 | 6.0 |
| | HB7 | 2.03 | 153 | 6.8 | 4.7 | 2.1 |
| **$(HF)_3(H_2O)_3$** | HB1 | 1.69 | 180 | 9.8 | 4.4 | 5.3 |
| **$(HF)_4(H_2O)_2$** | HB1 | 2.02 | 147 | 8.2 | 4.2 | 3.9 |
| **$(HF)_1(H_2O)_6$** | HB1 | 1.87 | 164 | 6.7 | 5.2 | 1.6 |
| | HB2 | 1.86 | 170 | 5.4 | 4.0 | 1.4 |
| | HB3 | 1.70 | 174 | 9.7 | 4.7 | 5.0 |
| | HB4 | 1.72 | 169 | 9.1 | 4.2 | 4.9 |
| | HB5 | 1.67 | 178 | 10.4 | 4.3 | 6.1 |
| | HB6 | 2.47 | 120 | 6.4 | 3.7 | 2.7 |
| **$(HF)_2(H_2O)_5$** | HB1 | 1.68 | 178 | 10.3 | 4.3 | 6.0 |
| | HB2 | 1.73 | 179 | 8.8 | 4.5 | 4.3 |
| | HB5 | 1.70 | 177 | 9.7 | 4.4 | 5.3 |
| **$(HF)_3(H_2O)_4$** | HB1 | 1.67 | 175 | 10.6 | 4.3 | 6.3 |
| **$(HF)_4(H_2O)_3$** | HB3 | 1.85 | 162 | 8.7 | 5.2 | 3.4 |
| | HB8 | 1.68 | 167 | 9.4 | 3.9 | 5.5 |
| **$(HF)_1(H_2O)_7$** | HB1 | 1.68 | 168 | 10.6 | 4.5 | 6.2 |
| | HB4 | 1.85 | 170 | 6.6 | 4.7 | 1.9 |
| | HB5 | 1.72 | 169 | 9.7 | 4.8 | 5.0 |
| | HB6 | 1.75 | 168 | 9.2 | 4.9 | 4.3 |
| | HB7 | 1.73 | 169 | 9.3 | 4.8 | 4.5 |
| | HB8 | 1.91 | 168 | 5.9 | 4.7 | 1.2 |
| | HB9 | 1.94 | 159 | 7.1 | 5.0 | 2.1 |
| | HB10 | 1.94 | 161 | 7.1 | 5.0 | 2.1 |
| **$(HF)_2(H_2O)_6$** | HB1 | 1.68 | 169 | 10.5 | 4.5 | 6.0 |
| | HB4 | 1.95 | 158 | 7.1 | 5.0 | 2.1 |
| | HB5 | 1.88 | 169 | 6.2 | 4.7 | 1.5 |
| | HB6 | 1.68 | 169 | 10.5 | 4.5 | 6.0 |
| | HB9 | 1.88 | 169 | 6.2 | 4.7 | 1.5 |
| | HB10 | 1.95 | 158 | 7.1 | 5.0 | 2.1 |
| **$(HF)_3(H_2O)_5$** | HB1 | 1.74 | 177 | 7.5 | 4.0 | 3.5 |
| | HB4 | 1.78 | 175 | 6.4 | 4.2 | 2.2 |
| | HB9 | 1.89 | 173 | 7.6 | 5.2 | 2.3 |
| **$(HF)_4(H_2O)_4$** | HB4 | 1.83 | 168 | 6.8 | 4.6 | 2.2 |
| | HB8 | 1.83 | 168 | 6.8 | 4.6 | 2.2 |
| | HB9 | 1.92 | 156 | 7.9 | 4.9 | 3.0 |
| | HB10 | 1.92 | 156 | 7.9 | 4.9 | 3.0 |
| **$(HF)_5(H_2O)_3$** | HB9 | 1.94 | 173 | 7.5 | 5.2 | 2.3 |

**Table S5:** The individual O-H…F HB energies (kcal/mol), distances (in Å) and angles (degrees), in cyclic $(HF)_m(H_2O)_n$-B clusters calculated at MP2/aVTZ level, along with the respective cooperativity contribution (kcal/mol). See Figures S1and text for details.

| Conformer B | HB Label | HB Distance | HB Angle | HB energy by MTA | HB energy in Dimer | Cooperativity |
|---|---|---|---|---|---|---|
| $(HF)_1(H_2O)_3$ | HB2 | 2.01 | 144 | 6.3 | 3.3 | 2.9 |
| $(HF)_2(H_2O)_2$ | HB2 | 1.84 | 159 | 6.3 | 2.7 | 3.6 |
| $(HF)_3(H_2O)_1$ | HB1 | 1.96 | 139 | 6.7 | 3.1 | 3.6 |
| $(HF)_2(H_2O)_3$ | HB2 | 1.82 | 159 | 6.8 | 2.4 | 4.3 |
| | HB4 | 1.80 | 161 | 10.0 | 2.8 | 7.2 |
| | HB6 | 2.18 | 133 | 6.2 | 3.6 | 2.6 |
| $(HF)_3(H_2O)_2$ | HB2 | 1.79 | 169 | 6.1 | 2.3 | 3.8 |
| $(HF)_4(H_2O)_1$ | HB1 | 2.35 | 119 | 6.5 | 3.0 | 3.5 |
| | HB5 | 1.81 | 156 | 7.0 | 2.4 | 4.6 |
| $(HF)_1(H_2O)_5$ | HB5 | 1.72 | 167 | 7.7 | 2.1 | 5.7 |
| $(HF)_2(H_2O)_4$ | HB2 | 1.72 | 166 | 7.5 | 2.1 | 5.5 |
| | HB5 | 1.87 | 161 | 3.2 | 1.1 | 2.1 |
| $(HF)_3(H_2O)_3$ | HB2 | 1.77 | 177 | 6.0 | 2.0 | 3.9 |
| | HB5 | 1.68 | 177 | 7.9 | 1.5 | 6.4 |
| $(HF)_4(H_2O)_2$ | HB2 | 1.72 | 170 | 7.0 | 1.9 | 5.1 |
| $(HF)_5(H_2O)_1$ | HB5 | 1.76 | 170 | 6.7 | 2.2 | 4.5 |
| | HB6 | 1.92 | 170 | 3.7 | 2.7 | 1.0 |
| $(HF)_1(H_2O)_6$ | HB7 | 1.97 | 161 | 5.0 | 2.6 | 2.4 |
| | HB9 | 1.86 | 1.52 | 5.8 | 2.8 | 3.0 |
| $(HF)_2(H_2O)_5$ | HB3 | 1.75 | 178 | 6.4 | 1.9 | 4.5 |
| | HB6 | 1.74 | 178 | 5.8 | 1.5 | 4.4 |
| $(HF)_3(H_2O)_4$ | HB3 | 1.66 | 177 | 8.5 | 1.2 | 7.3 |
| | HB5 | 1.77 | 164 | 5.6 | 2.2 | 3.4 |
| | HB7 | 1.86 | 165 | 2.9 | 1.0 | 1.8 |
| | HB8 | 1.97 | 162 | 5.9 | 2.8 | 3.1 |
| $(HF)_4(H_2O)_3$ | HB1 | 1.79 | 161 | 6.9 | 2.6 | 4.3 |
| | HB7 | 1.81 | 159 | 6.9 | 2.6 | 4.3 |
| $(HF)_5(H_2O)_2$ | HB3 | 1.71 | 176 | 7.1 | 1.7 | 5.4 |
| | HB6 | 1.74 | 178 | 6.4 | 1.7 | 4.7 |
| | HB7 | 1.94 | 166 | 3.7 | 2.8 | 0.9 |
| $(HF)_6(H_2O)_1$ | HB1 | 1.74 | 161 | 7.3 | 2.1 | 5.2 |
| | HB8 | 1.74 | 161 | 7.3 | 2.1 | 5.2 |
| $(HF)_1(H_2O)_7$ | HB3 | 1.75 | 165 | 7.3 | 2.3 | 4.9 |
| $(HF)_2(H_2O)_6$ | HB3 | 1.75 | 165 | 7.3 | 2.3 | 5.1 |
| | HB8 | 1.75 | 165 | 7.3 | 2.1 | 5.2 |
| $(HF)_3(H_2O)_5$ | HB2 | 1.79 | 170 | 6.3 | 2.4 | 3.8 |
| | HB5 | 1.68 | 174 | 7.4 | 1.5 | 5.9 |
| | HB7 | 1.66 | 175 | 8.9 | 1.3 | 7.6 |
| $(HF)_4(H_2O)_4$ | HB3 | 1.76 | 162 | 7.0 | 2.3 | 4.7 |
| | HB7 | 1.76 | 162 | 7.0 | 2.3 | 4.7 |
| $(HF)_5(H_2O)_3$ | HB2 | 1.67 | 174 | 8.3 | 1.5 | 6.9 |
| | HB4 | 1.62 | 176 | 8.7 | 0.7 | 8.0 |
| | HB8 | 1.81 | 173 | 3.9 | 1.3 | 2.6 |
| $(HF)_6(H_2O)_2$ | HB1 | 1.64 | 174 | 8.4 | 1.0 | 7.4 |
| | HB3 | 1.75 | 170 | 6.8 | 2.1 | 4.7 |
| | HB9 | 1.75 | 161 | 7.1 | 2.2 | 5.0 |
| $(HF)_7(H_2O)_1$ | HB8 | 1.72 | 177 | 6.5 | 1.7 | 4.7 |

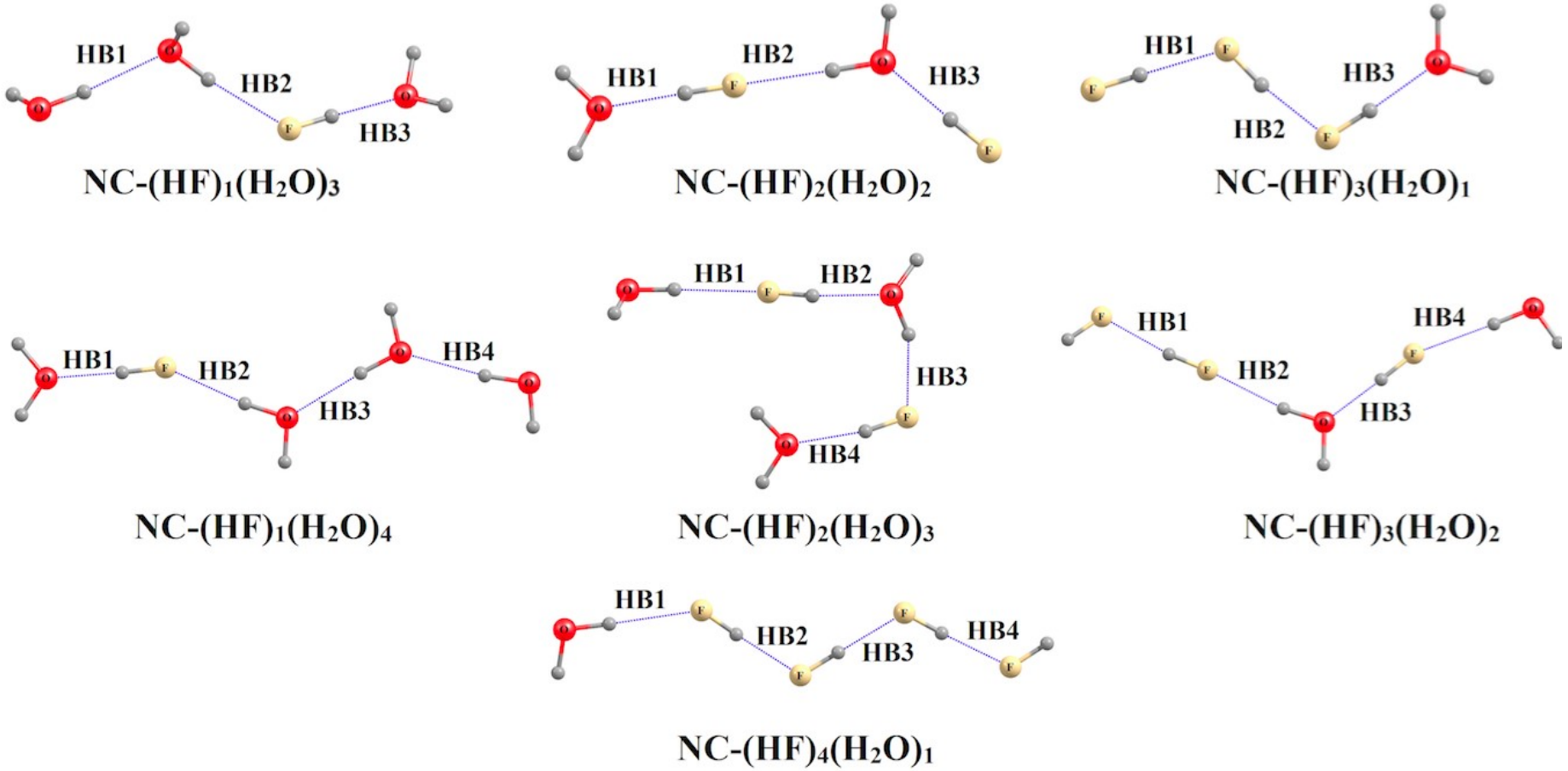


**Figure S2**: The MP2/aVDZ optimized geometries of linear non-cyclic NC-$(HF)_m(H_2O)_n$ (m + n = 4 and 5) clusters.

**Table S6:** The ZPE- and BSSE-corrected HB energies at MP2/aVTZ level of theory in some linear non-cyclic NC-$(HF)_m(H_2O)_n$ (m + n=4 and 5) clusters.

| H-bond label | HB Energy | ZPE-corrected HB Energy | BSSE-corrected HB Energy |
|---|---|---|---|
| | | **NC-$(HF)_1(H_2O)_3$** | |
| HB1 | 5.88 | 5.10 | 5.39 |
| HB2 | 4.26 | 3.85 | 3.84 |
| HB3 | 10.85 | 10.36 | 10.23 |
| | | **NC-$(HF)_2(H_2O)_2$** | |
| HB1 | 10.83 | 10.51 | 10.26 |
| HB2 | 4.37 | 4.57 | 3.98 |
| HB3 | 10.15 | 9.51 | 9.60 |
| | | **NC-$(HF)_3(H_2O)_1$ -A** | |
| HB1 | 6.53 | 6.31 | 5.98 |
| HB2 | 8.63 | 8.41 | 8.02 |
| HB3 | 12.05 | 12.22 | 11.46 |
| | | **NC-$(HF)_1(H_2O)_4$** | |
| HB1 | 10.68 | 9.88 | 10.10 |
| HB2 | 4.11 | 3.63 | 3.61 |
| HB3 | 1.60 | 1.84 | 1.57 |
| HB4 | 5.68 | 5.15 | 5.24 |
| | | **NC-$(HF)_2(H_2O)_3$** | |
| HB1 | 3.49 | 3.26 | 3.15 |
| HB2 | 12.48 | 11.76 | 11.87 |
| HB3 | 5.73 | 5.21 | 5.29 |
| HB4 | 10.87 | 10.39 | 10.36 |
| | | **NC-$(HF)_3(H_2O)_2$** | |
| HB1 | 5.65 | 5.25 | 5.11 |
| HB2 | 3.81 | 3.61 | 3.43 |
| HB3 | 11.38 | 10.75 | 10.78 |
| HB4 | 3.56 | 3.50 | 3.18 |
| | | **NC-$(HF)_4(H_2O)_1$** | |
| HB1 | 3.08 | 2.68 | 2.70 |
| HB2 | 6.98 | 6.42 | 6.42 |
| HB3 | 7.34 | 6.95 | 6.85 |
| HB4 | 6.28 | 5.84 | 5.73 |

**Note:** The energies of different types of respective HBs are much smaller in the linear non-cyclic clusters than those in the cyclic ones. The reasons for the smaller HB energies in non-cyclic clusters are twofold: (i) As compared to the respective cyclic clusters, there is one HB less in linear non-cyclic one. Because of this, the HB cooperativity contribution is expected to be smaller in later one. (ii) Another reason could be attributed to the fact that, the terminal HBs in linear non-cyclic clusters have only one adjacent neighbour in their cooperative network of HB. Evidently, the cooperativity contribution to such HB is much smaller. Thus much smaller cooperativity networking in linear non-cyclic clusters could be possible reason for the much weaker HB strengths as compared to the cyclic ones. Nevertheless, the energetic rank-ordering follows: F-H…O HB > F-H…F > O-H…O > O-H…F, in all the clusters studied this work.

**Table S7**: The F-H…O HB energies (kcal $mol^{-1}$), the unscaled F-H stretching frequencies ($cm^{-1}$) of the bond involved in the F-H…O HB and molecular electron density (MED) and molecular electrostatic potential (MESP) values (a. u.) at the corresponding bond critical point (BCP) in cyclic $(HF)_m(H_2O)_n$-A clusters, at MP2/aVTZ level.

| Conformers A | HB Labels | H-F Distance | HB energy (kcal/mol) | MESP at BCP | MED at BCP (a.u.) | F-H…O stretching frequency ($cm^{-1}$) |
|---|---|---|---|---|---|---|
| **$(HF)_1(H_2O)_1$ -A** | HB1 | 0.94 | 9.25 | 0.1658 | 0.0415 | 3675 |
| **$(HF)_1(H_2O)_2$ -A** | HB3 | 0.96 | 11.74 | 0.1873 | 0.0487 | 3386 |
| **$(HF)_2(H_2O)_1$ -A** | HB1 | 0.96 | 12.38 | 0.2214 | 0.0516 | 3321 |
| **$(HF)_1(H_2O)_3$ -A** | HB3 | 0.97 | 14.88 | 0.2241 | 0.0609 | 3099 |
| **$(HF)_2(H_2O)_2$ -A** | HB1 | 0.97 | 14.53 | 0.2352 | 0.0596 | 3193 |
| | HB3 | 0.97 | 14.53 | 0.2352 | 0.0596 | 3193 |
| **$(HF)_3(H_2O)_1$ -A** | HB4 | 0.98 | 16.12 | 0.2924 | 0.0701 | 2948 |
| **$(HF)_1(H_2O)_4$ -A** | HB4 | 0.98 | 16.00 | 0.2514 | 0.0688 | 3010 |
| **$(HF)_2(H_2O)_3$ -A** | HB2 | 0.98 | 17.09 | 0.3105 | 0.0816 | 2820 |
| | HB5 | 0.98 | 15.75 | 0.2889 | 0.0754 | 3001 |
| **$(HF)_3(H_2O)_2$ -A** | HB2 | 0.98 | 15.71 | 0.2599 | 0.0647 | 3044 |
| | HB5 | 0.99 | 17.57 | 0.2916 | 0.0718 | 2828 |
| **$(HF)_4(H_2O)_1$ -A** | HB1 | 0.99 | 17.87 | 0.3223 | 0.0771 | 2788 |
| **$(HF)_1(H_2O)_5$ -A** | HB5 | 0.98 | 16.28 | 0.2540 | 0.0695 | 3002 |
| **$(HF)_2(H_2O)_4$ -A** | HB2 | 0.98 | 16.34 | 0.2620 | 0.0700 | 3022 |
| | HB5 | 0.98 | 16.34 | 0.2620 | 0.0700 | 3022 |
| **$(HF)_3(H_2O)_3$ -A** | HB1 | 0.98 | 16.27 | 0.2732 | 0.0703 | 3034 |
| | HB3 | 0.98 | 15.98 | 0.2724 | 0.0700 | 3042 |
| | HB5 | 0.98 | 16.14 | 0.2709 | 0.0698 | 3042 |
| **$(HF)_4(H_2O)_2$ -A** | HB1 | 0.98 | 17.44 | 0.2949 | 0.0719 | 2877 |
| | HB4 | 0.98 | 17.44 | 0.2949 | 0.0719 | 2877 |
| **$(HF)_5(H_2O)_1$ -A** | HB1 | 0.99 | 18.44 | 0.3335 | 0.0794 | 2741 |
| **$(HF)_1(H_2O)_6$ -A** | HB7 | 0.98 | 16.66 | 0.2514 | 0.0719 | 2941 |
| **$(HF)_2(H_2O)_5$ -A** | HB5 | 0.98 | 16.96 | 0.2808 | 0.0695 | 2918 |
| | HB7 | 1.00 | 19.83 | 0.3028 | 0.0810 | 2599 |
| **$(HF)_3(H_2O)_4$ -A** | HB2 | 0.98 | 15.96 | 0.2645 | 0.0692 | 3007 |
| | HB4 | 1.01 | 19.93 | 0.3394 | 0.0890 | 2506 |
| | HB7 | 0.97 | 14.43 | 0.2678 | 0.0646 | 3120 |
| **$(HF)_4(H_2O)_3$ -A** | HB2 | 0.96 | 15.87 | 0.2723 | 0.0693 | 3039 |
| | HB5 | 0.99 | 18.29 | 0.3137 | 0.0788 | 2766 |
| | HB7 | 0.98 | 16.14 | 0.2780 | 0.0708 | 2976 |
| **$(HF)_5(H_2O)_2$ -A** | HB3 | 0.99 | 17.71 | 0.3124 | 0.0764 | 2839 |
| | HB7 | 0.99 | 18.31 | 0.3240 | 0.0793 | 2743 |
| **$(HF)_6(H_2O)_1$ -A** | HB1 | 0.99 | 18.71 | 0.3264 | 0.0766 | 2711 |
| **$(HF)_1(H_2O)_7$ -A** | HB2 | 1.00 | 18.76 | 0.2961 | 0.0817 | 2673 |
| **$(HF)_2(H_2O)_6$ -A** | HB10 | 0.99 | 18.13 | 0.2979 | 0.0794 | 2735 |
| | HB12 | 1.00 | 19.19 | 0.3133 | 0.0836 | 2621 |
| **$(HF)_3(H_2O)_5$ -A** | HB3 | 0.99 | 18.45 | 0.3129 | 0.0806 | 2770 |
| | HB5 | 1.00 | 18.68 | 0.3139 | 0.0820 | 2770 |
| | HB8 | 0.99 | 18.44 | 0.3129 | 0.0806 | 2770 |
| **$(HF)_4(H_2O)_4$ -A** | HB1 | 1.00 | 18.39 | 0.3260 | 0.0811 | 2820 |
| | HB3 | 1.00 | 18.39 | 0.3260 | 0.0811 | 2820 |
| | HB6 | 1.00 | 18.39 | 0.3260 | 0.0811 | 2820 |
| | HB10 | 1.00 | 18.39 | 0.3260 | 0.0811 | 2820 |
| **$(HF)_5(H_2O)_3$ -A** | HB1 | 0.97 | 14.57 | 0.2461 | 0.0572 | 3184 |
| | HB2 | 0.96 | 13.18 | 0.2218 | 0.0509 | 3320 |
| | HB4 | 0.97 | 15.01 | 0.2547 | 0.0619 | 3071 |
| | HB8 | 0.99 | 17.49 | 0.2965 | 0.0717 | 2835 |
| **$(HF)_6(H_2O)_2$ -A** | HB2 | 1.00 | 20.22 | 0.3460 | 0.0863 | 2563 |
| | HB6 | 0.97 | 14.24 | 0.2927 | 0.0633 | 3113 |
| **$(HF)_7(H_2O)_1$ -A** | HB1 | 0.97 | 15.57 | 0.2970 | 0.0640 | 3057 |
| | HB9 | 0.96 | 13.97 | 0.2690 | 0.0568 | 3216 |

**Table S8**: The F-H…F HB energies (kcal $mol^{-1}$), the unscaled F-H stretching frequencies ($cm^{-1}$) of the bond involved in the F-H…F HB and molecular electron density (MED) and molecular electrostatic potential (MESP) values (a. u.) at the corresponding bond critical point (BCP) in cyclic $(HF)_m$-$(H_2O)_n$-A clusters at MP2/aVTZ level.

| Conformers A | HB Labels | H-F Distance | HB energy (kcal/mol) | MESP at BCP (a.u.) | MED at BCP (a.u.) | F-H…F stretching frequency ($cm^{-1}$) |
|---|---|---|---|---|---|---|
| **$(HF)_2(H_2O)_1$ -A** | HB3 | 0.94 | 7.62 | 0.1677 | 0.0320 | 3745 |
| **$(HF)_3(H_2O)_1$ -A** | HB2 | 0.95 | 9.38 | 0.2263 | 0.0450 | 3570 |
| | HB3 | 0.96 | 11.29 | 0.2586 | 0.0532 | 3412 |
| **$(HF)_3(H_2O)_2$ -A** | HB4 | 0.96 | 11.33 | 0.2409 | 0.0503 | 3433 |
| **$(HF)_4(H_2O)_1$ -A** | HB2 | 0.96 | 12.71 | 0.2920 | 0.0598 | 3273 |
| | HB3 | 0.96 | 11.06 | 0.2733 | 0.0538 | 3437 |
| | HB4 | 0.95 | 9.83 | 0.2497 | 0.0486 | 3535 |
| **$(HF)_4(H_2O)_2$ -A** | HB2 | 0.96 | 11.41 | 0.2478 | 0.0512 | 3423 |
| | HB5 | 0.96 | 11.41 | 0.2478 | 0.0512 | 3423 |
| **$(HF)_5(H_2O)_1$ -A** | HB2 | 0.97 | 13.06 | 0.3063 | 0.0627 | 3216 |
| | HB3 | 0.96 | 11.27 | 0.2885 | 0.0565 | 3365 |
| | HB4 | 0.96 | 10.60 | 0.2761 | 0.0533 | 3472 |
| | HB5 | 0.95 | 9.76 | 0.2549 | 0.0490 | 3543 |
| **$(HF)_4(H_2O)_3$ -A** | HB4 | 0.96 | 11.37 | 0.2612 | 0.0565 | 3406 |
| **$(HF)_5(H_2O)_2$ -A** | HB2 | 0.96 | 11.57 | 0.2700 | 0.0570 | 3389 |
| | HB5 | 0.95 | 10.02 | 0.2544 | 0.0513 | 3502 |
| | HB6 | 0.96 | 12.49 | 0.2891 | 0.0607 | 3294 |
| **$(HF)_6(H_2O)_1$ -A** | HB2 | 0.97 | 13.11 | 0.3008 | 0.0598 | 3188 |
| | HB3 | 0.96 | 11.19 | 0.2824 | 0.0531 | 3313 |
| | HB4 | 0.96 | 11.04 | 0.2747 | 0.0511 | 3313 |
| | HB5 | 0.96 | 10.51 | 0.2689 | 0.0497 | 3542 |
| | HB6 | 0.95 | 9.51 | 0.2469 | 0.0455 | 3605 |
| **$(HF)_5(H_2O)_3$ -A** | HB7 | 0.96 | 11.66 | 0.2527 | 0.0517 | 3407 |
| **$(HF)_6(H_2O)_2$ -A** | HB3 | 0.97 | 14.05 | 0.3075 | 0.0654 | 3177 |
| | HB4 | 0.96 | 11.64 | 0.2844 | 0.0571 | 3374 |
| | HB7 | 0.95 | 10.60 | 0.2679 | 0.0506 | 3481 |
| | HB8 | 0.95 | 9.19 | 0.2393 | 0.0459 | 3633 |
| **$(HF)_7(H_2O)_1$ -A** | HB2 | 0.96 | 11.39 | 0.2870 | 0.0543 | 3351 |
| | HB3 | 0.96 | 10.69 | 0.2800 | 0.0525 | 3351 |
| | HB4 | 0.95 | 10.15 | 0.2690 | 0.0504 | 3351 |
| | HB7 | 0.95 | 9.42 | 0.2450 | 0.0456 | 3481 |
| | HB8 | 0.95 | 10.24 | 0.2580 | 0.0483 | 3481 |

**Table S9**: The O-H…O HB energies (kcal mol$^{-1}$), the unscaled F-H stretching frequencies (cm$^{-1}$) of the bond involved in the O-H…O HB and molecular electron density (MED) and molecular electrostatic potential (MESP) values (a. u.) at the corresponding bond critical point (BCP) in cyclic $(HF)_m(H_2O)_n$-A clusters at MP2/aVTZ level.

| Conformers $(HF)_m(H2O)_n$ | HB Labels | O-H Distance | HB energy (kcal/mol) | MESP at BCP (a.u.) | MED at BCP (a.u.) | O-H…O stretching frequency (cm$^{-1}$) |
|---|---|---|---|---|---|---|
| **$(HF)_1(H_2O)_2$ -A** | HB1 | 0.98 | 7.62 | 0.0904 | 0.0264 | 3578 |
| **$(HF)_1(H_2O)_3$ -A** | HB1 | 0.98 | 7.87 | 0.1005 | 0.0331 | 3488 |
| | HB2 | 0.99 | 9.47 | 0.1241 | 0.0398 | 3367 |
| **$(HF)_1(H_2O)_4$ -A** | HB1 | 0.98 | 8.68 | 0.1199 | 0.0399 | 3443 |
| | HB2 | 0.99 | 9.22 | 0.1280 | 0.0423 | 3379 |
| | HB3 | 0.99 | 10.19 | 0.1480 | 0.0463 | 3295 |
| **$(HF)_2(H_2O)_3$ -A** | HB3 | 0.99 | 10.16 | 0.1657 | 0.0476 | 3355 |
| **$(HF)_1(H_2O)_5$ -A** | HB1 | 0.99 | 8.63 | 0.1188 | 0.0400 | 3456 |
| | HB2 | 0.99 | 9.06 | 0.1220 | 0.0418 | 3415 |
| | HB3 | 0.99 | 9.36 | 0.1289 | 0.0429 | 3415 |
| | HB4 | 0.99 | 10.27 | 0.1489 | 0.0468 | 3361 |
| **$(HF)_2(H_2O)_4$ -A** | HB1 | 0.99 | 9.81 | 0.1528 | 0.0453 | 3349 |
| | HB4 | 0.99 | 9.81 | 0.1528 | 0.0453 | 3349 |
| **$(HF)_1(H_2O)_6$ -A** | HB1 | 0.98 | 4.87 | 0.0880 | 0.0268 | 3586 |
| | HB2 | 0.98 | 8.35 | 0.1259 | 0.0379 | 3410 |
| | HB3 | 0.99 | 6.61 | 0.1108 | 0.0323 | 3528 |
| | HB4 | 0.97 | 10.31 | 0.1506 | 0.0503 | 3155 |
| | HB5 | 0.98 | 7.28 | 0.1012 | 0.0356 | 3493 |
| | HB8 | 0.98 | 6.03 | 0.0899 | 0.0277 | 3586 |
| | HB9 | 0.97 | 5.59 | 0.0658 | 0.0212 | 3693 |
| **$(HF)_2(H_2O)_5$ -A** | HB1 | 0.98 | 6.34 | 0.1588 | 0.0364 | 3423 |
| | HB2 | 0.98 | 7.35 | 0.1040 | 0.0311 | 3520 |
| | HB3 | 0.98 | 5.44 | 0.1065 | 0.0288 | 3622 |
| | HB8 | 0.98 | 7.84 | 0.0994 | 0.0275 | 3576 |
| **$(HF)_3(H_2O)_4$ -A** | HB1 | 0.99 | 9.44 | 0.1474 | 0.0439 | 3345 |
| **$(HF)_1(H_2O)_7$ -A** | HB1 | 0.98 | 8.32 | 0.1112 | 0.0315 | 3518 |
| | HB4 | 1.00 | 10.28 | 0.1494 | 0.0482 | 3218 |
| | HB5 | 0.98 | 3.95 | 0.0942 | 0.0289 | 3593 |
| | HB6 | 0.99 | 10.03 | 0.1436 | 0.0468 | 3255 |
| | HB8 | 0.98 | 7.20 | 0.0888 | 0.0264 | 3615 |
| | HB9 | 1.00 | 10.44 | 0.1504 | 0.0485 | 3194 |
| | HB10 | 0.98 | 3.30 | 0.0886 | 0.0264 | 3594 |
| | HB11 | 0.98 | 7.24 | 0.0892 | 0.0344 | 3576 |
| | HB12 | 0.98 | 4.06 | 0.1144 | 0.0324 | 3561 |
| **$(HF)_2(H_2O)_6$ -A** | HB1 | 0.98 | 8.44 | 0.1213 | 0.0319 | 3520 |
| | HB2 | 0.98 | 3.72 | 0.1203 | 0.0310 | 3579 |
| | HB3 | 1.00 | 10.38 | 0.1616 | 0.0488 | 3206 |
| | HB4 | 0.98 | 3.68 | 0.1000 | 0.0275 | 3608 |
| | HB5 | 0.99 | 10.00 | 0.1555 | 0.0472 | 3243 |
| | HB11 | 0.98 | 8.31 | 0.1181 | 0.0305 | 3547 |
| **$(HF)_3(H_2O)_5$ -A** | HB1 | 1.00 | 10.14 | 0.1667 | 0.0475 | 3234 |
| | HB2 | 0.98 | 8.32 | 0.1313 | 0.0317 | 3523 |
| | HB9 | 0.98 | 8.32 | 0.1313 | 0.0317 | 3523 |
| **$(HF)_6(H_2O)_2$ -A** | HB1 | 0.97 | 7.75 | 0.1305 | 0.0260 | 3582 |

**Table S10**: The O-H…F HB energies (kcal mol$^{-1}$), the unscaled F-H stretching frequencies (cm$^{-1}$) of the bond involved in the O-H…F HB and molecular electron density (MED) and molecular electrostatic potential (MESP) values (a. u.) at the corresponding bond critical point (BCP) in cyclic $(HF)_m(H_2O)_n$-A clusters at MP2/aVTZ level.

| Conformers $(HF)_m(H2O)_n$ | HB Labels | O-H Distance | HB energy (kcal/mol) | MESP at BCP (a.u.) | MED at BCP (a.u.) | O-H…F stretching frequency (cm$^{-1}$) |
|---|---|---|---|---|---|---|
| **$(HF)_1(H_2O)_2$ -A** | HB2 | 0.97 | 6.31 | 0.0697 | 0.0154 | 3692 |
| **$(HF)_2(H_2O)_1$ -A** | HB2 | 0.97 | 6.78 | - | 0.0127 | 3699 |
| **$(HF)_1(H_2O)_3$ -A** | HB4 | 0.98 | 6.62 | 0.0952 | 0.0269 | 3606 |
| **$(HF)_2(H_2O)_2$ -A** | HB2 | 0.98 | 7.42 | 0.1242 | 0.0296 | 3567 |
| | HB4 | 0.98 | 7.42 | 0.1242 | 0.0296 | 3567 |
| **$(HF)_3(H_2O)_1$ -A** | HB1 | 0.98 | 6.94 | 0.1413 | 0.0289 | 3570 |
| **$(HF)_1(H_2O)_4$ -A** | HB5 | 0.98 | 6.65 | 0.1182 | 0.0323 | 3585 |
| **$(HF)_2(H_2O)_3$ -A** | HB1 | 0.98 | 8.21 | 0.1558 | 0.0387 | 3556 |
| | HB4 | 0.98 | 7.17 | 0.1315 | 0.0340 | 3624 |
| **$(HF)_3(H_2O)_2$ -A** | HB1 | 0.98 | 7.80 | 0.1540 | 0.0351 | 3512 |
| | HB3 | 0.98 | 6.90 | 0.1427 | 0.0314 | 3576 |
| **$(HF)_4(H_2O)_1$ -A** | HB5 | 0.98 | 6.93 | 0.1686 | 0.0338 | 3535 |
| **$(HF)_1(H_2O)_5$ -A** | HB6 | 0.98 | 6.55 | 0.1192 | 0.0323 | 3594 |
| **$(HF)_2(H_2O)_4$ -A** | HB3 | 0.98 | 6.78 | 0.1332 | 0.0339 | 3575 |
| | HB6 | 0.98 | 6.78 | 0.1332 | 0.0339 | 3575 |
| **$(HF)_3(H_2O)_3$ -A** | HB2 | 0.98 | 7.57 | 0.1588 | 0.0373 | 3522 |
| | HB4 | 0.98 | 7.24 | 0.1574 | 0.0370 | 3531 |
| | HB6 | 0.98 | 7.36 | 0.1575 | 0.0367 | 3537 |
| **$(HF)_4(H_2O)_2$ -A** | HB3 | 0.98 | 7.00 | 0.1541 | 0.0330 | 3560 |
| | HB6 | 0.98 | 7.00 | 0.1541 | 0.0330 | 3560 |
| **$(HF)_5(H_2O)_1$ -A** | HB6 | 0.98 | 6.72 | 0.1754 | 0.0342 | 3543 |
| **$(HF)_1(H_2O)_6$ -A** | HB6 | 0.98 | 6.83 | 0.1086 | 0.0321 | 3579 |
| **$(HF)_2(H_2O)_5$ -A** | HB4 | 0.98 | 7.24 | 0.1603 | 0.0356 | 3492 |
| | HB6 | 0.99 | 8.86 | 0.1633 | 0.0393 | 3438 |
| **$(HF)_3(H_2O)_4$ -A** | HB3 | 0.98 | 6.49 | 0.1506 | 0.0367 | 3518 |
| | HB5 | 0.97 | 4.13 | 0.0784 | 0.0210 | 3679 |
| | HB6 | 0.98 | 7.16 | 0.1374 | 0.0301 | 3583 |
| | HB8 | 0.97 | 1.99 | 0.0778 | 0.0175 | 3679 |
| | HB9 | 0.97 | 5.83 | 0.0952 | 0.0169 | 3730 |
| **$(HF)_4(H_2O)_3$ -A** | HB1 | 0.98 | 7.22 | 0.1622 | 0.0375 | 3524 |
| | HB3 | 0.98 | 6.22 | 0.1533 | 0.0344 | 3576 |
| | HB6 | 0.98 | 7.44 | 0.1694 | 0.0389 | 3504 |
| **$(HF)_5(H_2O)_2$ -A** | HB1 | 0.98 | 6.71 | 0.1735 | 0.0362 | 3553 |
| | HB4 | 0.98 | 6.42 | 0.1669 | 0.0345 | 3587 |
| **$(HF)_6(H_2O)_1$ -A** | HB7 | 0.98 | 6.49 | 0.1655 | 0.0323 | 3542 |
| **$(HF)_1(H_2O)_7$ -A** | HB3 | 0.97 | 5.99 | 0.0739 | 0.0210 | 3699 |
| | HB7 | 0.97 | 1.85 | 0.0778 | 0.0219 | 3722 |
| **$(HF)_2(H_2O)_6$ -A** | HB6 | 0.97 | 2.13 | 0.0898 | 0.0225 | 3742 |
| | HB7 | 0.97 | 5.99 | 0.0824 | 0.0209 | 3712 |
| | HB8 | 0.97 | 6.05 | 0.0806 | 0.0202 | 3659 |
| | HB9 | 0.98 | 2.20 | 0.1097 | 0.0260 | 3652 |
| **$(HF)_3(H_2O)_5$ -A** | HB4 | 0.98 | 7.13 | 0.1191 | 0.0258 | 3611 |
| | HB6 | 0.98 | 6.96 | 0.1121 | 0.0239 | 3657 |
| | HB7 | 0.98 | 6.96 | 0.1121 | 0.0239 | 3657 |
| | HB10 | 0.97 | 5.93 | 0.0920 | 0.0206 | 3666 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | HB11 | 0.97 | 5.93 | 0.0920 | 0.0206 | 3666 |
| | HB12 | 0.98 | 7.13 | 0.1191 | 0.0258 | 3611 |

**Table S10**: Continued…

| **Conformers $(HF)_m(H2O)_n$** | **HB Labels** | **O-H Distance** | **HB energy (kcal/mol)** | **MESP at BCP (a.u.)** | **MED at BCP (a.u.)** | **O-H….F stretching frequency ($cm^{-1}$)** |
|---|---|---|---|---|---|---|
| **$(HF)_4(H_2O)_4$ -A** | HB2 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB4 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB5 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB7 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB8 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB9 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB11 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| | HB12 | 0.98 | 7.04 | 0.1230 | 0.0242 | 3618 |
| **$(HF)_5(H_2O)_3$ -A** | HB3 | 0.98 | 6.99 | 0.1280 | 0.0314 | 3594 |
| | HB5 | 0.98 | 7.83 | 0.1640 | 0.0356 | 3504 |
| | HB6 | 0.98 | 7.13 | 0.1712 | 0.0355 | 3538 |
| | HB9 | 0.98 | 7.35 | 0.1543 | 0.0331 | 3544 |
| **$(HF)_6(H_2O)_2$ -A** | HB5 | 0.99 | 7.63 | 0.2162 | 0.0419 | 3469 |
| | HB9 | 0.98 | 4.29 | 0.1521 | 0.0311 | 3582 |
| **$(HF)_7(H_2O)_1$ -A** | HB5 | 0.98 | 7.27 | 0.2110 | 0.0394 | 3506 |
| | HB6 | 0.98 | 7.27 | 0.1910 | 0.0356 | 3506 |

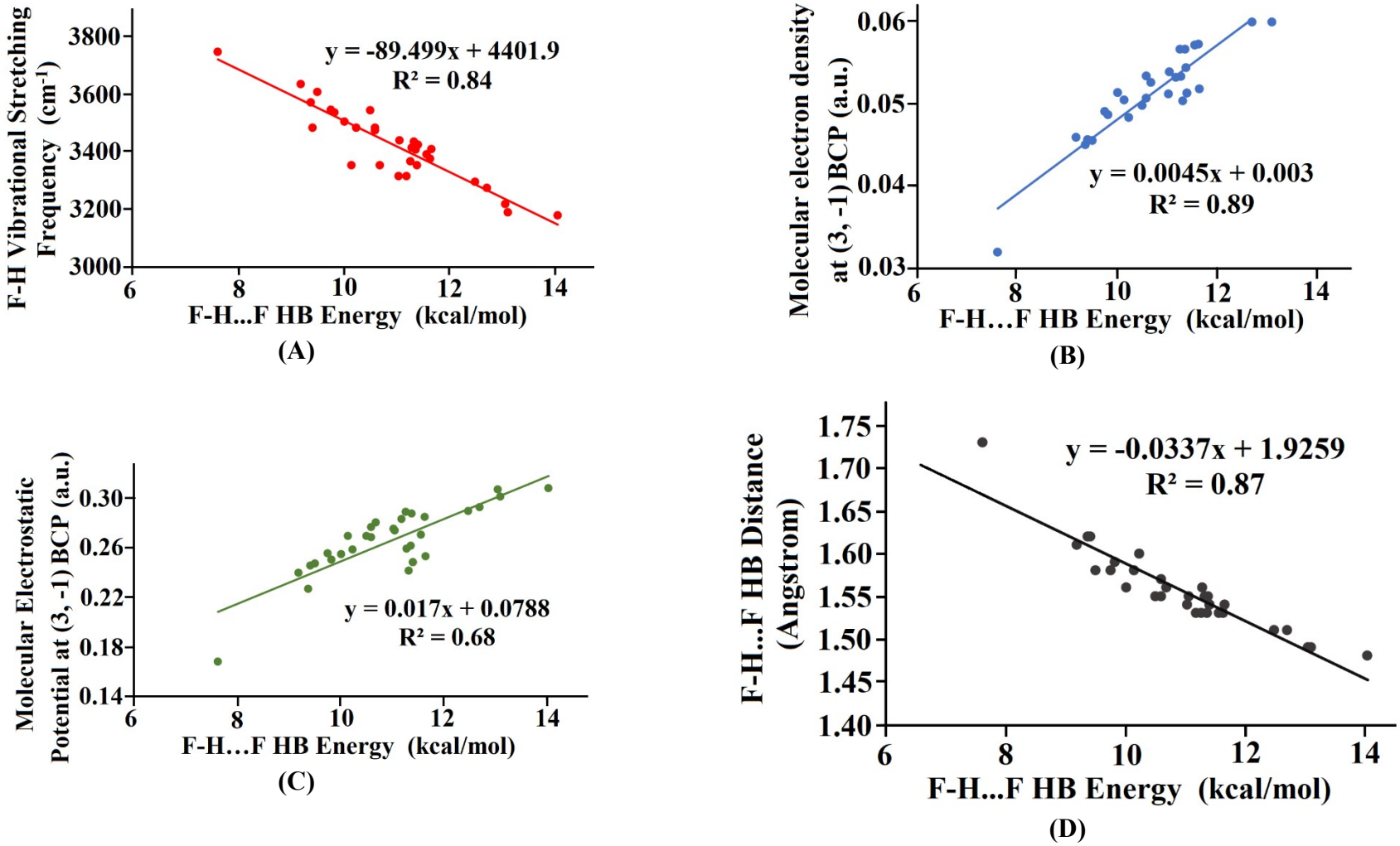


**Figure S3:** Correlation plots between the F-H…F hydrogen bond energy and **(A)** F-H stretching frequency (in $cm^{-1}$), **(B)**, molecular electron density (MED) value (in a.u.) at (3,-1) bond critical point (BCP), **(C)** molecular electrostatic potential (V(**r**)) value (in a.u.) at (3,-1) bond critical point (BCP) and **(D)** F-H…F hydrogen bond (HB) distances (in angstrom), in cyclic $(HF)_m(H_2O)_n$-A clusters.

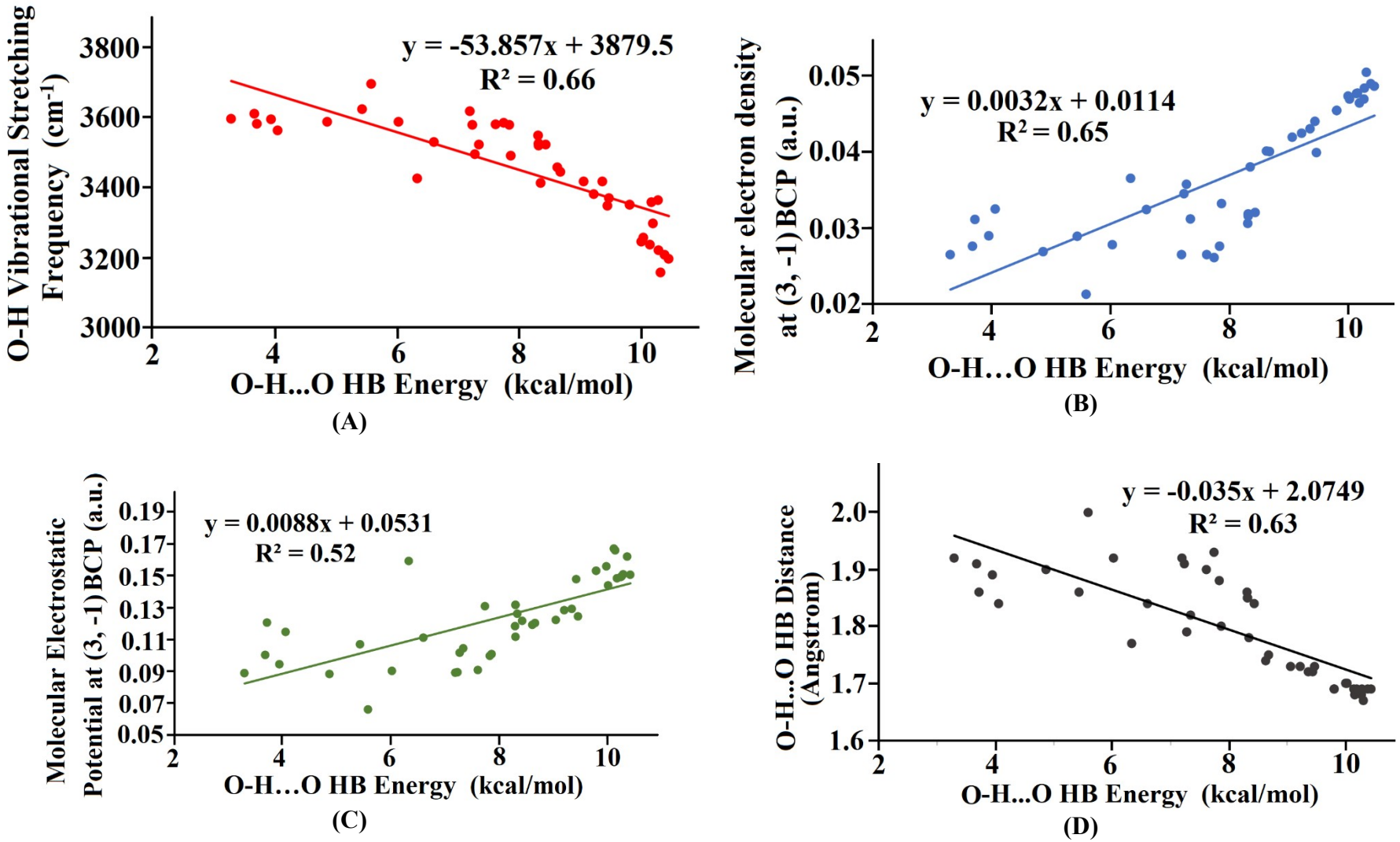


**Figure S4:** Correlation plots between the O-H…O hydrogen bond energy and **(A)** F-H stretching frequency (in $cm^{-1}$), **(B)**, molecular electron density (MED) value (in a.u.) at (3,-1) bond critical point (BCP), **(C)** molecular electrostatic potential (V(**r**)) value (in a.u.) at (3,-1) bond critical point (BCP) and **(D)** O-H…O hydrogen bond (HB) distances (in angstrom), in cyclic $(HF)_m(H_2O)_n$-A cluster.

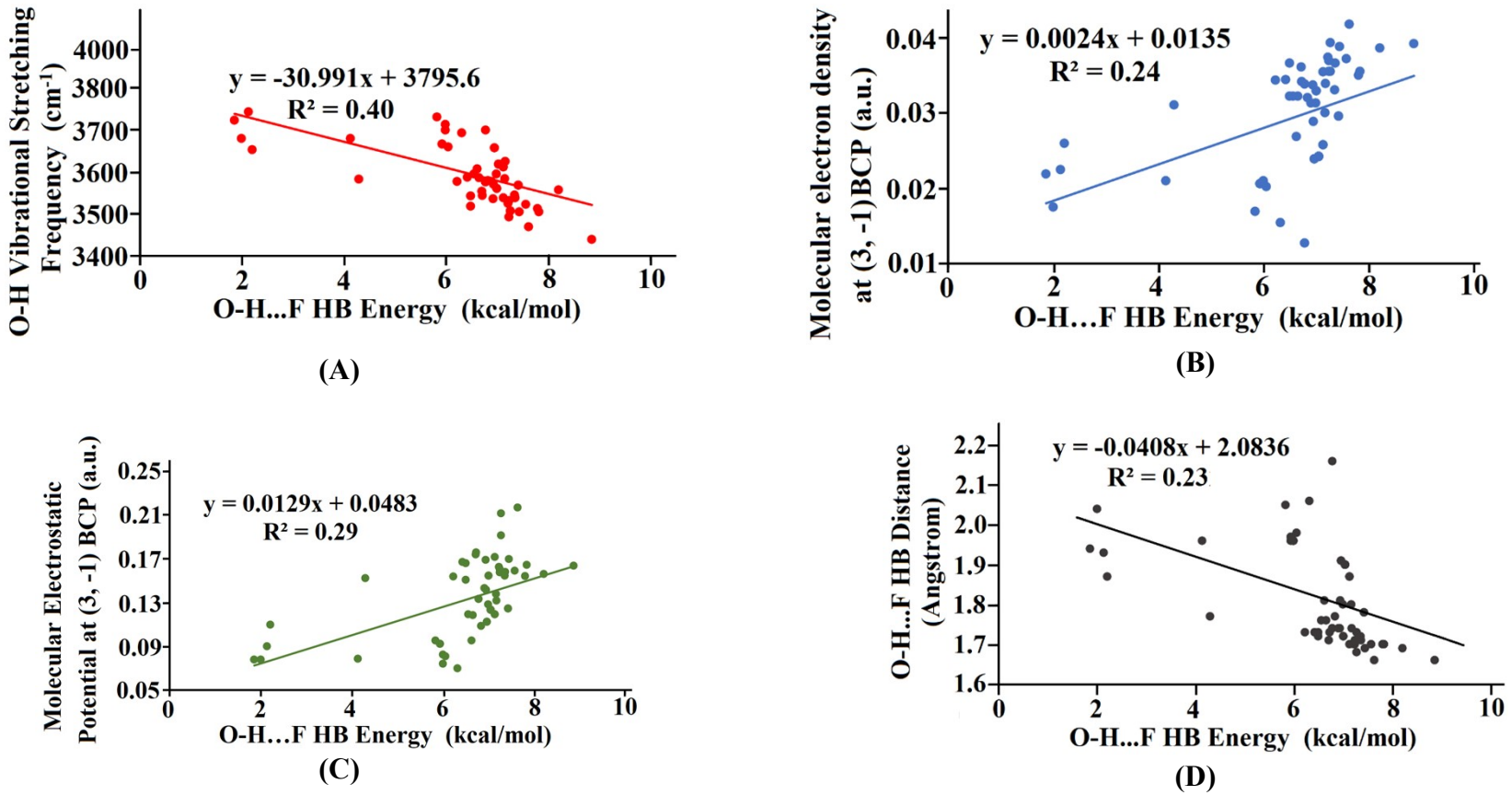


**Figure S5:** Correlation plots between the F-H…O hydrogen bond energy and **(A)** F-H stretching frequency (in $cm^{-1}$), **(B)**, molecular electron density (MED) value (in a.u.) at (3,-1) bond critical point (BCP), **(C)** molecular electrostatic potential (V(**r**)) value (in a.u.) at (3,-1) bond critical point (BCP) and **(D)** F-H…O hydrogen bond (HB) distances (in angstrom), in cyclic $(HF)_m(H_2O)_n$-A clusters.

**Note:** The correlation coefficients for the plots between O-H..F HB energy by MTA and other indirect measure is small. This may be attributed to the fact that there exists many bifurcated anti-cooperative O-H…F HBs in these clusters. As discussed in main text, the strength of these bifurcated anti-cooperative HBs is much smaller as compared to the ones which are not bifurcated. These smaller HB energies of bifurcated anti-cooperative HBs could be possible reason for deviation from the linearity with other measures of HB strengths.

**A Check on the MTA-Method: How Authentic are Hydrogen Bond Energies?**

**Table S11:** Error in the estimation of total energy of cyclic $(HF)_m(H_2O)_n$-A clusters calculated at MP2/aVTZ level of theory. See text for details.

| Conformer A | $\sum E_{HB}$ (a.u.) | $\sum E_{monomer}$ ‡ (a.u.) | $E_{calculated}$ (a.u.) | $E_{actual}$ (a.u.) | Error (a.u.) | Error (kcal/mol) | Error/HB (kcal/mol) |
|---|---|---|---|---|---|---|---|
| $(HF)_1(H_2O)_2$ | 0.04091 | -252.99706 | -253.03797 | -253.02876 | 0.00921 | 5.8 | 1.9 |
| $(HF)_2(H_2O)_1$ | 0.04268 | -277.00861 | -277.05129 | -277.04050 | 0.01079 | 6.8 | 2.3 |
| $(HF)_1(H_2O)_3$ | 0.06190 | -329.32384 | -329.38574 | -329.37725 | 0.00849 | 5.3 | 1.3 |
| $(HF)_2(H_2O)_2$ | 0.06997 | -353.33441 | -353.40434 | -353.39269 | 0.01170 | 7.3 | 1.8 |
| $(HF)_3(H_2O)_1$ | 0.06969 | -377.34593 | -377.41562 | -377.40249 | 0.01313 | 8.2 | 2.1 |
| $(HF)_1(H_2O)_4$ | 0.08086 | -405.65151 | -405.73237 | -405.72270 | 0.00967 | 6.1 | 1.2 |
| $(HF)_2(H_2O)_3$ | 0.09303 | -429.65987 | -429.75291 | -429.73852 | 0.01439 | 9.0 | 1.8 |
| $(HF)_3(H_2O)_2$ | 0.09451 | -453.67189 | -453.76640 | -453.75162 | 0.01478 | 9.3 | 1.9 |
| $(HF)_4(H_2O)_1$ | 0.09307 | -477.68405 | -477.77713 | -477.76051 | 0.01662 | 10.4 | 2.1 |
| $(HF)_1(H_2O)_5$ | 0.09588 | -481.97990 | -482.07578 | -482.06485 | 0.01094 | 6.9 | 1.1 |
| $(HF)_2(H_2O)_4$ | 0.10498 | -505.98959 | -506.09457 | -506.08161 | 0.01296 | 8.1 | 1.4 |
| $(HF)_3(H_2O)_3$ | 0.11245 | -529.99951 | -530.11196 | -530.09697 | 0.01499 | 9.4 | 1.6 |
| $(HF)_4(H_2O)_2$ | 0.11428 | -554.01044 | -554.12472 | -554.10755 | 0.01717 | 10.8 | 1.8 |
| $(HF)_5(H_2O)_1$ | 0.11133 | -578.02307 | -578.13440 | -578.11578 | 0.01862 | 11.7 | 2.0 |
| $(HF)_1(H_2O)_6$ | 0.11558 | -558.30758 | -558.42316 | -558.41339 | 0.00976 | 6.1 | 0.7 |
| $(HF)_2(H_2O)_5$ | 0.12726 | -582.31512 | -582.44239 | -582.42781 | 0.01458 | 9.2 | 1.1 |
| $(HF)_3(H_2O)_4$ | 0.13604 | -606.32462 | -606.46066 | -606.44250 | 0.01815 | 11.4 | 1.3 |
| $(HF)_4(H_2O)_3$ | 0.13156 | -630.33771 | -630.46927 | -630.45253 | 0.01675 | 10.5 | 1.5 |
| $(HF)_5(H_2O)_2$ | 0.13265 | -654.34911 | -654.48176 | -654.46250 | 0.019266 | 12.1 | 1.7 |
| $(HF)_6(H_2O)_1$ | 0.12840 | -678.36224 | -678.49069 | -678.47034 | 0.02030 | 12.7 | 1.8 |
| $(HF)_1(H_2O)_7$ | 0.15213 | -634.63316 | -634.78530 | -634.76891 | 0.01639 | 10.3 | 0.9 |
| $(HF)_2(H_2O)_6$ | 0.15652 | -658.64126 | -658.79778 | -658.78381 | 0.01397 | 8.8 | 0.7 |
| $(HF)_3(H_2O)_5$ | 0.19506 | -682.64948 | -682.84453 | -682.79737 | 0.04716 | 29.6 | 2.5 |
| $(HF)_4(H_2O)_4$ | 0.20701 | -706.65776 | -706.86478 | -706.80991 | 0.05486 | 34.4 | 2.9 |
| $(HF)_5(H_2O)_3$ | 0.16131 | -730.67829 | -730.83960 | -730.81233 | 0.02727 | 17.1 | 1.9 |
| $(HF)_6(H_2O)_2$ | 0.15873 | -754.68868 | -754.84740 | -754.82092 | 0.02648 | 16.6 | 1.9 |
| $(HF)_7(H_2O)_1$ | 0.15297 | -778.70438 | -778.85736 | -778.82796 | 0.02940 | 18.5 | 2.1 |

‡ Monomer geometries were taken from those in the respective cluster.

In order to authenticate the values of energies of different types of HBs obtained by MTA method, the molecular energy of a given cluster is approximately obtained by adding the sum of monomer energies to the sum of HB energies. For instance, the sum of energies of four HBs (0.06997 a.u.) when subtracted from the sum of energies of monomers (-353.33441 a.u.) in the HF-water cyclic tetramer $(HF)_2$-$(H_2O)_2$-A, yield the calculated energy of -353.40434 a.u. The actual energy of this cluster at the MP2/aVTZ level is -353.39269 a.u. The difference in these two energies (calculated - actual) is moderate (0.01170 a.u.), suggesting that HB energies

calculated with MTA-based method are indeed reliable. The MP2/aVTZ molecular energies of cyclic $(HF)_m(H_2O)_n$, clusters estimated in this way are in good agreement with the respective actual energies. The typical absolute error falls between 0.5 to 54 miliHartrees (mHs); see Tables S11 and S12in SI, respectively for all the cyclic $(HF)_m(H_2O)_n$ clusters. Another important result noticed from these Tables is that the error in the estimation of molecular energy of a cluster using the estimated HB energies is, in general, found to be increases with increase in size of these mixed HF-water clusters. Nevertheless, the average error per HB (the total error divided by the number of HB) is small (typically less than 2.9 kcal/mol) for all HF-water mixed clusters studied here.

**Table S12:** Error in the estimation of total energy of cyclic $(HF)_m(H_2O)_n$-B clusters calculated at MP2/aug-cc-pVTZ level of theory. See text for details

| Conformer B | $\sum E_{HB}$ (a.u.) | $\sum E_{monomers}$ ‡ (a.u.) | $E_{calculated}$ (a.u.) | $E_{actual}$ (a.u.) | Error (a.u.) | Error (kcal/mol) | Error/HB (kcal/mol) |
|---|---|---|---|---|---|---|---|
| $(HF)_1(H_2O)_3$ | 0.05348 | -329.32500 | -329.37847 | -329.36845 | 0.00998 | 6.3 | 1.6 |
| $(HF)_2(H_2O)_2$ | 0.06812 | -353.33422 | -353.40235 | -353.39127 | 0.01108 | 7.0 | 1.7 |
| $(HF)_3(H_2O)_1$ | 0.05230 | -377.34992 | -377.40221 | -377.39053 | 0.01169 | 7.3 | 1.8 |
| $(HF)_1(H_2O)_4$ | 0.07424 | -405.65303 | -405.72727 | -405.71947 | 0.00780 | 4.9 | 1.0 |
| $(HF)_2(H_2O)_3$ | 0.09378 | -429.66063 | -429.75441 | -429.73306 | 0.02135 | 13.4 | 2.2 |
| $(HF)_3(H_2O)_2$ | 0.09250 | -453.67188 | -453.76438 | -453.74947 | 0.01490 | 9.4 | 1.9 |
| $(HF)_4(H_2O)_1$ | 0.09929 | -477.68115 | -477.78043 | -477.75280 | 0.02763 | 17.3 | 2.9 |
| $(HF)_1(H_2O)_5$ | 0.10037 | -481.97820 | -482.07857 | -482.06630 | 0.01227 | 7.7 | 1.1 |
| $(HF)_2(H_2O)_4$ | 0.10346 | -505.98976 | -506.09269 | -506.08269 | 0.01052 | 6.6 | 0.9 |
| $(HF)_3(H_2O)_3$ | 0.11036 | -529.99947 | -530.10982 | -530.09512 | 0.01470 | 9.2 | 1.5 |
| $(HF)_4(H_2O)_2$ | 0.10770 | -554.01232 | -554.12002 | -554.10514 | 0.01488 | 9.3 | 1.6 |
| $(HF)_5(H_2O)_1$ | 0.10343 | -578.02310 | -578.12654 | -578.10858 | 0.01795 | 11.3 | 1.9 |
| $(HF)_1(H_2O)_6$ | 0.12289 | -558.30573 | -558.42862 | -558.40839 | 0.02023 | 12.7 | 1.4 |
| $(HF)_2(H_2O)_5$ | 0.11705 | -582.31793 | -582.43498 | -582.42327 | 0.01171 | 7.4 | 1.1 |
| $(HF)_3(H_2O)_4$ | 0.13291 | -606.32552 | -606.44118 | -606.44176 | 0.01662 | 10.5 | 1.3 |
| $(HF)_4(H_2O)_3$ | 0.13423 | -630.34001 | -630.47431 | -630.45084 | 0.02348 | 14.7 | 1.8 |
| $(HF)_5(H_2O)_2$ | 0.12313 | -654.34992 | -654.47305 | -654.45515 | 0.01790 | 11.2 | 1.6 |
| $(HF)_6(H_2O)_1$ | 0.13099 | -678.36645 | -678.49745 | -678.47034 | 0.02710 | 17.0 | 2.1 |
| $(HF)_1(H_2O)_7$ | 0.14179 | -634.63583 | -637.77762 | -634.75678 | 0.02085 | 13.1 | 1.3 |
| $(HF)_2(H_2O)_6$ | 0.15080 | -658.64537 | -658.79617 | -658.77298 | 0.02318 | 14.6 | 1.5 |
| $(HF)_3(H_2O)_5$ | 0.15286 | -682.65337 | -682.80623 | -682.78792 | 0.01830 | 11.5 | 1.3 |
| $(HF)_4(H_2O)_4$ | 0.16601 | -706.66480 | -706.83080 | -706.80085 | 0.02996 | 18.8 | 1.9 |
| $(HF)_5(H_2O)_3$ | 0.15787 | -730.67714 | -730.83501 | -730.81157 | 0.02349 | 14.7 | 1.6 |
| $(HF)_6(H_2O)_2$ | 0.15756 | -754.69108 | -754.84865 | -754.82038 | 0.02826 | 17.7 | 2.0 |
| $(HF)_7(H_2O)_1$ | 0.14505 | -778.70171 | -778.84675 | -778.82476 | 0.02199 | 13.8 | 1.7 |

‡ Monomer geometries were taken from those in the respective cluster.

**Table S13:** Cartesian Coordinates of cyclic $(HF)_m(H_2O)_n$-A clusters optimized at MP2/aug-cc-pVDZ level of theory along with single point energy at MP2/aug-cc-pVTZ level

**$(HF)_1(H_2O)_1$ -A**
**MP2/aug-cc-pVTZ = -176.6841045 a.u.**

| | | | |
|---|---|---|---|
| O | -1.244914000 | 0.000368000 | -0.12437500 |
| H | -1.649100000 | 0.765438000 | 0.30679500 |
| H | -1.647791000 | -0.765399000 | 0.30680000 |
| F | 1.408111000 | -0.000356000 | 0.020178000 |
| H | 0.467932000 | -0.000050000 | -0.04951600 |

**$(HF)_1(H_2O)_2$ -A**
**MP2/aug-cc-pVTZ = -253.0287586 a.u.**

| | | | |
|---|---|---|---|
| O | 1.636242000 | 0.060448000 | 0.10369600 |
| H | 2.377032000 | -0.081664000 | -0.49839900 |
| H | 1.108561000 | -0.755119000 | 0.05301200 |
| O | -0.852903000 | 1.235815000 | -0.12714800 |
| H | 0.122702000 | 1.191890000 | -0.05456600 |
| H | -1.144618000 | 1.756688000 | 0.63218600 |
| F | -0.867229000 | -1.330843000 | 0.00700300 |
| H | -1.042224000 | -0.390985000 | -0.03624300 |

**$(HF)_2(H_2O)_1$-A**
**MP2/aug-cc-pVTZ = -277.0405054 a.u.**

| | | | |
|---|---|---|---|
| O | -1.434006000 | -0.600006000 | -0.117583000 |
| H | -0.678133000 | -1.209325000 | -0.059621000 |
| H | -2.020276000 | -0.850507000 | 0.608660000 |
| F | 0.077986000 | 1.444108000 | 0.010096000 |
| H | -0.637981000 | 0.803828000 | -0.024830000 |
| F | 1.433548000 | -0.783221000 | 0.016242000 |
| H | 1.205275000 | 0.130514000 | 0.017950000 |

**$(HF)_1(H_2O)_3$-A**
**MP2/aug-cc-pVTZ = -329.3772544 a.u.**

| | | | |
|---|---|---|---|
| O | 1.521648000 | -1.123411000 | 0.190121000 |
| H | 2.086725000 | -1.761799000 | -0.260525000 |
| H | 0.608571000 | -1.444067000 | 0.053723000 |
| O | 1.115843000 | 1.588886000 | 0.014202000 |
| H | 1.544340000 | 2.007631000 | -0.742367000 |
| H | 1.447197000 | 0.663207000 | 0.021154000 |
| O | -1.528712000 | 1.009260000 | -0.021754000 |
| H | -0.601297000 | 1.353186000 | -0.007624000 |
| H | -1.942066000 | 1.349777000 | 0.781887000 |
| F | -1.194292000 | -1.484933000 | -0.124913000 |
| H | -1.400397000 | -0.536890000 | -0.080163000 |

**$(HF)_2(H_2O)_2$-A**
**MP2/aug-cc-pVTZ = -353.3926877 a.u.**

| | | | |
|---|---|---|---|
| O | 1.662044000 | 0.782523000 | -0.107946000 |
| H | 0.817640000 | 1.277160000 | -0.056868000 |
| H | 2.212011000 | 1.133639000 | 0.603837000 |
| O | -1.662047000 | -0.782541000 | -0.107764000 |
| H | -0.817641000 | -1.277169000 | -0.056625000 |
| H | -2.211993000 | -1.133536000 | 0.604094000 |
| F | 0.922839000 | -1.626039000 | 0.009922000 |
| H | 1.292601000 | -0.730198000 | -0.023679000 |
| F | -0.922839000 | 1.626041000 | 0.009671000 |
| H | -1.292601000 | 0.730194000 | -0.023765000 |

**$(HF)_3(H_2O)_1$-A**
**MP2/aug-cc-pVTZ = -377.4024912 a.u.**

| | | | |
|---|---|---|---|
| O | 1.707122000 | 0.679204000 | -0.099602000 |
| H | 0.913210000 | 1.249376000 | -0.057468000 |
| H | 2.274226000 | 0.964516000 | 0.628686000 |
| F | -0.852185000 | 1.663441000 | -0.017793000 |
| H | -1.273710000 | 0.812719000 | 0.004624000 |
| F | -1.631881000 | -0.770543000 | 0.042057000 |
| H | -0.782243000 | -1.212518000 | 0.015782000 |
| F | 0.728322000 | -1.610361000 | -0.022545000 |
| H | 1.198985000 | -0.751366000 | -0.041615000 |

**$(HF)_1(H_2O)_4$-A**
**MP2/aug-cc-pVTZ = -405.7226973 a.u.**

| | | | |
|---|---|---|---|
| O | 1.605371000 | -1.638892000 | -0.069855000 |
| H | 1.903374000 | -2.123480000 | -0.849200000 |
| H | 0.646264000 | -1.824386000 | -0.013280000 |
| O | 2.059822000 | 1.048164000 | 0.138021000 |
| H | 2.572068000 | 1.174498000 | 0.946021000 |
| H | 1.950684000 | 0.071984000 | 0.056900000 |
| O | -0.374687000 | 2.219128000 | -0.121539000 |
| H | -0.327306000 | 2.765352000 | -0.915750000 |
| H | 0.532846000 | 1.843264000 | -0.015270000 |
| O | -2.219276000 | 0.274067000 | -0.005242000 |
| H | -1.561724000 | 1.014983000 | -0.059913000 |
| H | -2.769540000 | 0.476861000 | 0.761722000 |
| F | -1.108366000 | -1.963651000 | 0.086925000 |
| H | -1.558075000 | -1.098422000 | 0.055692000 |

**$(HF)_2(H_2O)_3$-A**
**MP2/aug-cc-pVTZ = -429.73852 a.u.**

| | | | |
|---|---|---|---|
| O | -2.020496000 | -0.918223000 | 0.099235000 |
| H | -2.573474000 | -1.240070000 | -0.623689000 |
| H | -1.182353000 | -1.424987000 | 0.030068000 |
| O | 1.074646000 | 1.967792000 | -0.045301000 |
| H | 0.100550000 | 1.905592000 | 0.030510000 |
| H | 1.229772000 | 2.553037000 | -0.796728000 |
| O | 2.185402000 | -0.480856000 | 0.026136000 |
| H | 2.716006000 | -0.514013000 | 0.832317000 |
| H | 1.819409000 | 0.438863000 | -0.011033000 |
| F | 0.357263000 | -2.166985000 | -0.089606000 |
| H | 1.093781000 | -1.523888000 | -0.039391000 |
| F | -1.615109000 | 1.556157000 | 0.153507000 |
| H | -1.798393000 | 0.601229000 | 0.125672000 |

**$(HF)_3(H_2O)_2$-A**
**MP2/aug-cc-pVTZ = -453.7516203 a.u.**

| | | | |
|---|---|---|---|
| O | -1.592857000 | -1.479695000 | -0.055370000 |
| H | -1.972909000 | -1.918903000 | 0.716234000 |
| H | -0.638288000 | -1.712866000 | -0.048083000 |
| O | 2.214739000 | 0.282141000 | 0.098745000 |
| H | 1.564239000 | 1.014334000 | 0.122189000 |
| H | 2.812049000 | 0.493358000 | -0.630126000 |
| F | 1.051379000 | -1.926507000 | -0.041180000 |
| F | -1.940083000 | 0.964799000 | -0.172015000 |
| F | 0.242871000 | 2.151328000 | 0.143625000 |
| H | -0.613510000 | 1.741878000 | 0.023387000 |
| H | 1.534971000 | -1.080970000 | 0.005547000 |

| | | | |
|---|---|---|---|
| H | -1.823987000 | -0.012387000 | -0.118591000 |

**$(HF)_4(H_2O)_1$-A**
**MP2/aug-cc-pVTZ = -477.7605089 a.u.**

| | | | |
|---|---|---|---|
| O | 2.045349000 | 0.796528000 | -0.074984000 |
| H | 1.254712000 | 1.375287000 | -0.077480000 |
| H | 2.588593000 | 1.097964000 | 0.664761000 |
| F | 1.408444000 | -1.586263000 | -0.058582000 |
| F | -1.052521000 | -1.836770000 | 0.018302000 |
| F | -2.132274000 | 0.423027000 | 0.067716000 |
| F | -0.297233000 | 2.166526000 | -0.078131000 |
| H | 1.688789000 | -0.639130000 | -0.056250000 |
| H | -0.090904000 | -1.779961000 | -0.014636000 |
| H | -1.763332000 | -0.460351000 | 0.049740000 |
| H | -1.028823000 | 1.559821000 | -0.027338000 |

**$(HF)_1(H_2O)_5$-A**
**MP2/aug-cc-pVTZ = -482.0648464 a.u.**

| | | | |
|---|---|---|---|
| O | -1.372016000 | -2.294777000 | 0.042873000 |
| H | -1.534482000 | -2.873098000 | 0.797664000 |
| H | -0.398556000 | -2.274921000 | -0.048808000 |
| O | -2.727956000 | 0.066089000 | -0.152411000 |
| H | -3.229185000 | -0.014017000 | -0.973007000 |
| H | -2.238948000 | -0.785356000 | -0.073648000 |
| O | -1.278737000 | 2.332187000 | 0.230635000 |
| H | -1.620977000 | 2.704552000 | 1.052115000 |
| H | -1.805142000 | 1.510122000 | 0.085564000 |
| O | 1.397779000 | 2.212686000 | -0.144221000 |
| H | 0.421787000 | 2.246625000 | 0.005569000 |
| H | 1.543431000 | 2.732470000 | -0.944031000 |
| O | 2.676457000 | -0.131529000 | 0.013206000 |
| H | 3.203051000 | -0.060849000 | 0.818917000 |
| H | 2.181075000 | 0.725416000 | -0.052337000 |
| F | 1.353010000 | -2.236300000 | -0.174699000 |
| H | 1.860526000 | -1.406210000 | -0.097082000 |

**$(HF)_2(H_2O)_4$-A**
**MP2/aug-cc-pVTZ = -506.0816119 a.u.**

| | | | |
|---|---|---|---|
| O | 1.211657000 | -2.281979000 | -0.078809000 |
| H | 1.328763000 | -2.854378000 | -0.846599000 |
| H | 0.242545000 | -2.227703000 | 0.048921000 |
| O | 2.680037000 | -0.040764000 | 0.078992000 |
| H | 3.156447000 | -0.119156000 | 0.914845000 |
| H | 2.127752000 | -0.859920000 | 0.013667000 |
| O | -2.680053000 | 0.040746000 | -0.078878000 |
| H | -3.156414000 | 0.119276000 | -0.914749000 |
| H | -2.127740000 | 0.859881000 | -0.013458000 |
| O | -1.211685000 | 2.281961000 | 0.078760000 |
| H | -1.328803000 | 2.854540000 | 0.846414000 |
| H | -1.946623000 | -1.270373000 | 0.117120000 |
| F | -1.480291000 | -2.117681000 | 0.253170000 |
| H | -0.242574000 | 2.227679000 | -0.048965000 |
| F | 1.480267000 | 2.117595000 | -0.253303000 |
| H | 1.946629000 | 1.270320000 | -0.117123000 |

**$(HF)_3(H_2O)_3$-A**
**MP2/aug-cc-pVTZ = -530.0969724 a.u.**

| | | | |
|---|---|---|---|
| O | -2.029332000 | -1.623828000 | 0.156199000 |
| H | -2.279846000 | -2.059793000 | 0.980413000 |
| H | -1.109049000 | -1.915433000 | -0.019780000 |
| O | -0.332441000 | 2.419129000 | -0.523576000 |
| H | -1.104679000 | 1.855095000 | -0.300421000 |
| H | -0.603038000 | 3.320193000 | -0.306976000 |
| O | 2.449784000 | -0.915927000 | 0.039142000 |
| H | 2.233389000 | 0.026371000 | 0.208133000 |
| H | 3.079794000 | -0.904451000 | -0.692419000 |
| F | -2.405553000 | 0.837316000 | 0.114377000 |
| H | -2.257883000 | -0.128649000 | 0.135055000 |
| F | 1.811794000 | 1.655728000 | 0.490654000 |
| H | 0.969374000 | 1.970438000 | 0.109740000 |
| F | 0.494869000 | -2.423149000 | -0.306367000 |
| H | 1.257862000 | -1.827815000 | -0.175833000 |

**$(HF)_4(H_2O)_2$-A**
**MP2/aug-cc-pVTZ = -554.1075485 a.u.**

| | | | |
|---|---|---|---|
| O | 2.135840000 | 0.827425000 | 1.068880000 |
| H | 2.711065000 | 0.847001000 | 1.844336000 |
| H | 1.245436000 | 1.076806000 | 1.395133000 |
| O | -2.135840000 | -0.827425000 | -1.068880000 |
| H | -1.245436000 | -1.076806000 | -1.395133000 |
| H | -2.711065000 | -0.847001000 | -1.844336000 |
| F | 2.188656000 | -1.260687000 | -0.248938000 |
| H | 2.173994000 | -0.435759000 | 0.289648000 |
| F | 0.348324000 | -1.447326000 | -1.926995000 |
| H | 1.070102000 | -1.387797000 | -1.300514000 |
| F | -2.188656000 | 1.260687000 | 0.248938000 |
| H | -2.173994000 | 0.435759000 | -0.289648000 |
| F | -0.348324000 | 1.447326000 | 1.926995000 |
| H | -1.070102000 | 1.387797000 | 1.300514000 |

**$(HF)_5(H_2O)_1$-A**
**MP2/aug-cc-pVTZ = -578.1157831 a.u.**

| | | | |
|---|---|---|---|
| O | 2.180445000 | 1.321034000 | -0.045729000 |
| H | 1.302256000 | 1.752573000 | -0.090460000 |
| H | 2.593019000 | 1.648927000 | 0.763675000 |
| F | 2.187098000 | -1.116418000 | -0.349400000 |
| H | 2.186139000 | -0.134769000 | -0.218316000 |
| F | 0.189717000 | -2.289121000 | 0.479833000 |
| H | 0.984767000 | -1.847661000 | 0.152766000 |
| F | -1.958660000 | -1.379902000 | -0.388273000 |
| H | -1.139062000 | -1.760932000 | -0.065292000 |
| F | -2.302613000 | 1.012376000 | 0.277366000 |
| H | -2.202825000 | 0.094645000 | 0.026895000 |
| F | -0.273695000 | 2.462218000 | -0.163437000 |
| H | -1.053226000 | 1.939359000 | -0.006575000 |

**$(HF)_1(H_2O)_6$ -A**
**MP2/aug-cc-pVTZ = -558.4133976 a.u.**

| | | | |
|---|---|---|---|
| O | -1.225805000 | -0.291167000 | 1.740797000 |
| H | -1.430780000 | -0.523629000 | 2.654703000 |
| H | -2.091680000 | -0.242289000 | 1.271550000 |
| O | 0.209897000 | -1.763375000 | -0.227672000 |
| H | -0.199306000 | -1.227778000 | -0.935003000 |
| H | -0.216012000 | -1.414566000 | 0.580515000 |
| O | -3.268277000 | -0.108307000 | -0.052695000 |
| H | -2.660761000 | 0.068061000 | -0.802644000 |
| H | -3.908043000 | 0.614312000 | -0.074874000 |
| O | -1.085672000 | 0.282209000 | -1.722049000 |
| H | -0.611693000 | 0.942842000 | -1.140971000 |
| H | -0.981510000 | 0.591881000 | -2.630006000 |
| O | 0.033525000 | 1.785226000 | 0.150921000 |
| H | -0.284599000 | 1.283771000 | 0.922482000 |
| H | 1.011921000 | 1.717621000 | 0.207855000 |
| O | 2.750960000 | 1.307365000 | 0.350588000 |
| H | 2.860235000 | 0.359441000 | 0.133557000 |
| H | 3.486323000 | 1.755018000 | -0.083763000 |
| F | 2.669032000 | -1.368320000 | -0.205074000 |
| H | 1.706774000 | -1.553853000 | -0.212631000 |

**$(HF)_2(H_2O)_5$ -A**
**MP2/aug-cc-pVTZ = -582.427812 a.u.**

| | | | |
|---|---|---|---|
| O | -0.571357000 | 1.327873000 | 1.038619000 |
| H | -1.390668000 | 1.454826000 | 0.505248000 |
| H | -0.505035000 | 0.359276000 | 1.147767000 |
| O | -2.865643000 | 1.365008000 | -0.468455000 |
| H | -2.930687000 | 0.406257000 | -0.666064000 |
| H | -2.880296000 | 1.803401000 | -1.328157000 |
| O | -2.724603000 | -1.401433000 | -0.571313000 |
| H | -1.907156000 | -1.587799000 | -0.067808000 |
| H | -2.731694000 | -2.042987000 | -1.291766000 |
| O | -0.404264000 | -1.515499000 | 1.020419000 |
| H | -0.393326000 | -2.023574000 | 1.841562000 |
| H | 0.437718000 | -1.740423000 | 0.566024000 |
| O | 3.123800000 | 0.176106000 | -0.491035000 |
| H | 3.563756000 | 0.352695000 | -1.331876000 |
| H | 2.541178000 | 0.955726000 | -0.329759000 |
| F | 1.454720000 | 2.179102000 | -0.033143000 |
| H | 0.615800000 | 1.855294000 | 0.401968000 |
| F | 1.868647000 | -1.956871000 | -0.325253000 |
| H | 2.382299000 | -1.124802000 | -0.414181000 |

**$(HF)_3(H_2O)_4$ -A**
**MP2/aug-cc-pVTZ = -606.4425054 a.u.**

| | | | |
|---|---|---|---|
| O | -0.205592000 | 1.803058000 | -0.340024000 |
| H | 0.180400000 | 1.178612000 | -0.978147000 |
| H | 0.274523000 | 1.600784000 | 0.480199000 |
| O | -2.798142000 | 1.152272000 | 0.055037000 |
| H | -3.368277000 | 1.561844000 | -0.607337000 |
| H | -1.880525000 | 1.473933000 | -0.132530000 |
| O | -0.003325000 | -1.668355000 | 0.214999000 |
| H | -0.984840000 | -1.633572000 | 0.237135000 |
| H | 0.292503000 | -1.182934000 | 1.003438000 |
| O | 3.167874000 | -0.026885000 | -0.070992000 |
| H | 2.600532000 | -0.171735000 | -0.855179000 |
| H | 3.819708000 | 0.638038000 | -0.326461000 |
| F | -2.676915000 | -1.333934000 | 0.214066000 |
| H | -2.792184000 | -0.367629000 | 0.134494000 |
| F | 1.007045000 | -0.469139000 | -1.648282000 |
| H | 0.558768000 | -1.012015000 | -0.928960000 |
| F | 1.410689000 | 0.399627000 | 1.668671000 |
| H | 2.167550000 | 0.279643000 | 1.071398000 |

**$(HF)_4(H_2O)_3$-A**
**MP2/aug-cc-pVTZ = -630.4525265 a.u.**

| | | | |
|---|---|---|---|
| O | 0.208325000 | 2.553673000 | 0.655630000 |
| H | -0.601375000 | 2.287503000 | 0.168176000 |
| H | 0.160228000 | 3.515176000 | 0.727608000 |
| O | -3.012833000 | -0.392113000 | -0.016149000 |
| H | -2.367809000 | -1.064347000 | 0.286245000 |
| H | -3.533119000 | -0.828980000 | -0.702303000 |
| O | 2.760242000 | -0.986808000 | -0.028172000 |
| H | 2.607940000 | -0.018568000 | -0.102465000 |
| H | 3.142631000 | -1.121988000 | 0.848005000 |
| F | -1.989771000 | 1.785491000 | -0.675015000 |
| H | -2.392771000 | 0.931882000 | -0.427212000 |
| F | -1.180145000 | -2.202665000 | 0.826875000 |
| H | -0.392691000 | -2.307419000 | 0.291183000 |
| F | 0.856502000 | -2.438415000 | -0.586597000 |
| H | 1.617088000 | -1.849525000 | -0.355688000 |
| F | 2.354151000 | 1.644675000 | -0.213235000 |
| H | 1.507737000 | 2.015311000 | 0.106095000 |

**$(HF)_5(H_2O)_2$-A**
**MP2/aug-cc-pVTZ = -654.4624961 a.u.**

| | | | |
|---|---|---|---|
| O | -2.161859000 | -1.792392000 | -0.540497000 |
| H | -2.799007000 | -2.450084000 | -0.233621000 |
| H | -1.322222000 | -1.999085000 | -0.077491000 |
| O | 2.943917000 | 0.707740000 | -0.176062000 |
| H | 3.433603000 | 0.974492000 | 0.612332000 |
| H | 2.213110000 | 1.354223000 | -0.263103000 |
| F | 0.137818000 | -2.245137000 | 0.778340000 |
| H | 0.981025000 | -2.042235000 | 0.368802000 |
| F | 2.311189000 | -1.673217000 | -0.287865000 |
| H | 2.560315000 | -0.720553000 | -0.236592000 |
| F | 0.918833000 | 2.486817000 | -0.422944000 |
| H | 0.089373000 | 2.332385000 | 0.020855000 |
| F | -1.236386000 | 2.030772000 | 0.795558000 |
| H | -1.880693000 | 1.463783000 | 0.356840000 |
| F | -2.861923000 | 0.554573000 | -0.334496000 |
| H | -2.589893000 | -0.394804000 | -0.405565000 |

**$(HF)_6(H_2O)_1$-A**
**MP2/aug-cc-pVTZ = -678.4703356 a.u.**

| | | | |
|---|---|---|---|
| O | 2.955779000 | 0.431700000 | -0.176663000 |
| H | 2.312993000 | 1.168365000 | -0.238233000 |
| H | 3.492716000 | 0.615380000 | 0.604845000 |
| F | 2.021329000 | -1.829391000 | -0.336905000 |
| H | 2.396825000 | -0.914083000 | -0.262643000 |
| F | -0.104288000 | -2.198530000 | 0.830341000 |
| H | 0.737611000 | -2.068997000 | 0.370855000 |
| F | -2.184295000 | -1.723109000 | -0.442404000 |
| H | -1.379939000 | -1.940864000 | 0.034913000 |
| F | -2.766646000 | 0.705631000 | -0.415225000 |
| H | -2.564058000 | -0.231248000 | -0.426180000 |
| F | -1.091596000 | 2.143927000 | 0.768841000 |
| H | -1.745686000 | 1.608724000 | 0.320688000 |
| F | 1.152465000 | 2.439973000 | -0.362875000 |
| H | 0.298083000 | 2.353646000 | 0.046405000 |

**$(HF)_1(H_2O)_7$-A**
**MP2/aug-cc-pVTZ = -634.7689147 a.u.**

| | | | |
|---|---|---|---|
| O | -2.049908000 | -0.071736000 | -1.395971000 |
| H | -2.913932000 | 0.023262000 | -1.815269000 |
| H | -2.005664000 | 0.626510000 | -0.686843000 |
| O | -0.958241000 | -1.997972000 | 0.311888000 |
| H | -1.455964000 | -1.483751000 | -0.358405000 |
| H | -0.064375000 | -2.099444000 | -0.078907000 |
| O | -1.577909000 | 1.633483000 | 0.599741000 |
| H | -1.404103000 | 1.053023000 | 1.361474000 |
| H | -0.700435000 | 2.014032000 | 0.395679000 |
| O | 1.100601000 | 2.200054000 | -0.131340000 |
| H | 1.637379000 | 2.996634000 | -0.038099000 |
| H | 1.503789000 | 1.523539000 | 0.476165000 |
| O | 1.909971000 | 0.150233000 | 1.392862000 |
| H | 1.130308000 | -0.090917000 | 1.923629000 |
| H | 1.992578000 | -0.587437000 | 0.758555000 |
| O | 1.604832000 | -1.715813000 | -0.746367000 |
| H | 2.190974000 | -2.317660000 | -1.221174000 |
| H | 1.341272000 | -1.008603000 | -1.397300000 |
| O | 0.663959000 | 0.304795000 | -2.209763000 |
| H | 0.856663000 | 1.094937000 | -1.668076000 |
| H | -0.306621000 | 0.215483000 | -2.152781000 |
| F | -0.724436000 | -0.538514000 | 2.279206000 |
| H | -0.845766000 | -1.168328000 | 1.517554000 |

**$(HF)_2(H_2O)_6$-A**
**MP2/aug-cc-pVTZ = -658.7838148 a.u.**

| | | | |
|---|---|---|---|
| O | 1.797931000 | 1.633215000 | -0.351116000 |
| H | 2.597880000 | 2.143185000 | -0.529328000 |
| H | 2.005265000 | 0.692972000 | -0.601881000 |
| O | 0.505453000 | 0.853617000 | 1.995045000 |
| H | 1.029173000 | 1.291364000 | 1.290507000 |
| H | -0.425135000 | 1.060694000 | 1.768213000 |
| O | -2.037007000 | 1.081813000 | 0.848888000 |
| H | -2.824559000 | 1.605462000 | 1.041749000 |
| H | -1.696980000 | 1.395135000 | -0.034192000 |
| O | -0.826123000 | 1.632251000 | -1.455828000 |
| H | -0.791966000 | 0.774406000 | -1.914442000 |
| H | 0.104761000 | 1.800245000 | -1.211277000 |
| O | -1.590671000 | -1.607062000 | 0.195284000 |
| H | -0.849341000 | -1.801827000 | 0.799825000 |
| H | -1.937643000 | -0.748792000 | 0.515962000 |
| O | 1.985758000 | -0.981007000 | -0.876245000 |
| H | 1.766972000 | -1.405234000 | -0.028529000 |
| H | 1.217238000 | -1.184505000 | -1.438649000 |
| F | 0.782977000 | -1.564656000 | 1.677721000 |
| H | 0.696229000 | -0.586941000 | 1.862447000 |
| F | -0.617734000 | -1.174210000 | -2.030596000 |
| H | -1.043732000 | -1.391609000 | -1.160937000 |

**$(HF)_3(H_2O)_5$-A**
**MP2/aug-cc-pVTZ = -682.7973725 a.u.**

| | | | |
|---|---|---|---|
| O | 1.841245000 | -0.002124000 | 1.510673000 |
| H | 1.267501000 | 0.763727000 | 1.686548000 |
| H | 1.266548000 | -0.767562000 | 1.685252000 |
| O | 2.147804000 | -0.000242000 | -1.140203000 |
| H | 2.196807000 | -0.001008000 | -0.145793000 |
| H | 3.058590000 | -0.000494000 | -1.460611000 |
| O | 0.122117000 | -1.919951000 | -1.185095000 |
| H | 0.905412000 | -1.352310000 | -1.344874000 |
| H | -0.628813000 | -1.398292000 | -1.523877000 |
| O | -2.074656000 | 0.000366000 | 0.985786000 |
| H | -1.557520000 | -0.770521000 | 1.288251000 |
| H | -1.556688000 | 0.770241000 | 1.289410000 |
| O | 0.124146000 | 1.921672000 | -1.182168000 |
| H | 0.906823000 | 1.353430000 | -1.342830000 |
| H | -0.627349000 | 1.401362000 | -1.521766000 |
| F | -0.175475000 | -2.032110000 | 1.258180000 |
| H | -0.048615000 | -2.053194000 | 0.271601000 |
| F | -1.919318000 | 0.002124000 | -1.468891000 |
| H | -2.052359000 | 0.001464000 | -0.480562000 |
| F | -0.173399000 | 2.030432000 | 1.261281000 |
| H | -0.046458000 | 2.052874000 | 0.274749000 |

**$(HF)_4(H_2O)_4$-A**
**MP2/aug-cc-pVTZ = -706.8099142 a.u.**

| | | | |
|---|---|---|---|
| O | -0.218971000 | -1.948088000 | 1.195587000 |
| H | 0.606289000 | -1.497623000 | 1.455741000 |
| H | -0.923668000 | -1.325873000 | 1.456155000 |
| O | 1.948088000 | -0.218972000 | -1.195591000 |
| H | 1.325874000 | -0.923670000 | -1.456158000 |
| H | 1.497623000 | 0.606287000 | -1.455744000 |
| O | -1.948091000 | 0.218973000 | -1.195584000 |
| H | -1.497622000 | -0.606286000 | -1.455736000 |
| H | -1.325879000 | 0.923673000 | -1.456154000 |
| O | 0.218975000 | 1.948090000 | 1.195587000 |
| H | -0.606283000 | 1.497622000 | 1.455740000 |
| H | 0.923675000 | 1.325878000 | 1.456156000 |
| F | -0.224940000 | -2.001337000 | -1.265766000 |
| H | -0.230871000 | -2.050738000 | -0.271184000 |
| F | 2.001342000 | -0.224937000 | 1.265763000 |
| H | 2.050740000 | -0.230872000 | 0.271182000 |
| F | -2.001335000 | 0.224938000 | 1.265769000 |
| H | -2.050738000 | 0.230875000 | 0.271187000 |
| F | 0.224936000 | 2.001339000 | -1.265767000 |
| H | 0.230875000 | 2.050739000 | -0.271186000 |

**$(HF)_5(H_2O)_3$-A**
**MP2/aug-cc-pVTZ = -730.8123317 a.u.**

| | | | |
|---|---|---|---|
| O | -0.485414000 | -0.013182000 | 0.079307000 |
| H | 0.082938000 | 0.789190000 | 0.083664000 |
| H | -1.052865000 | 0.049042000 | -0.723066000 |
| O | -4.202823000 | -0.075340000 | -0.100254000 |
| H | -4.838678000 | 0.649342000 | -0.041823000 |
| H | -3.714839000 | -0.068811000 | 0.747985000 |
| O | 3.605510000 | -1.220163000 | -0.058996000 |
| H | 4.017974000 | -1.642082000 | -0.823688000 |
| H | 2.701177000 | -1.596447000 | -0.004798000 |
| F | 1.038864000 | -2.043494000 | 0.088796000 |
| H | 0.427846000 | -1.295468000 | 0.073400000 |
| F | -2.317267000 | -0.084382000 | 1.882264000 |
| H | -1.563036000 | -0.044629000 | 1.290240000 |
| F | -2.367800000 | 0.051135000 | -1.807623000 |
| H | -3.139886000 | 0.017726000 | -1.216669000 |
| F | 1.208492000 | 2.055012000 | 0.160941000 |
| H | 2.125945000 | 1.791006000 | 0.075034000 |
| F | 3.559853000 | 1.251109000 | -0.073215000 |
| H | 3.603546000 | 0.266703000 | -0.078175000 |

**$(HF)_6(H_2O)_2$-A**
**MP2/aug-cc-pVTZ = -754.8209233 a.u.**

| | | | |
|---|---|---|---|
| O | 0.148042000 | 1.414997000 | 1.125051000 |
| H | -0.680697000 | 1.741250000 | 0.722068000 |
| H | 0.032287000 | 0.451813000 | 1.212329000 |
| O | -0.047370000 | -1.472403000 | 1.139533000 |
| H | 0.055303000 | -1.918078000 | 1.992144000 |
| H | 0.746092000 | -1.728779000 | 0.611751000 |
| F | 2.216255000 | 2.006397000 | -0.022075000 |
| H | 1.355616000 | 1.784714000 | 0.437969000 |
| F | 3.328725000 | 0.040430000 | -0.968890000 |
| H | 2.914649000 | 0.841881000 | -0.612730000 |
| F | 2.092093000 | -2.016282000 | -0.313816000 |
| H | 2.596562000 | -1.246531000 | -0.588104000 |
| F | -2.236192000 | -1.978068000 | -0.008823000 |
| H | -1.385692000 | -1.818718000 | 0.428016000 |
| F | -3.274338000 | 0.047544000 | -1.095253000 |
| H | -2.909307000 | -0.743797000 | -0.707249000 |
| F | -2.241197000 | 2.123584000 | -0.028466000 |
| H | -2.672567000 | 1.395974000 | -0.458105000 |

**$(HF)_7(H_2O)_1$-A**
**MP2/aug-cc-pVTZ = -778.827959 a.u.**

| | | | |
|---|---|---|---|
| O | 0.465253000 | 0.036458000 | -0.014263000 |
| H | -0.107833000 | 0.837371000 | -0.020105000 |
| H | 1.033677000 | 0.099686000 | 0.785736000 |
| F | -1.033017000 | -1.993671000 | -0.023779000 |
| H | -0.431183000 | -1.231868000 | -0.005864000 |
| F | -3.446031000 | -1.341125000 | 0.084182000 |
| H | -2.536151000 | -1.638836000 | 0.043423000 |
| F | -3.607595000 | 1.165352000 | 0.067132000 |
| H | -3.605231000 | 0.209062000 | 0.075082000 |
| F | -1.255697000 | 2.062777000 | -0.114765000 |
| H | -2.165125000 | 1.783298000 | -0.047365000 |
| F | 2.417726000 | 0.077964000 | 1.823491000 |
| H | 3.168999000 | 0.052730000 | 1.241355000 |
| F | 4.152447000 | 0.003667000 | -0.042158000 |
| H | 3.571402000 | -0.015127000 | -0.798234000 |
| F | 2.311434000 | -0.031807000 | -1.778997000 |
| H | 1.540041000 | 0.009414000 | -1.202393000 |

**Table S14:** Cartesian coordinates of cyclic $(HF)_m(H_2O)_n$ -B clusters optimized at MP2/aug-cc-pVDZ level of theory along with single point energy at MP2/aug-cc-pVTZ level

**$(HF)_1(H_2O)_3$ -B**
**MP2/aug-cc-pVTZ = -329.368492 a.u.**

| | | | |
|---|---|---|---|
| O | -1.931445000 | -1.216400000 | -0.330703000 |
| H | -2.787544000 | -1.564646000 | -0.053320000 |
| H | -2.079156000 | -0.263365000 | -0.461245000 |
| O | 0.312378000 | -0.068266000 | 0.935161000 |
| H | -0.243302000 | -0.826312000 | 0.676294000 |
| H | 1.173381000 | -0.205874000 | 0.495732000 |
| O | 2.829732000 | -0.291385000 | -0.348260000 |
| H | 2.885162000 | 0.211014000 | -1.172267000 |
| H | 3.595872000 | -0.001087000 | 0.164290000 |
| F | -1.247663000 | 1.553341000 | -0.209371000 |
| H | -0.573914000 | 1.043539000 | 0.263902000 |

**$(HF)_2(H_2O)_2$-B**
**MP2/aug-cc-pVTZ = -353.3912671 a.u.**

| | | | |
|---|---|---|---|
| O | -0.041054000 | 1.816402000 | -0.050786000 |
| H | -0.099079000 | 2.380413000 | 0.731344000 |
| H | -0.837067000 | 1.230515000 | -0.019593000 |
| O | -1.919944000 | -0.124914000 | 0.049241000 |
| H | -1.321687000 | -0.896597000 | 0.055212000 |
| H | -2.555910000 | -0.304263000 | -0.654427000 |
| F | 0.251560000 | -1.859413000 | 0.089149000 |
| H | 0.921329000 | -1.185627000 | 0.016653000 |
| F | 1.794840000 | 0.141374000 | -0.094042000 |
| H | 1.131681000 | 0.865206000 | -0.069433000 |

**$(HF)_3(H_2O)_1$-B**
**MP2/aug-cc-pVTZ = -377.39053 a.u.**

| | | | |
|---|---|---|---|
| O | 0.469951000 | -0.105834000 | 0.786260000 |
| H | 0.622919000 | -0.187970000 | 1.738354000 |
| H | -0.100991000 | -0.860881000 | 0.546679000 |
| F | -1.827343000 | -1.199986000 | -0.322941000 |
| H | -1.984831000 | -0.278387000 | -0.428523000 |
| F | -1.454526000 | 1.390336000 | -0.169048000 |
| H | -0.652972000 | 1.085240000 | 0.237842000 |
| F | 2.868135000 | -0.061929000 | -0.478172000 |
| H | 2.021336000 | -0.081819000 | -0.076847000 |

**$(HF)_1(H_2O)_4$-B**
**MP2/aug-cc-pVTZ = -405.719471 a.u.**

| | | | |
|---|---|---|---|
| O | -0.322655000 | -1.729056000 | 0.622854000 |
| H | -0.981092000 | -1.777524000 | -0.088322000 |
| H | -0.573560000 | -0.905260000 | 1.073095000 |
| O | 2.147325000 | -0.954336000 | -0.301967000 |
| H | 2.854633000 | -1.394451000 | 0.184541000 |
| H | 1.311406000 | -1.364250000 | 0.020515000 |
| O | 1.449338000 | 1.669168000 | -0.210714000 |
| H | 1.513276000 | 2.011039000 | -1.111521000 |
| H | 1.831016000 | 0.759482000 | -0.259087000 |
| O | -0.968769000 | 1.131630000 | 0.788883000 |
| H | -0.097771000 | 1.443623000 | 0.424280000 |
| H | -1.326464000 | 1.862712000 | 1.307020000 |
| F | -2.316689000 | -0.189385000 | -0.955941000 |
| H | -1.884397000 | 0.401939000 | -0.344332000 |

**$(HF)_2(H_2O)_3$-B**
**MP2/aug-cc-pVTZ = -429.7330597 a.u.**

| | | | |
|---|---|---|---|
| O | -2.451832000 | -0.001437000 | -0.892883000 |
| H | -2.178156000 | -0.816335000 | -0.443422000 |
| H | -3.394932000 | -0.113379000 | -1.064793000 |
| O | -0.621707000 | 1.162781000 | 0.878675000 |
| H | 0.204082000 | 1.476231000 | 0.458340000 |
| H | -1.311331000 | 1.235522000 | 0.193289000 |
| O | 1.929305000 | -1.134753000 | -0.335390000 |
| H | 1.947313000 | -1.578575000 | -1.192881000 |
| H | 1.083577000 | -1.401335000 | 0.079053000 |
| F | 1.838902000 | 1.402257000 | -0.332957000 |
| H | 1.947872000 | 0.443939000 | -0.379674000 |
| F | -0.517280000 | -1.293279000 | 0.891183000 |
| H | -0.540007000 | -0.300657000 | 0.979095000 |

**$(HF)_3(H_2O)_2$-B**
**MP2/aug-cc-pVTZ = -453.7494861 a.u.**

| | | | |
|---|---|---|---|
| O | 1.995099000 | -0.870573000 | 0.070307000 |
| H | 2.477477000 | -1.006845000 | 0.896009000 |
| H | 1.841217000 | 0.107376000 | 0.004565000 |
| O | 1.433482000 | 1.741647000 | -0.084106000 |
| H | 0.470699000 | 1.876515000 | 0.012898000 |
| H | 1.682938000 | 2.255198000 | -0.862393000 |
| F | -0.108285000 | -2.116644000 | -0.124140000 |
| H | 0.753780000 | -1.629376000 | -0.035903000 |
| F | -2.068647000 | -0.603940000 | -0.074016000 |
| H | -1.327422000 | -1.218502000 | -0.097392000 |
| F | -1.302440000 | 1.794319000 | 0.214617000 |
| H | -1.639299000 | 0.910426000 | 0.109838000 |

**$(HF)_4(H_2O)_1$-B**
**MP2/aug-cc-pVTZ = -477.7528015 a.u.**

| | | | |
|---|---|---|---|
| O | -0.466238000 | 1.385051000 | 0.704016000 |
| H | 0.389098000 | 1.565638000 | 0.262626000 |
| H | -1.155076000 | 1.627256000 | 0.063978000 |
| F | -2.539161000 | -0.053962000 | -0.816737000 |
| H | -2.058372000 | -0.701921000 | -0.344939000 |
| F | -0.627497000 | -1.022001000 | 0.798983000 |
| H | -0.557916000 | -0.001561000 | 0.837488000 |
| F | 1.653940000 | -1.404662000 | -0.229466000 |
| H | 0.791561000 | -1.415267000 | 0.176714000 |
| F | 1.993331000 | 1.135677000 | -0.466959000 |
| H | 2.009577000 | 0.188372000 | -0.444811000 |

**$(HF)_1(H_2O)_5$-B**
**MP2/aug-cc-pVTZ = -482.0662984 a.u.**

| | | | |
|---|---|---|---|
| O | 2.034510000 | -1.364542000 | -0.630414000 |
| H | 2.730848000 | -1.938054000 | -0.286603000 |
| H | 1.248399000 | -1.496862000 | -0.028444000 |
| O | -0.048376000 | -1.392764000 | 1.009445000 |
| H | -0.921819000 | -1.518433000 | 0.577294000 |
| H | -0.060330000 | -0.457158000 | 1.276413000 |
| O | 0.191029000 | 1.524221000 | 0.992390000 |
| H | -3.324719000 | -1.553009000 | 0.060951000 |
| H | -2.474471000 | -0.389895000 | -0.499838000 |
| O | -2.469627000 | -1.359350000 | -0.342132000 |
| H | -1.949506000 | 1.758252000 | -1.474795000 |
| H | -1.301155000 | 1.545877000 | -0.092955000 |
| O | -2.120068000 | 1.379641000 | -0.603222000 |
| H | 1.027943000 | 1.495491000 | 0.478870000 |
| H | 0.323726000 | 2.207007000 | 1.661492000 |
| F | 2.377072000 | 1.086392000 | -0.519965000 |
| H | 2.315986000 | 0.106695000 | -0.595359000 |

**$(HF)_2(H_2O)_4$-B**
**MP2/aug-cc-pVTZ = -506.0826946 a.u.**

| | | | |
|---|---|---|---|
| O | 2.093722000 | 1.232126000 | -0.628203000 |
| H | 1.289576000 | 1.451636000 | -0.108407000 |
| H | 1.903927000 | 1.518277000 | -1.530986000 |
| O | -0.131819000 | 1.506714000 | 0.987515000 |
| H | -0.982944000 | 1.502536000 | 0.495963000 |
| H | -0.216918000 | 2.203689000 | 1.649936000 |
| O | -2.042014000 | -1.329255000 | -0.641509000 |
| H | -2.750244000 | -1.904356000 | -0.325567000 |
| H | -1.266080000 | -1.491843000 | -0.038695000 |
| O | 0.042503000 | -1.417420000 | 1.014184000 |
| H | 0.079791000 | -0.486484000 | 1.293942000 |
| H | 0.914208000 | -1.567186000 | 0.603117000 |
| F | 2.521039000 | -1.250561000 | -0.290036000 |
| H | 2.414747000 | -0.308688000 | -0.465687000 |
| F | -2.338625000 | 1.126315000 | -0.490807000 |
| H | -2.300407000 | 0.147461000 | -0.580481000 |

**$(HF)_3(H_2O)_3$-B**
**MP2/aug-cc-pVTZ = -530.0951202 a.u.**

| | | | |
|---|---|---|---|
| O | -2.575241000 | -0.621489000 | -0.182561000 |
| H | -3.133918000 | -0.492689000 | -0.959428000 |
| H | -2.232662000 | 0.277970000 | 0.050309000 |
| O | -1.635045000 | 1.811745000 | 0.448871000 |
| H | -0.728426000 | 2.041076000 | 0.166023000 |
| H | -1.696151000 | 2.117322000 | 1.362152000 |
| O | 1.545274000 | -1.604863000 | 0.622369000 |
| H | 0.688631000 | -1.900930000 | 0.239629000 |
| H | 2.114318000 | -2.384775000 | 0.620548000 |
| F | -0.798107000 | -2.330809000 | -0.416279000 |
| H | -1.511284000 | -1.659635000 | -0.337196000 |
| F | 2.499079000 | 0.422116000 | -0.414464000 |
| H | 2.128779000 | -0.400146000 | -0.017449000 |
| F | 0.927182000 | 2.377902000 | -0.359645000 |
| H | 1.544524000 | 1.649516000 | -0.384674000 |

**$(HF)_4(H_2O)_2$-B**
**MP2/aug-cc-pVTZ = -554.105141 a.u.**

| | | | |
|---|---|---|---|
| O | 0.846384000 | -1.640672000 | -0.664798000 |
| H | 1.445345000 | -1.633437000 | 0.102484000 |
| H | 1.002826000 | -0.763272000 | -1.057939000 |
| O | 1.460991000 | 1.177980000 | -0.738747000 |
| H | 0.637408000 | 1.637121000 | -0.466461000 |
| H | 1.942056000 | 1.805233000 | -1.293339000 |
| F | -1.526030000 | -1.887697000 | -0.067863000 |
| H | -0.564628000 | -1.812893000 | -0.300379000 |
| F | -2.548095000 | 0.309760000 | 0.412699000 |
| H | -2.179977000 | -0.564387000 | 0.236791000 |
| F | -0.902660000 | 2.178087000 | 0.063206000 |
| H | -1.555024000 | 1.495783000 | 0.210016000 |
| F | 2.593771000 | -0.251710000 | 1.099976000 |
| H | 2.262479000 | 0.411497000 | 0.504935000 |

**$(HF)_5(H_2O)_1$-B**
**MP2/aug-cc-pVTZ = -578.1085853 a.u.**

| | | | |
|---|---|---|---|
| O | 1.319012000 | 0.045921000 | 0.772524000 |
| H | 2.088598000 | 0.124905000 | 0.187253000 |
| H | 0.788379000 | 0.856858000 | 0.640459000 |
| F | -0.026697000 | -1.965859000 | 0.452236000 |
| H | 0.540979000 | -1.153225000 | 0.578263000 |
| F | -2.274627000 | -1.406240000 | -0.374704000 |
| H | -1.400039000 | -1.662458000 | -0.050150000 |
| F | -2.541515000 | 1.076724000 | -0.481379000 |
| H | -2.481497000 | 0.120528000 | -0.453678000 |
| F | -0.394447000 | 2.130635000 | 0.367529000 |
| H | -1.223368000 | 1.793995000 | 0.044320000 |
| F | 3.763761000 | 0.059760000 | -0.752838000 |
| H | 4.555697000 | -0.114222000 | -0.303004000 |

**$(HF)_1(H_2O)_6$-B**
**MP2/aug-cc-pVTZ = -558.4083929 a.u.**

| | | | |
|---|---|---|---|
| O | -1.933340000 | 1.630186000 | -0.995179000 |
| H | -1.522648000 | 1.806822000 | -1.851119000 |
| H | -2.145048000 | 0.675619000 | -1.008782000 |
| O | -0.127786000 | 1.679318000 | 1.177015000 |
| H | -0.781014000 | 1.770247000 | 0.452528000 |
| H | -0.333234000 | 0.811999000 | 1.562612000 |
| O | 2.306890000 | 1.767278000 | 0.031258000 |
| H | 1.435105000 | 1.771164000 | 0.503588000 |
| H | 2.880309000 | 2.345308000 | 0.547955000 |
| O | 2.705194000 | -0.757257000 | -0.832800000 |
| H | 2.677191000 | 0.174779000 | -0.503162000 |
| H | 3.571498000 | -1.096674000 | -0.577838000 |
| O | 0.531868000 | -2.105077000 | -0.070897000 |
| H | -0.074323000 | -2.068033000 | -0.825523000 |
| H | 1.353069000 | -1.622500000 | -0.356033000 |
| O | -2.344861000 | -1.133293000 | -0.558907000 |
| H | -3.228236000 | -1.523097000 | -0.570373000 |
| H | -2.075535000 | -1.140063000 | 0.379522000 |
| F | -0.789385000 | -1.093350000 | 1.721219000 |
| H | -0.182392000 | -1.512203000 | 1.049762000 |

**$(HF)_2(H_2O)_5$-B**
**MP2/aug-cc-pVTZ = -582.4232679 a.u.**

| | | | |
|---|---|---|---|
| O | -2.863114000 | -0.886825000 | 0.197856000 |
| H | -2.679254000 | 0.073194000 | 0.371512000 |
| H | -3.724983000 | -0.903866000 | -0.237106000 |
| O | -2.397074000 | 1.707414000 | 0.616580000 |
| H | -1.578810000 | 2.094628000 | 0.224488000 |
| H | -2.447890000 | 2.079305000 | 1.505288000 |
| O | -0.161023000 | 2.807838000 | -0.452790000 |
| H | 0.719646000 | 2.427692000 | -0.264183000 |
| H | -0.135837000 | 3.037756000 | -1.389168000 |
| O | 3.056039000 | -0.547897000 | 0.411570000 |
| H | 2.369478000 | -1.257588000 | 0.347853000 |
| H | 3.758087000 | -0.820881000 | -0.192164000 |
| O | 1.254811000 | -2.532149000 | 0.225737000 |
| H | 0.404970000 | -2.382603000 | -0.236604000 |
| H | 1.024203000 | -3.036767000 | 1.014840000 |
| F | 2.324900000 | 1.814805000 | 0.087299000 |
| H | 2.591282000 | 0.884004000 | 0.206531000 |
| F | -1.085814000 | -2.077398000 | -1.075699000 |
| H | -1.786197000 | -1.597999000 | -0.590154000 |

**$(HF)_3(H_2O)_4$-B**
**MP2/aug-cc-pVTZ = -606.4417651 a.u.**

| | | | |
|---|---|---|---|
| O | 1.081173000 | 1.348708000 | -0.579191000 |
| H | 0.736704000 | 0.538220000 | -0.988175000 |
| H | 1.774401000 | 1.026204000 | 0.025784000 |
| O | -0.888130000 | 2.796158000 | 0.469918000 |
| H | -0.116439000 | 2.295481000 | 0.089789000 |
| H | -0.933090000 | 3.624462000 | -0.024053000 |
| O | -2.187314000 | -1.135173000 | -0.067496000 |
| H | -2.216669000 | -1.582371000 | 0.788219000 |
| H | -2.485397000 | -0.211827000 | 0.109929000 |
| O | 1.920078000 | -2.279795000 | 0.367245000 |
| H | 1.234718000 | -2.059467000 | -0.294436000 |
| H | 2.508176000 | -2.910954000 | -0.066602000 |
| F | -2.897895000 | 1.369323000 | 0.412082000 |
| H | -2.116819000 | 1.973547000 | 0.433886000 |
| F | 2.889570000 | -0.030993000 | 1.074723000 |
| H | 2.584128000 | -0.914663000 | 0.849289000 |
| F | -0.034527000 | -1.253357000 | -1.234633000 |
| H | -0.909672000 | -1.219027000 | -0.762209000 |

**$(HF)_4(H_2O)_3$-B**
**MP2/aug-cc-pVTZ = -630.450837 a.u.**

| | | | |
|---|---|---|---|
| O | 1.808436000 | 1.797334000 | -0.541791000 |
| H | 1.920249000 | 2.686004000 | -0.182894000 |
| H | 2.647588000 | 1.329518000 | -0.357399000 |
| O | 2.059474000 | -1.749017000 | 0.544282000 |
| H | 2.036687000 | -2.551261000 | 0.006812000 |
| H | 1.203552000 | -1.297636000 | 0.387030000 |
| O | -0.066207000 | 0.000494000 | 0.037071000 |
| H | -0.628640000 | 0.253137000 | 0.796287000 |
| H | 0.540190000 | 0.767971000 | -0.141990000 |
| F | 3.800772000 | 0.012478000 | 0.024451000 |
| H | 3.201164000 | -0.718233000 | 0.227284000 |
| F | -2.136318000 | 0.501975000 | 1.766591000 |
| H | -2.825740000 | 0.325777000 | 1.137341000 |
| F | -1.767554000 | -0.518018000 | -1.687287000 |
| H | -1.032421000 | -0.302852000 | -1.066898000 |
| F | -3.701552000 | -0.046940000 | -0.175147000 |
| H | -3.049665000 | -0.253539000 | -0.847715000 |

**$(HF)_5(H_2O)_2$-B**
**MP2/aug-cc-pVTZ = -654.4551504 a.u.**

| | | | |
|---|---|---|---|
| O | -1.776034000 | -0.071985000 | -0.823413000 |
| H | -1.192423000 | -0.857287000 | -0.823474000 |
| H | -2.406763000 | -0.201893000 | -0.098745000 |
| O | 3.130474000 | 0.163342000 | 0.196953000 |
| H | 3.889781000 | 0.327367000 | 0.770452000 |
| H | 2.537242000 | 0.935724000 | 0.316657000 |
| F | -0.652659000 | 2.099948000 | -0.823855000 |
| H | -1.104466000 | 1.213071000 | -0.816871000 |
| F | 1.420477000 | 2.214475000 | 0.532928000 |
| H | 0.615220000 | 2.192712000 | 0.008804000 |
| F | 1.996957000 | -2.010888000 | 0.496742000 |
| H | 2.458677000 | -1.146925000 | 0.393795000 |
| F | -0.115692000 | -2.220299000 | -0.833211000 |
| H | 0.697591000 | -2.164635000 | -0.333956000 |
| F | -3.928041000 | -0.180972000 | 1.099547000 |
| H | -4.761288000 | -0.013364000 | 0.729035000 |

**$(HF)_6(H_2O)_1$-B**
**MP2/aug-cc-pVTZ = -678.4703452 a.u.**

| | | | |
|---|---|---|---|
| O | 0.000005000 | 0.043198000 | 0.000035000 |
| H | -0.585164000 | 0.627791000 | -0.531007000 |
| H | 0.585246000 | 0.628036000 | 0.530729000 |
| F | -2.004484000 | 1.296623000 | -1.271786000 |
| H | -2.736326000 | 0.862160000 | -0.848261000 |
| H | -1.033337000 | -0.811947000 | 0.863485000 |
| H | -3.073283000 | -0.596313000 | 0.598291000 |
| F | -3.678211000 | -0.076072000 | 0.075252000 |
| F | -1.786948000 | -1.255447000 | 1.271573000 |
| F | 1.786796000 | -1.256466000 | -1.270686000 |
| H | 1.033242000 | -0.812599000 | -0.862891000 |
| F | 3.678207000 | -0.076597000 | -0.075087000 |
| H | 3.073214000 | -0.597083000 | -0.597808000 |
| F | 2.004651000 | 1.297140000 | 1.271101000 |
| H | 2.736439000 | 0.862321000 | 0.847845000 |

**$(HF)_1(H_2O)_7$-B**
**MP2/aug-cc-pVTZ = -634.7567758 a.u.**

| | | | |
|---|---|---|---|
| O | 0.979095000 | -1.246737000 | -0.922659000 |
| H | 0.918586000 | -0.281775000 | -1.050072000 |
| H | 0.221241000 | -1.463636000 | -0.343064000 |
| O | 3.376939000 | -1.350775000 | 0.231821000 |
| H | 2.485728000 | -1.433760000 | -0.206353000 |
| H | 3.990389000 | -1.848176000 | -0.323582000 |
| O | 1.232155000 | 1.611270000 | -0.733271000 |
| H | 2.134974000 | 1.594969000 | -0.350427000 |
| H | 1.249282000 | 2.309011000 | -1.399827000 |
| O | -1.198241000 | -1.574609000 | 0.831277000 |
| H | -2.089143000 | -1.582378000 | 0.397575000 |
| H | -1.243050000 | -2.232018000 | 1.536280000 |
| O | -3.595383000 | -1.273795000 | -0.365693000 |
| H | -3.659789000 | -0.287835000 | -0.377084000 |
| H | -3.707625000 | -1.542409000 | -1.286022000 |
| O | -3.429222000 | 1.440062000 | -0.269843000 |
| H | -2.559652000 | 1.508357000 | 0.197391000 |
| H | -4.036366000 | 1.983847000 | 0.246757000 |
| O | -1.035980000 | 1.290918000 | 0.996912000 |
| H | -0.980099000 | 0.326257000 | 1.128050000 |
| H | -0.239983000 | 1.511233000 | 0.478688000 |
| F | 3.678111000 | 1.124238000 | 0.336810000 |
| H | 3.637801000 | 0.146880000 | 0.316826000 |

**$(HF)_2(H_2O)_6$-B**
**MP2/aug-cc-pVTZ = -658.7729858 a.u.**

| | | | |
|---|---|---|---|
| O | -1.009331000 | 1.236292000 | -0.988859000 |
| H | -0.936942000 | 0.271332000 | -1.106725000 |
| H | -0.222083000 | 1.478732000 | -0.464252000 |
| O | -3.360483000 | 1.343043000 | 0.260121000 |
| H | -2.489397000 | 1.427372000 | -0.215106000 |
| H | -3.999661000 | 1.833465000 | -0.272102000 |
| O | -1.224957000 | -1.623040000 | -0.726245000 |
| H | -2.120799000 | -1.602967000 | -0.326233000 |
| H | -1.250904000 | -2.332709000 | -1.379915000 |
| O | 1.009331000 | -1.236292000 | 0.988860000 |
| H | 0.936942000 | -0.271332000 | 1.106726000 |
| H | 0.222083000 | -1.478732000 | 0.464253000 |
| O | 3.360483000 | -1.343043000 | -0.260122000 |
| H | 2.489396000 | -1.427372000 | 0.215106000 |
| H | 3.999661000 | -1.833465000 | 0.272101000 |
| O | 1.224957000 | 1.623040000 | 0.726246000 |
| H | 2.120800000 | 1.602967000 | 0.326233000 |
| H | 1.250905000 | 2.332709000 | 1.379915000 |
| F | -3.636686000 | -1.132058000 | 0.399173000 |
| H | -3.607381000 | -0.154330000 | 0.367088000 |
| F | 3.636686000 | 1.132058000 | -0.399173000 |
| H | 3.607380000 | 0.154329000 | -0.367089000 |

**$(HF)_3(H_2O)_5$-B**
**MP2/aug-cc-pVTZ = -682.787925 a.u.**

| | | | |
|---|---|---|---|
| O | 0.031589000 | 1.458558000 | 1.133276000 |
| H | -0.849003000 | 1.717132000 | 0.772083000 |
| H | 0.004073000 | 0.487832000 | 1.228924000 |
| O | -2.427348000 | 2.100225000 | 0.136476000 |
| H | -2.811244000 | 1.360873000 | -0.373890000 |
| H | -2.520422000 | 2.872762000 | -0.434329000 |
| O | -2.138536000 | -2.157962000 | -0.141625000 |
| H | -1.321528000 | -1.937776000 | 0.358211000 |
| H | -1.879539000 | -2.845844000 | -0.768044000 |
| O | 0.112729000 | -1.395958000 | 1.272037000 |
| H | 0.221506000 | -1.757300000 | 2.161583000 |
| H | 0.938796000 | -1.636218000 | 0.792937000 |
| O | 3.488176000 | 0.099960000 | -0.795676000 |
| H | 3.734872000 | 0.182393000 | -1.725419000 |
| H | 2.953717000 | 0.904409000 | -0.592585000 |
| F | 1.950593000 | 2.166041000 | -0.205630000 |
| H | 1.155471000 | 1.895700000 | 0.334029000 |
| F | 2.274380000 | -1.959686000 | -0.170465000 |
| H | 2.771900000 | -1.153339000 | -0.441654000 |
| F | -3.309236000 | -0.166559000 | -1.157525000 |
| H | -2.865025000 | -0.939428000 | -0.780837000 |

**$(HF)_4(H_2O)_4$-B**
**MP2/aug-cc-pVTZ = -706.8008463 a.u.**

| | | | |
|---|---|---|---|
| O | -1.021890000 | -1.231651000 | 0.989840000 |
| H | -0.921760000 | -0.272863000 | 1.147108000 |
| H | -0.255715000 | -1.477249000 | 0.430864000 |
| O | -1.128368000 | 1.601355000 | 0.767532000 |
| H | -2.019466000 | 1.603994000 | 0.358145000 |
| H | -1.139757000 | 2.310630000 | 1.422965000 |
| O | 1.021856000 | 1.231661000 | -0.989775000 |
| H | 0.921720000 | 0.272874000 | -1.147039000 |
| H | 0.255693000 | 1.477265000 | -0.430786000 |
| O | 1.128331000 | -1.601344000 | -0.767469000 |
| H | 2.019439000 | -1.603986000 | -0.358102000 |
| H | 1.139704000 | -2.310618000 | -1.422904000 |
| F | -3.172764000 | -1.379901000 | -0.184461000 |
| H | -2.300252000 | -1.391540000 | 0.293792000 |
| F | -3.501180000 | 1.085510000 | -0.432927000 |
| H | -3.480761000 | 0.128258000 | -0.385738000 |
| F | 3.501173000 | -1.085506000 | 0.432933000 |
| H | 3.480756000 | -0.128254000 | 0.385743000 |
| F | 3.172760000 | 1.379906000 | 0.184472000 |
| H | 2.300236000 | 1.391548000 | -0.293758000 |

**$(HF)_5(H_2O)_3$-B**
**MP2/aug-cc-pVTZ = -730.8115173 a.u.**

| | | | |
|---|---|---|---|
| O | 0.095387000 | 1.474049000 | 1.144559000 |
| H | -0.694161000 | 1.769639000 | 0.653061000 |
| H | -0.000400000 | 0.508469000 | 1.222912000 |
| O | 3.410595000 | -0.053568000 | -0.902092000 |
| H | 3.519693000 | 0.111431000 | -1.847339000 |
| H | 3.046595000 | 0.781126000 | -0.526285000 |
| O | -0.041882000 | -1.428694000 | 1.175810000 |
| H | 0.094728000 | -1.849929000 | 2.035740000 |
| H | 0.745748000 | -1.681602000 | 0.629752000 |
| F | 2.294533000 | 2.093807000 | 0.187359000 |
| H | 1.410233000 | 1.881125000 | 0.559804000 |
| F | 2.032904000 | -2.001000000 | -0.298474000 |
| H | 2.593555000 | -1.229130000 | -0.561733000 |
| F | -2.233660000 | -2.008603000 | 0.106771000 |
| H | -1.373262000 | -1.817550000 | 0.520997000 |
| F | -3.260369000 | -0.075558000 | -1.129185000 |
| H | -2.895634000 | -0.832874000 | -0.675336000 |
| F | -2.190649000 | 2.094193000 | -0.302994000 |
| H | -2.631929000 | 1.325803000 | -0.640265000 |

**$(HF)_6(H_2O)_2$-B**
**MP2/aug-cc-pVTZ = -754.8203833 a.u.**

| | | | |
|---|---|---|---|
| O | -0.454251000 | -0.012865000 | -0.047916000 |
| H | -0.996294000 | -0.078371000 | 0.768420000 |
| H | 0.131219000 | -0.810261000 | -0.066094000 |
| O | 3.563389000 | -1.302840000 | 0.159858000 |
| H | 3.625955000 | -0.325852000 | 0.175796000 |
| H | 4.205801000 | -1.595791000 | -0.499181000 |
| F | 1.212562000 | -2.032373000 | -0.168814000 |
| H | 2.151378000 | -1.774979000 | -0.050630000 |
| F | 3.438751000 | 1.414831000 | 0.203233000 |
| H | 2.541738000 | 1.711343000 | 0.086024000 |
| F | 1.007598000 | 2.051939000 | -0.110965000 |
| H | 0.424870000 | 1.279068000 | -0.073361000 |
| F | -2.321085000 | 0.014394000 | -1.766620000 |
| H | -1.540473000 | -0.010025000 | -1.194575000 |
| F | -4.134033000 | -0.040316000 | -0.011853000 |
| H | -3.557401000 | -0.017022000 | -0.772608000 |
| F | -2.379099000 | -0.066720000 | 1.840008000 |
| H | -3.134284000 | -0.060015000 | 1.263244000 |

**$(HF)_7(H_2O)_1$-B**
**MP2/aug-cc-pVTZ = -778.8247594 a.u.**

| | | | |
|---|---|---|---|
| O | 3.196935000 | 0.009471000 | -0.626657000 |
| H | 4.142750000 | 0.106068000 | -0.456166000 |
| H | 2.766117000 | 0.766749000 | -0.178205000 |
| F | 2.237199000 | -2.185667000 | -0.103334000 |
| H | 2.633723000 | -1.297422000 | -0.300060000 |
| F | 0.091223000 | -2.158872000 | 1.086680000 |
| H | 0.940734000 | -2.179274000 | 0.623813000 |
| F | -1.986734000 | -2.352685000 | -0.255246000 |
| H | -1.173263000 | -2.309609000 | 0.254225000 |
| F | -3.047120000 | -0.159259000 | -0.785993000 |
| H | -2.646645000 | -1.005822000 | -0.577989000 |
| F | -2.295670000 | 1.818223000 | 0.543929000 |
| H | -2.598123000 | 1.060333000 | 0.042514000 |
| F | -0.214275000 | 2.951519000 | -0.275964000 |
| H | -1.018082000 | 2.533306000 | 0.028913000 |
| F | 1.950851000 | 2.035446000 | 0.653140000 |
| H | 1.137132000 | 2.397246000 | 0.316639000 |

**Table S15:** Cartesian coordinates of linear non-cyclic N-C $(HF)_m(H_2O)_n$, (m + n = 4 and 5) clusters optimized at MP2/aug-cc-pVDZ level of theory along with single point energy at MP2/aug-cc-pVTZ level

**NC-$(HF)_1(H_2O)_3$**
**MP2/aug-cc-pVTZ = -329.3586702 a.u.**

| | | | |
|---|---|---|---|
| O | 3.856675000 | -0.396989000 | 0.072114000 |
| H | 2.955400000 | -0.031324000 | 0.066203000 |
| H | 4.211247000 | -0.122994000 | 0.927758000 |
| O | 1.265991000 | 0.833663000 | -0.067194000 |
| H | 0.468479000 | 0.283848000 | -0.046411000 |
| H | 1.219175000 | 1.280971000 | -0.924283000 |
| F | -1.174506000 | -0.649501000 | -0.218394000 |
| H | -2.067368000 | -0.377733000 | -0.039678000 |
| O | -3.633266000 | 0.061709000 | 0.225275000 |
| H | -4.286703000 | -0.096794000 | -0.449504000 |
| H | -3.844878000 | 0.922473000 | 0.589903000 |

**NC-$(HF)_2(H_2O)_2$**
**MP2/aug-cc-pVTZ = -353.3768061 a.u.**

| | | | |
|---|---|---|---|
| O | -3.727339000 | -0.358040000 | 0.000000000 |
| H | -4.454448000 | 0.274662000 | 0.000005000 |
| H | -4.129693000 | -1.234982000 | -0.000004000 |
| F | -1.196731000 | 0.217145000 | 0.000000000 |
| H | -2.122396000 | 0.019734000 | 0.000000000 |
| O | 1.593067000 | 0.812110000 | 0.000000000 |
| H | 0.646347000 | 0.602048000 | 0.000000000 |
| H | 1.650207000 | 1.774670000 | 0.000000000 |
| F | 3.702168000 | -0.757094000 | 0.000000000 |
| H | 2.935224000 | -0.209149000 | 0.000000000 |

**NC-$(HF)_3(H_2O)_1$**
**MP2/aug-cc-pVTZ = -377.3901312 a.u.**

| | | | |
|---|---|---|---|
| F | -0.215795000 | 3.481772000 | 0.000000000 |
| H | -0.407350000 | 2.565762000 | 0.000000000 |
| F | -0.739120000 | 0.868126000 | 0.000000000 |
| H | 0.000000000 | 0.274854000 | 0.000000000 |
| F | 1.115604000 | -0.889783000 | 0.000000000 |
| H | 0.683458000 | -1.743552000 | 0.000000000 |
| O | -0.112767000 | -3.125539000 | 0.000000000 |
| H | 0.253463000 | -4.017953000 | 0.000000000 |
| H | -1.073631000 | -3.215838000 | 0.000000000 |

**NC-$(HF)_1(H_2O)_4$**
**MP2/aug-cc-pVTZ = -405.696311a.u.**

| | | | |
|---|---|---|---|
| O | 5.037884000 | -0.722349000 | 0.000000000 |
| H | 5.532429000 | -1.550837000 | 0.000000000 |
| H | 5.692371000 | -0.013667000 | 0.000000000 |
| F | 2.445925000 | -0.569018000 | 0.000000000 |
| H | 3.392888000 | -0.601698000 | 0.000000000 |
| O | -0.008987000 | 0.905682000 | 0.000000000 |
| H | 0.856017000 | 0.466287000 | 0.000000000 |
| H | 0.186945000 | 1.849517000 | 0.000000000 |
| O | -5.321464000 | 0.941924000 | 0.000000000 |
| H | -4.392297000 | 0.646680000 | 0.000000000 |
| H | -5.259882000 | 1.904288000 | 0.000000000 |
| O | -2.653328000 | -0.128182000 | 0.000000000 |
| H | -1.730350000 | 0.187013000 | 0.000000000 |
| H | -2.588793000 | -1.090057000 | 0.000000000 |

**NC-$(HF)_2(H_2O)_3$**
**MP2/aug-cc-pVTZ = -429.7182711 a.u.**

| | | | |
|---|---|---|---|
| O | 3.729237000 | 0.129634000 | -0.231531000 |
| H | 2.828407000 | -0.234258000 | -0.167955000 |
| H | 3.851002000 | 0.562433000 | 0.615641000 |
| F | 0.981386000 | -0.913186000 | 0.007265000 |
| H | 0.100599000 | -1.195321000 | 0.218607000 |
| O | -1.434485000 | -1.809258000 | 0.237656000 |
| H | -2.074760000 | -1.113374000 | 0.009680000 |
| H | -1.686112000 | -2.608488000 | -0.238238000 |
| F | -2.683925000 | 0.581859000 | -0.327270000 |
| H | -1.964318000 | 1.142964000 | -0.121907000 |
| O | -0.510110000 | 1.937663000 | 0.232990000 |
| H | 0.309048000 | 1.498565000 | 0.453531000 |
| H | -0.318150000 | 2.865109000 | 0.197751000 |

**NC-$(HF)_3(H_2O)_2$**
**MP2/aug-cc-pVTZ = -453.7155941 a.u.**

| | | | |
|---|---|---|---|
| F | 4.433449000 | -2.118952000 | 0.082096000 |
| H | 5.311160000 | -1.818761000 | 0.037140000 |
| F | 2.455019000 | -0.331094000 | -0.014282000 |
| H | 3.195529000 | -0.902426000 | 0.013941000 |
| O | 0.223080000 | 1.493099000 | -0.107547000 |
| H | 1.029202000 | 0.957381000 | -0.083740000 |
| H | 0.499541000 | 2.412234000 | -0.187858000 |
| F | -2.164132000 | 0.530472000 | 0.026450000 |
| H | -1.290495000 | 0.901981000 | -0.024130000 |
| O | -5.067119000 | 0.248985000 | 0.118070000 |
| H | -4.103958000 | 0.361235000 | 0.086159000 |
| H | -5.403237000 | 1.150992000 | 0.053701000 |

**NC-$(HF)_4(H_2O)_1$**
**MP2/aug-cc-pVTZ =** -477.727297 **a.u.**

| | | | |
|---|---|---|---|
| O | -4.933988000 | 1.123185000 | 0.000000000 |
| H | -4.035966000 | 0.757724000 | 0.000000000 |
| H | -4.792521000 | 2.077576000 | 0.000000000 |
| F | -2.194194000 | -0.037384000 | 0.000000000 |
| H | -1.311956000 | 0.283887000 | 0.000000000 |
| F | 0.298832000 | 0.799523000 | 0.000000000 |
| H | 0.940452000 | 0.107960000 | 0.000000000 |
| F | 2.071884000 | -1.099655000 | 0.000000000 |
| H | 2.983882000 | -0.871069000 | 0.000000000 |
| F | 4.651537000 | -0.532935000 | 0.000000000 |
| H | 5.264619000 | -1.231028000 | 0.000000000 |