Supplementary Information For: Concerted Proton Transfer in Homogeneous and Heterogeneous Cyclic Hydrogen-Bonded Clusters of H_2O, HF, and HCl

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1 Comparison to Benchmark Data

Table S1 Barrier height energies (in kcal mol^{-1}) of the homogeneous trimers, tetramers, and pentamers, compared between CCSD(T)-F12/haQZ-F12//MP2/haTZ and CCSD(T)-F12/haQZ-F12//CCSD(T)/aQZ, as well as the difference between them.

System	This Work	Ref 52*	Deviation	% Deviation
$(HF)_3$	20.65	20.68	-0.031	-0.15%
$(HF)_4$	14.73	14.80	-0.068	-0.46%
$(HF)_5$	14.74	14.84	-0.099	-0.66%
$(H_2O)_3$	29.99	29.99	-0.004	-0.01%
$(H_2O)_4$	26.85	26.88	-0.033	-0.12%
$(H_2O)_5$	30.37	30.41	-0.046	-0.15%
$(HCl)_3$	27.36	27.35	$+0.006$	$+0.02\%$
$(HCl)_4$	30.86	30.88	-0.020	-0.07%
$(HCl)_5$	37.87	37.90	-0.033	-0.09%

*Deviations between CCSD(T)-F12/haQZ-F12 and CCSD(T)-F12/ha5Z-F12 energetics were found to be less than 0.1 kcal mol^{-1} in all systems

Table S2 Imaginary harmonic vibrational frequencies (in cm^{-1}) of the homogeneous trimers, tetramers, and pentamers, compared between MP2/haTZ and CCSD(T)/aTZ, as well as their absolute difference.

System	MP2	CCSD(T)	Deviation	%Deviation
$(HF)_3$	$1695i$	$1775i$	$-80i$	-4.51%
$(HF)_4$	$1441i$	$1515i$	$-74i$	-4.88%
$(HF)_5$	$1369i$	$1433i$	$-64i$	-4.47%
$(H_2O)_3$	$1814i$	$1915i$	$-101i$	-5.27%
$(H_2O)_4$	$1653i$	$1753i$	$-100i$	-5.70%
$(H_2O)_5$	$1624i$	$1724i$	$-100i$	-5.80%
$(HCl)_3$	$1504i$	$1652i$	$-148i$	-8.96%
$(HCl)_4$	$1467i$	$1602i$	$-135i$	-8.43%
$(HCl)_5$	$1460i$	$1597i$	$-137i$	-8.58%

Table S3 Symmetric HX stretch harmonic vibrational frequencies (in cm^{-1}) of the homogeneous trimers, tetramers, and pentamers, compared between MP2/haTZ and CCSD(T)/aTZ, as well as their absolute difference.

System	MP2	CCSD(T)	Deviation	%Deviation
$(HF)_3$	3714	3751	−37	−0.99%
$(HF)_4$	3360	3426	−66	−1.93%
$(HF)_5$	3221	3291	−70	−2.13%
$(H_2O)_3$	3582	3605	−23	−0.64%
$(H_2O)_4$	3401	3448	−47	−1.36%
$(H_2O)_5$	3359	3413	−54	−1.58%
$(HCl)_3$	2889	2871	+18	+0.63%
$(HCl)_4$	2831	2828	+3	+0.11%
$(HCl)_5$	2826	2825	+1	+0.04%

2 Energetics of Isomers

For heterogeneous systems containing 2 or 3 H_2O fragments, there are isomers which differ only by the relative orientations of the free hydrogen atoms that do not participate in hydrogen bonding about the (pseudo-)plane formed by the heavy atoms. The relative orientation of these dangling hydrogen atoms is given in the following tables by $H_2O\uparrow$ or $H_2O\downarrow$, denoting which fragments have a free hydrogen atom pointing "up" or "down" (arbitrarily defined), respectively.

Table S4 CCSD(T)-F12/haQZ-F12 relative energies of products, barrier heights of transition states for CPT, and dissociation energies of reactants (ΔE, $\Delta E^{\ddagger}$, and D_e, respectively, in kcal mol^{-1}) for each $(HF)_x(H_2O)_y(HCl)_z$ trimer configuration containing two H_2O fragments, with the fragment labels ($f1$, $f2$, $f3$) denoting the direction of the hydrogen bond network in the reactant.

$f1$	$f2$	$f3$	ΔE	$\Delta E^{\ddagger}$	D_e
HF	$H_2O\uparrow$	$H_2O\downarrow$	0.0	21.7	18.2
HF	$H_2O\uparrow$	$H_2O\uparrow$	0.0	22.3	17.9[a]
$H_2O\uparrow$	$H_2O\downarrow$	HCl	0.0	11.9	13.8
$H_2O\uparrow$	$H_2O\uparrow$	HCl	0.0	12.5	13.4[b]

[a] 0.3 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the FOO plane

[b] 0.4 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the OOCl plane

Table S5 CCSD(T)-F12/haQZ-F12 relative energies of products, barrier heights of transition states for CPT, and dissociation energies of reactants (ΔE, $\Delta E^{\ddagger}$, and D_e, respectively, in kcal mol^{-1}) for each $(HF)_x(H_2O)_y(HCl)_z$ tetramer configuration containing two or three H_2O fragments, with the fragment labels ($f1$, $f2$, $f3$, $f4$) denoting the direction of the hydrogen bond network in the reactant. No stationary points were found at the MP2/haTZ level of theory for the $(HF)_1(H_2O)_3$ or $(HCl)_1(H_2O)_3$ conformer in which all free hydrogen atoms were on the same side of the (pseudo-)plane.

$f1$	$f2$	$f3$	$f4$	ΔE	$\Delta E^{\ddagger}$	D_e
HF	HF	$H_2O\uparrow$	$H_2O\downarrow$	0.0	13.4	31.2
HF	HF	$H_2O\uparrow$	$H_2O\uparrow$	0.0	13.9	30.6[a]
HF	$H_2O\uparrow$	HF	$H_2O\downarrow$	0.0	14.2	32.3
HF	$H_2O\uparrow$	HF	$H_2O\uparrow$	0.0	14.4	32.1[b]
HF	$H_2O\uparrow$	$H_2O\downarrow$	HCl	2.4	9.9	26.0
HF	$H_2O\uparrow$	$H_2O\uparrow$	HCl	2.4	10.3	25.4[c]
HF	$H_2O\uparrow$	HCl	$H_2O\downarrow$	0.0	8.1	25.9
HF	$H_2O\uparrow$	HCl	$H_2O\uparrow$	0.0	8.2	25.8[d]
HF	$H_2O\uparrow$	$H_2O\downarrow$	$H_2O\uparrow$	0.0	18.4	30.2
HF	$H_2O\downarrow$	$H_2O\uparrow$	$H_2O\uparrow$	0.1	18.8	29.9[e]
$H_2O\uparrow$	$H_2O\downarrow$	$H_2O\uparrow$	HCl	0.0	7.9	24.1
$H_2O\downarrow$	$H_2O\uparrow$	$H_2O\uparrow$	HCl	0.0	8.2	23.7[f]
$H_2O\uparrow$	$H_2O\downarrow$	HCl	HCl	0.0	8.7	19.9
$H_2O\uparrow$	$H_2O\uparrow$	HCl	HCl	0.0	9.5	19.3[g]

[a] 0.6 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the FFOO plane
[b] 0.2 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the FOFO plane
[c] 0.6 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the FOOCl plane
[d] 0.1 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the FOClO plane
[e] 0.3 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the FOOO plane
[f] 0.4 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the OOClCl plane
[g] 0.6 kcal mol^{-1} higher than the conformer with the dangling hydrogen atoms on opposite sides of the OOOCl plane

3 Cartesian Coordinates of Optimized Geometries

Table S6 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	-0.939131	1.177031	0.000000	0.000000	-1.297481	0.000000
F	1.488904	0.224796	0.000000	1.123652	0.648741	0.000000
F	-0.549773	-1.401827	0.000000	-1.123652	0.648741	0.000000
H	0.000000	1.180024	0.000000	0.000000	0.915953	0.000000
H	1.021931	-0.590012	0.000000	-0.793238	-0.457976	0.000000
H	-1.021931	-0.590012	0.000000	0.793238	-0.457976	0.000000

Table S7 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_2(HCl)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	1.873361	0.359753	0.000000	0.000000	1.130077	-1.130130
F	0.369556	-1.815169	0.000000	0.000000	-1.130077	-1.130130
Cl	-1.258370	0.812344	0.000000	0.000000	0.000000	1.281093
H	1.592898	-0.532860	0.000000	0.000000	0.000000	-1.349569
H	0.000000	1.085577	0.000000	0.000000	0.938553	-0.043338
H	-0.386862	-1.263808	0.000000	0.000000	-0.938553	-0.043338

Table S8 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_1(HCl)_2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	-1.076990	-1.711369	0.000000	0.000000	0.000000	1.701340
Cl	1.861330	-0.446581	0.000000	0.000000	1.530404	-0.482787
Cl	-1.258788	1.409312	0.000000	0.000000	-1.530404	-0.482787
H	0.869450	-1.264559	0.000000	0.000000	-0.820514	0.939071
H	-1.419753	-0.843187	0.000000	0.000000	0.820514	0.939071
H	0.000000	1.143631	0.000000	0.000000	0.000000	-0.775425

Table S9 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_2(H_2O)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	1.421297	-0.605419	-0.093904	0.028959	1.342937	0.000000
H	0.662002	-1.204931	-0.046842	0.014346	0.581017	0.765078
H	2.000819	-0.861522	0.630176	-0.817284	1.807492	0.000000
F	-0.066862	1.434820	0.008891	0.028959	-0.710167	-1.128889
H	0.645180	0.793157	-0.016165	0.014346	0.581017	-0.765078
F	-1.430781	-0.770712	0.010358	0.028959	-0.710167	1.128889
H	-1.199588	0.139673	0.010823	0.035654	-0.930024	0.000000

Table S10 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of trans $(HF)_1(H_2O)_2$, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-1.633691	0.018142	0.091844	0.000000	-1.183222	-0.653832
H	-1.088661	-0.781636	0.048419	0.025128	-0.884595	0.392308
H	-2.352878	-0.130198	-0.528184	0.839655	-1.600889	-0.874489
O	0.817766	1.242285	-0.108984	0.000000	1.183222	-0.653832
H	-0.153427	1.173888	-0.045400	0.000000	0.000000	-0.930597
H	1.094043	1.771623	0.644794	-0.839655	1.600889	-0.874489
F	0.886982	-1.305792	0.005172	0.000000	0.000000	1.372918
H	1.045484	-0.364966	-0.029054	-0.025128	0.884595	0.392308

Table S11 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of cis $(HF)_1(H_2O)_2$, i.e. $(HF)_1(H_2O{\uparrow})_2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	1.625346	-0.084140	-0.055900	0.057034	-0.656593	1.181196
H	1.126584	0.744238	-0.003825	0.053666	0.390430	0.883962
H	2.453713	0.080621	0.401449	-0.752891	-0.841119	1.668422
O	-0.875873	-1.210839	-0.090089	0.057034	-0.656593	-1.181196
H	0.094603	-1.211946	-0.004235	-0.027390	-0.934766	0.000000
H	-1.206570	-1.724121	0.652644	-0.752891	-0.841119	-1.668422
F	-0.826959	1.340480	0.015555	0.057034	1.371293	0.000000
H	-1.021486	0.406726	-0.018114	0.053666	0.390430	-0.883962

Table S12 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_1(H_2O)_1(HCl)_1$*

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
Cl	1.577222	-0.141590	0.005200	-1.331694	-0.121171	0.005849	1.444153	-0.006047	0.004992
F	-1.128108	1.418970	0.008433	0.940115	1.287310	0.009473	-1.272982	1.467410	0.009279
O	-1.633637	-1.090711	-0.091354	1.361264	-1.008948	-0.100204	-1.231426	-1.392942	-0.092326
H	-0.722431	-1.413258	-0.063232	0.336420	-1.077330	-0.091050	-1.703185	-0.549348	-0.034388
H	0.669496	0.774894	0.010088	1.680370	-1.385706	0.731862	-1.592803	-1.938193	0.613603
H	-1.456364	0.524994	-0.022269	1.377331	0.101600	-0.038193	0.401670	-0.802193	-0.014420
H	-2.081409	-1.524639	0.641949	-0.106469	0.907134	0.014331	-0.348045	1.329380	0.005441

*The reactant and product of this structure are not equivalent

Table S13 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(H_2O)_3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	0.169306	1.595577	0.108999	0.028304	1.369079	0.000000
O	-1.472461	-0.646198	-0.082860	0.028304	-0.688010	1.185487
O	1.301926	-0.943125	-0.092177	0.028304	-0.688010	-1.185487
H	-0.631841	1.043140	0.056078	0.861628	1.851002	0.000000
H	-0.604947	-1.085503	-0.027801	-0.061429	-0.951329	0.000000
H	1.219641	0.025564	-0.021409	0.039426	0.472391	-0.821467
H	0.078087	2.241910	-0.596222	0.039426	0.472391	0.821467
H	-2.024958	-1.084540	0.569447	-0.779171	-0.894460	-1.666604
H	1.973842	-1.190601	0.548208	-0.779171	-0.894460	1.666604

Table S14 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of trans $(H_2O)_2(HCl)_1$, i.e. $(H_2O{\uparrow})_1(H_2O{\downarrow})_1(HCl)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-0.942898	1.524419	-0.106862	0.000000	1.192450	-1.186132
H	0.574452	0.698130	-0.034642	0.004592	1.068412	-0.156661
H	-1.193226	2.070712	0.644529	-0.850579	1.591001	-1.411636
O	-1.684210	-1.138905	0.093032	0.000000	-1.192450	-1.186132
H	-1.476983	0.711675	-0.030688	0.000000	0.000000	-1.390755
H	-2.101063	-1.698900	-0.568586	0.850579	-1.591001	-1.411636
Cl	1.527124	-0.205124	0.001824	0.000000	0.000000	1.382674
H	-0.747418	-1.378624	0.069015	-0.004592	-1.068412	-0.156661

Table S15 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of cis $(H_2O)_2(HCl)_1$, i.e. $(H_2O\uparrow)_2(HCl)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	0.940115	1.535732	-0.089630	0.043757	-1.188092	1.190375
H	-0.569290	0.692891	-0.023007	0.072509	-0.159089	1.063509
H	1.173624	2.097118	0.655861	-0.775189	-1.383618	1.663083
O	1.674736	-1.134781	-0.059238	0.043757	-1.188092	-1.190375
H	1.496693	0.740666	-0.005163	-0.038608	-1.396376	0.000000
H	2.142492	-1.813026	0.435909	-0.775189	-1.383618	-1.663083
Cl	-1.523789	-0.208141	0.008717	0.043757	1.381839	0.000000
H	0.742082	-1.386855	-0.020841	0.072509	-0.159089	-1.063509

Table S16 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(H_2O)_1(HCl)_2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-0.395218	2.010647	-0.090590	0.018483	1.805968	0.000000
H	0.528566	1.727594	-0.051212	0.029210	1.108120	0.790433
H	-0.495396	2.642812	0.628712	-0.854315	2.229019	0.000000
Cl	-1.686127	-0.757049	0.004849	0.018483	-0.533585	-1.542070
H	-1.290135	0.487301	-0.024400	0.029210	1.108120	-0.790433
Cl	1.904802	-0.423111	0.004744	0.018483	-0.533585	1.542070
H	0.701231	-0.880165	0.008548	0.019618	-0.751092	0.000000

Table S17 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HCl)_3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	-1.272380	1.686169	0.000000	0.000000	-1.770142	0.000000
Cl	2.096455	0.258829	0.000000	1.532988	0.885071	0.000000
Cl	-0.824075	-1.944998	0.000000	-1.532988	0.885071	0.000000
H	0.000000	1.506925	0.000000	0.000000	1.121559	0.000000
H	1.305035	-0.753462	0.000000	-0.971299	-0.560779	0.000000
H	-1.305035	-0.753462	0.000000	0.971299	-0.560779	0.000000

Table S18 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_4$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	1.258960	1.258960	0.000000	1.135547	-1.135547	0.000000
F	1.258960	-1.258960	0.000000	1.135547	1.135547	0.000000
F	-1.258960	-1.258960	0.000000	-1.135547	1.135547	0.000000
F	-1.258960	1.258960	0.000000	-1.135547	-1.135547	0.000000
H	1.415828	0.320373	0.000000	0.000000	1.250986	0.000000
H	0.320373	-1.415828	0.000000	-1.250986	0.000000	0.000000
H	-1.415828	-0.320373	0.000000	0.000000	-1.250986	0.000000
H	-0.320373	1.415828	0.000000	1.250986	0.000000	0.000000

Table S19 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_3(HCl)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	-1.297367	1.329004	0.000000	0.000000	0.000000	1.629974
F	1.736893	0.926978	0.000000	0.000000	1.700778	-0.459523
F	1.567767	-1.628424	0.000000	0.000000	0.000000	-1.973742
F	-0.987942	-1.674414	0.000000	0.000000	-1.700778	-0.459523
H	0.000000	1.340009	0.000000	0.000000	-1.113583	0.455311
H	1.810839	-0.014716	0.000000	0.000000	1.113583	0.455311
H	0.632817	-1.771865	0.000000	0.000000	0.886860	-1.292542
H	-1.238877	-0.763764	0.000000	0.000000	-0.886860	-1.292542

Table S20 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_3(H_2O)_1$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-1.683240	0.706671	-0.077583	0.026492	-1.659117	0.000000
F	1.613068	-0.802977	0.023354	0.003033	1.624214	0.000000
F	0.884847	1.628778	-0.009585	0.026492	0.057037	-1.649737
F	-0.748470	-1.576030	-0.010339	0.026492	0.057037	1.649737
H	-0.880947	1.259566	-0.044587	0.020693	-0.986586	0.830721
H	0.754012	-1.223441	0.008277	0.017974	0.884716	-0.930812
H	1.292874	0.773606	0.001208	0.020693	-0.986586	-0.830721
H	-1.204557	-0.709382	-0.025521	0.017974	0.884716	0.930812
H	-2.240466	0.998343	0.650421	-0.793428	-2.167914	0.000000

Table S21 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating $(HF)_2(HCl)_2$, i.e. $f1 = f2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	-1.253022	1.644984	0.000000	0.000000	1.546542	-0.960414
Cl	2.066903	0.379943	0.000000	0.000000	-1.546542	-0.960414
F	0.476659	-2.284965	0.000000	0.000000	-1.139266	1.703904
F	-1.931781	-1.327506	0.000000	0.000000	1.139266	1.703904
H	0.000000	1.321641	0.000000	0.000000	1.390513	0.645351
H	1.535464	-0.798566	0.000000	0.000000	0.000000	-1.061429
H	-0.432929	-2.044225	0.000000	0.000000	-1.390513	0.645351
H	-1.842421	-0.390368	0.000000	0.000000	0.000000	1.754517

Table S22 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating $(HF)_2(HCl)_2$, i.e. $f1 = f3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	1.510330	-1.816569	0.000000	0.000000	0.000000	2.002237
F	1.510330	1.294572	0.000000	0.000000	1.794850	0.000000
Cl	-1.510330	1.816569	0.000000	0.000000	0.000000	-2.002237
F	-1.510330	-1.294572	0.000000	0.000000	-1.794850	0.000000
H	1.656351	-0.532342	0.000000	0.000000	-1.109677	0.882761
H	0.615783	1.580864	0.000000	0.000000	1.109677	0.882761
H	-1.656351	0.532342	0.000000	0.000000	1.109677	-0.882761
H	-0.615783	-1.580864	0.000000	0.000000	-1.109677	-0.882761

Table S23 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating $(HF)_2(H_2O)_1(HCl)_1$*, i.e. $f1 = f2$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
O	-0.829706	1.849550	-0.037522	-0.715225	1.713557	-0.066369	-0.254181	1.951077	-0.073138
F	-0.365770	-1.922915	0.067345	-0.267439	-1.731229	0.043021	-0.637662	-1.870851	0.027157
Cl	1.914937	0.124285	-0.023095	1.682277	0.109509	-0.012279	1.790370	-0.139268	-0.006596
F	-2.220922	-0.220138	-0.065358	-1.993185	-0.252783	-0.034777	-2.290941	0.093704	-0.017330
H	-1.736173	0.620677	-0.050420	-1.391762	0.818197	-0.045156	-1.094948	1.460214	-0.048466
H	1.059668	-0.849364	0.019438	0.632524	-1.005576	0.020953	0.209127	-1.444928	0.015153
H	0.095707	1.552649	-0.036370	0.221679	1.301077	-0.068608	0.912236	0.871928	-0.020256
H	-1.136393	-1.370929	0.013172	-1.189403	-1.040219	0.001696	-1.782519	-0.701187	-0.003536
H	-0.918871	2.425206	0.729080	-0.804334	2.212528	0.756604	-0.289304	2.567236	0.665897

*The reactant and product of this structure are not equivalent

Table S24 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating $(HF)_2(H_2O)_1(HCl)_1$, i.e. $f1 = f3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	2.299985	-0.006336	-0.076667	0.251473	-1.998052	0.000000
Cl	-1.864208	-0.089776	0.009750	-0.090708	1.635820	0.000000
F	0.583790	-1.827661	-0.006796	-0.090708	-0.423274	1.795216
F	0.368030	1.981169	-0.006678	-0.090708	-0.423274	-1.795216
H	1.792783	0.822139	-0.040582	0.110092	-1.379360	-0.836042
H	-0.888202	-0.954480	-0.001326	-0.111018	0.433288	1.220654
H	1.298662	-1.175658	-0.026003	0.110092	-1.379360	0.836042
H	-0.415942	1.460860	-0.004795	-0.111018	0.433288	-1.220654
H	2.937976	0.042448	0.641559	1.164862	-2.313450	0.000000

Table S25 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating trans $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_1(H_2O\downarrow)_1$ with $f1 = f2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-0.040050	1.801373	-0.038877	0.780050	0.909637	-1.175243
F	0.257439	-1.854750	0.068421	-0.780050	-0.825046	1.223504
F	1.778504	0.142087	-0.072259	0.780050	0.825046	1.223504
O	-1.906068	-0.131753	0.034998	-0.780050	-0.909637	-1.175243
H	-0.834705	1.218043	-0.018581	0.000000	0.000000	-1.288346
H	-1.311485	-0.901641	0.041925	-0.862989	-0.978079	-0.127375
H	-0.099589	2.364254	0.738809	0.408532	1.738225	-1.497266
H	0.924484	-1.179489	0.012270	0.000000	0.000000	1.318443
H	1.114533	0.864872	-0.050525	0.862989	0.978079	-0.127375
H	-2.547782	-0.309024	-0.658315	-0.408532	-1.738225	-1.497266

Table S26 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating cis $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_2$ with $f1 = f2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-0.416377	-1.767489	-0.055193	-0.040218	-1.174456	1.197028
F	0.212862	1.871579	0.045954	-0.040218	1.224868	-1.135215
F	-1.752899	0.303574	-0.027787	-0.040218	1.224868	1.135215
O	1.865514	-0.339247	-0.095792	-0.040218	-1.174456	-1.197028
H	0.503146	-1.419367	-0.013857	0.026072	-1.297027	0.000000
H	1.492988	0.556799	-0.034327	-0.042611	-0.125480	-1.300554
H	-0.518671	-2.355564	0.698752	0.735389	-1.514281	1.655627
H	-0.598976	1.378265	0.014784	-0.044225	1.320227	0.000000
H	-1.291585	-0.561823	-0.033467	-0.042611	-0.125480	1.300554
H	2.680334	-0.320799	0.412495	0.735389	-1.514281	-1.655627

Table S27 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating trans $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_1(H_2O\downarrow)_1$ with $f1 = f3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	-0.960803	1.573104	-0.002208	0.000000	0.000000	1.656250
F	0.960803	-1.573104	0.002208	0.000000	0.000000	-1.656250
O	-1.638792	-0.831754	0.098470	0.000000	-1.671374	0.000000
O	1.638792	0.831754	-0.098470	0.000000	1.671374	0.000000
H	-0.779414	-1.293999	0.056125	-0.012132	-0.974111	0.855132
H	0.779414	1.293999	-0.056125	0.012132	0.974111	-0.855132
H	-1.309441	0.669863	0.027727	0.012132	0.974111	0.855132
H	1.309441	-0.669863	-0.027727	-0.012132	-0.974111	-0.855132
H	-2.164786	-1.185796	-0.624510	-0.815249	-2.184369	0.000000
H	2.164786	1.185796	0.624510	0.815249	2.184369	0.000000

Table S28 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating cis $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_2$ with $f1 = f3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	-1.249078	1.354255	0.025455	1.654273	0.000000	0.019746
F	1.249078	-1.354255	0.025455	-1.654273	0.000000	0.019746
O	-1.249078	-1.349527	-0.097215	0.000000	1.669111	-0.097804
O	1.249078	1.349527	-0.097215	0.000000	-1.669111	-0.097804
H	-1.460624	-0.397373	-0.048417	0.854965	0.974479	-0.034722
H	1.460624	0.397373	-0.048417	-0.854965	-0.974479	-0.034722
H	-0.285572	1.444063	-0.010441	0.854965	-0.974479	-0.034722
H	0.285572	-1.444063	-0.010441	-0.854965	0.974479	-0.034722
H	-1.750787	-1.769177	0.607487	0.000000	2.244855	0.674165
H	1.750787	1.769177	0.607487	0.000000	-2.244855	0.674165

Table S29 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HF)_1(HCl)_3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	-1.729343	-1.795346	0.000000	0.000000	2.086211	-0.372274
Cl	-1.282703	1.766491	0.000000	0.000000	0.000000	1.912568
Cl	2.249958	1.101542	0.000000	0.000000	-2.086211	-0.372274
F	1.356299	-1.912736	0.000000	0.000000	0.000000	-2.071922
H	-1.670963	-0.505742	0.000000	0.000000	0.891803	-1.409105
H	0.000000	1.627515	0.000000	0.000000	1.099336	0.804591
H	1.998282	-0.163057	0.000000	0.000000	-1.099336	0.804591
H	0.421486	-1.979769	0.000000	0.000000	-0.891803	-1.409105

Table S30 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating $(HF)_1(H_2O)_1(HCl)_2$*, i.e. $f3 = f4$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
O	1.230067	2.065127	0.013508	0.504116	2.021536	0.169596	1.637299	1.698290	-0.077022
Cl	-1.779482	-1.088660	0.051770	-1.172867	-1.353010	0.127792	-1.894806	-0.883488	0.008853
Cl	1.784342	-1.164019	-0.040332	1.835109	-0.530474	-0.111512	1.585921	-1.272854	-0.002062
F	-1.287261	1.907954	-0.112464	-1.700794	1.269175	-0.287873	-1.134235	2.088625	-0.007559
H	-0.333013	2.018913	-0.064027	-0.516139	1.727763	-0.039026	0.716542	2.005570	-0.044512
H	0.496185	-1.263439	-0.005299	0.479002	-0.998643	-0.007840	-0.625188	-1.153288	0.001947
H	1.589604	1.164118	0.004769	1.075734	1.179287	0.057714	1.664863	0.049238	-0.022990
H	-1.683641	0.203794	-0.028699	-1.593435	0.225650	-0.150397	-1.482979	1.217062	-0.006214
H	1.593053	2.479565	0.802923	0.570940	2.290304	1.096877	2.087527	2.155285	0.640518

*The reactant and product of this structure are not equivalent

Table S31 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating $(HF)_1(H_2O)_1(HCl)_2$, i.e. $f2 = f4$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	2.390358	0.039260	-0.077016	0.034836	-0.053559	2.055159
Cl	-2.300361	-0.092311	-0.084700	0.034836	-0.053559	-2.055159
F	0.044106	-1.992141	0.159299	-0.076243	-1.779048	0.000000
O	-0.216050	2.023552	0.047203	0.034836	1.897319	0.000000
H	0.654217	1.595770	0.000709	0.053985	1.251169	0.830276
H	1.506040	-0.897341	0.023867	-0.029510	-1.095778	0.907146
H	-1.410568	0.886780	-0.017690	0.053985	1.251169	-0.830276
H	-0.755677	-1.500214	0.082490	-0.029510	-1.095778	-0.907146
H	-0.192503	2.557721	0.848479	-0.825870	2.343104	0.000000

Table S32 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating trans $(HF)_1(H_2O)_2(HCl)_1$*, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$ with $f2 = f3$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
O	0.722440	1.981285	-0.010412	0.765372	1.789385	-0.064602	0.339901	-1.897579	0.000683
F	0.388133	-1.885282	-0.132131	0.154832	-1.793341	-0.202865	0.468450	1.979688	0.104425
Cl	-1.923971	0.046918	0.057819	-1.680932	0.153300	0.091418	-1.814926	0.027698	-0.055170
O	2.264791	-0.255599	0.033290	1.997836	-0.321623	0.102335	2.341327	-0.084037	-0.015107
H	1.820225	0.620540	0.027537	1.527228	0.642991	0.011869	1.148617	-1.334338	-0.011313
H	1.162963	-1.303680	-0.060239	1.210293	-1.041513	-0.030138	1.855901	0.756661	0.014707
H	0.727979	2.587440	-0.757466	0.810868	2.267346	-0.900294	0.394112	-2.420482	0.807480
H	-1.007065	-0.872333	-0.036600	-0.657422	-1.076222	-0.096959	-0.328505	1.475853	0.056351
H	-0.175991	1.616050	0.010500	-0.163569	1.413280	-0.011312	-0.851101	-0.921283	-0.016284
H	2.788343	-0.283574	0.839506	2.349301	-0.414006	0.996635	2.968842	0.008455	-0.737481

*The reactant and product of this structure are not equivalent

Table S33 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating cis $(HF)_1(H_2O)_2(HCl)_1$*, i.e. $(HF)_1(H_2O\uparrow)_2(HCl)_1$ with $f2 = f3$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
O	0.704714	1.971388	-0.081862	-0.759933	1.758676	-0.261416	0.320911	-1.923561	-0.000353
F	0.401655	-1.877890	-0.007769	-0.157173	-1.798914	-0.211400	0.481395	1.991301	0.101263
Cl	-1.938400	0.032624	0.013933	1.675049	0.154559	0.106745	-1.809082	0.041575	-0.044158
O	2.286622	-0.246506	-0.067843	-1.993927	-0.314345	0.135146	2.311748	-0.095415	-0.148240
H	1.856362	0.633579	-0.018888	-1.527304	0.654055	0.020952	1.142182	-1.382917	-0.006022
H	1.175648	-1.292282	-0.028703	-1.216844	-1.030284	-0.024936	1.857091	0.756559	-0.051048
H	0.671908	2.764332	0.460790	-0.799907	2.510714	0.339245	0.352326	-2.445134	0.808265
H	-1.007583	-0.876848	0.002948	0.647690	-1.093944	-0.099580	-0.315484	1.487906	0.055116
H	-0.192524	1.604499	-0.054147	0.169487	1.383963	-0.181177	-0.857724	-0.916241	-0.018391
H	2.903400	-0.285945	0.668701	-2.303524	-0.416432	1.043602	3.182179	0.023155	0.240148

*The reactant and product of this structure are not equivalent

Table S34 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating trans $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$ with $f2 = f4$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	1.857259	-0.267692	-0.016894	0.000000	0.000000	1.713982
F	-2.268902	0.334326	-0.037040	0.000000	0.000000	-2.028142
O	-0.080886	1.949178	0.129484	0.000000	1.780038	-0.502782
O	-0.953926	-1.811390	-0.065554	0.000000	-1.780038	-0.502782
H	1.034719	0.778798	0.039353	-0.017941	1.239225	0.389434
H	-1.825153	-0.521608	-0.044680	-0.012561	-0.975734	-1.292099
H	-0.018650	-1.541717	-0.061842	0.017941	-1.239225	0.389434
H	-0.954071	1.518542	0.062562	0.012561	0.975734	-1.292099
H	-0.055765	2.595704	-0.583026	0.835999	2.263310	-0.517290
H	-1.055858	-2.390190	0.696741	-0.835999	-2.263310	-0.517290

Table S35 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating cis $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O\uparrow)_2(HCl)_1$ with $f2 = f4$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	1.857397	-0.270139	0.009176	0.175991	-1.703261	0.000000
F	-2.268885	0.336638	0.017949	-0.154508	2.019012	0.000000
O	-0.076527	1.954199	-0.090203	-0.154508	0.490957	-1.777742
O	-0.957264	-1.809596	-0.088751	-0.154508	0.490957	1.777742
H	1.038160	0.779411	-0.017434	-0.048893	-0.395524	-1.237842
H	-1.827489	-0.519502	-0.016430	-0.149062	1.283005	0.975938
H	-0.021185	-1.543404	-0.075444	-0.048893	-0.395524	1.237842
H	-0.951748	1.524962	-0.047609	-0.149062	1.283005	-0.975938
H	-0.064756	2.592713	0.629656	0.633376	0.577029	-2.329257
H	-1.058444	-2.428385	0.641367	0.633376	0.577029	2.329257

Table S36 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of the isomer of $(HF)_1(H_2O)_3$ with alternating relative orientations of dangling hydrogen atoms, i.e. $f2 = f4 = H_2O\uparrow$ and $f3 = H_2O\downarrow$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
F	1.116013	-1.511400	-0.067087	-0.045492	-1.680294	0.000000
O	-1.036954	1.602497	0.040530	0.040722	1.669327	0.000000
O	1.570343	0.944591	-0.027090	0.040722	-0.028261	1.705645
O	-1.597127	-1.071335	-0.020920	0.040722	-0.028261	-1.705645
H	-1.394019	0.688782	0.031897	0.031043	0.946770	0.888130
H	0.660822	1.325930	-0.004496	-0.006791	-0.857411	1.021002
H	-0.686095	-1.415198	-0.040616	0.031043	0.946770	-0.888130
H	1.370630	-0.576166	-0.043033	-0.006791	-0.857411	-1.021002
H	-1.466317	2.052493	-0.692217	0.866637	2.165477	0.000000
H	2.023823	1.293631	0.745440	-0.741527	-0.061994	2.264502
H	-2.043066	-1.572896	0.666652	-0.741527	-0.061994	-2.264502

Table S37 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of the isomer of $(HF)_1(H_2O)_3$* with adjacent dangling hydrogen atoms on the same side of the ring, i.e. $f2 = f3 = H_2O\uparrow$ and $f4 = H_2O\downarrow$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
F	-1.219985	-1.434729	-0.092602	-0.032045	-1.679520	0.075132	1.087532	-1.528731	0.071753
O	1.146780	1.539895	0.012339	0.031154	1.671304	-0.040317	-1.012140	1.616756	-0.035476
O	-1.499272	1.046384	-0.020749	1.705306	-0.056509	0.048874	1.587630	0.909692	-0.149430
O	1.502605	-1.171199	0.149493	-1.693818	0.000462	-0.157667	-1.619303	-1.047837	0.044291
H	1.458772	0.611103	0.011107	0.902700	0.930630	-0.011572	-1.380125	0.707536	-0.010822
H	-0.565777	1.364319	-0.010746	1.007177	-0.873053	0.057999	0.699698	1.326902	-0.059708
H	0.577552	-1.458980	0.051276	-0.875309	0.969099	-0.039387	-0.712532	-1.403001	0.057355
H	-1.406412	-0.483726	-0.059601	-1.027172	-0.840009	-0.050502	1.356728	-0.601231	-0.008772
H	1.597602	1.966767	-0.721041	0.044183	2.207512	0.759585	-1.482707	2.103911	0.645911
H	-1.908097	1.404651	0.772393	2.247305	-0.145301	-0.741130	2.141572	1.306263	0.528646
H	2.025326	-1.812216	-0.338632	-2.351623	-0.055249	0.541691	-2.059921	-1.510694	-0.673470

*The reactant and product of this structure are not equivalent

Table S38 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(H_2O)_4$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-1.367088	1.367088	0.008505	1.695984	0.000000	0.048116
O	1.367088	-1.367088	0.008505	-1.695984	0.000000	0.048116
O	1.367088	1.367088	-0.008505	0.000000	-1.695984	-0.048116
O	-1.367088	-1.367088	-0.008505	0.000000	1.695984	-0.048116
H	-1.506077	0.395454	-0.006204	0.928651	0.928651	0.000000
H	1.506077	-0.395454	-0.006204	-0.928651	0.928651	0.000000
H	0.395454	1.506077	0.006204	-0.928651	-0.928651	0.000000
H	-0.395454	-1.506077	0.006204	0.928651	-0.928651	0.000000
H	-1.879688	1.685418	0.756260	-2.272111	0.000000	-0.722449
H	1.879688	-1.685418	0.756260	2.272111	0.000000	-0.722449
H	1.685418	1.879688	-0.756260	0.000000	2.272111	0.722449
H	-1.685418	-1.879688	-0.756260	0.000000	-2.272111	0.722449

Table S39 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of the isomer of $(H_2O)_3(HCl)_1$ with alternating relative orientations of dangling hydrogen atoms, i.e. $f1 = f3 = H_2O\uparrow$ and $f2 = H_2O\downarrow$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	1.890387	0.161035	-0.054200	-0.110480	1.727512	0.000000
O	-2.330838	-0.330866	-0.018915	0.037912	-2.045862	0.000000
O	-0.813851	1.959009	0.017332	0.037912	-0.478912	1.855310
O	-0.155422	-1.929030	0.020064	0.037912	-0.478912	-1.855310
H	-1.908476	0.552806	-0.005650	0.061646	-1.385207	0.885379
H	0.087983	1.600249	-0.021869	-0.036109	0.391625	1.324424
H	-1.011963	-1.440535	0.004009	0.061646	-1.385207	-0.885379
H	0.994485	-0.833778	-0.004509	-0.036109	0.391625	-1.324424
H	-2.922098	-0.320971	-0.776683	-0.794571	-2.533426	0.000000
H	-0.802823	2.573620	0.756969	0.855891	-0.408814	2.360204
H	-0.172803	-2.461893	0.821279	0.855891	-0.408814	-2.360204

Table S40 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of the isomer of $(H_2O)_3(HCl)_1$* with adjacent dangling hydrogen atoms on the same side of the ring, i.e. $f1 = f2 = H_2O\uparrow$ and $f3 = H_2O\downarrow$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
Cl	-1.897426	0.148634	-0.063734	1.720572	-0.012114	0.112955	1.888554	0.171014	0.077618
O	2.346310	-0.324688	-0.040760	-2.033967	0.027730	0.162090	-2.330142	-0.338586	0.064378
O	0.798634	1.940953	0.179518	-0.464520	1.811642	-0.308378	-0.822722	1.958102	-0.031979
O	0.167614	-1.920554	0.020689	-0.506033	-1.850727	-0.114425	-0.146829	-1.913152	-0.235188
H	1.938123	0.564071	-0.017131	-1.371577	0.908510	0.006902	-1.905200	0.543663	0.038549
H	-0.102611	1.585730	0.110730	0.405102	1.278733	-0.202221	0.080164	1.603615	0.017074
H	1.021179	-1.427491	-0.002328	-1.402659	-0.853335	0.010952	-1.008192	-1.463047	-0.076344
H	-0.989779	-0.836305	-0.017131	0.372243	-1.342161	-0.032939	0.998237	-0.818263	-0.061024
H	2.928230	-0.322633	-0.805529	-2.343446	0.013482	1.075666	-2.947383	-0.304463	0.799945
H	0.776513	2.775499	-0.297054	-0.387987	2.565241	0.287266	-0.825381	2.512048	-0.818384
H	0.184127	-2.431344	0.836341	-0.485243	-2.273690	-0.980153	-0.100125	-2.631700	0.402982

*The reactant and product of this structure are not equivalent

Table S41 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating trans $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_2$ with $f1 = f2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-0.946972	2.251167	-0.118835	0.250686	1.174448	1.792921
Cl	1.533782	-1.325913	-0.109037	0.250686	-1.527598	-1.029651
Cl	-1.948841	-0.883121	0.096884	-0.250686	1.527598	-1.029651
O	1.695155	1.594536	0.135540	-0.250686	-1.174448	1.792921
H	-1.429949	1.412137	-0.076784	0.000000	0.000000	1.839569
H	1.655655	-0.002020	0.017750	0.000000	0.000000	-1.101219
H	-0.683535	-1.152024	0.013017	0.089507	1.435647	0.818959
H	0.773956	1.924168	0.056889	-0.089507	-1.435647	0.818959
H	-1.265385	2.682326	-0.917799	1.184525	1.343896	1.972555
H	2.019789	1.923356	0.979897	-1.184525	-1.343896	1.972555

Table S42 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of non-alternating cis $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_2(HCl)_2$ with $f1 = f2$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	-1.705800	1.527253	-0.366040	-1.566735	1.430228	-0.410700
Cl	1.976626	-0.830376	-0.115487	1.766948	-0.614357	-0.148215
Cl	-1.496941	-1.361170	0.143527	-1.217119	-1.381259	0.157899
O	0.879421	2.273045	0.183026	0.662217	2.023972	0.253177
H	-0.839660	1.918386	-0.125707	-0.474338	1.791070	-0.021704
H	0.721646	-1.137458	-0.020663	0.306043	-1.063514	0.004061
H	-1.646379	-0.055428	-0.080506	-1.573137	0.419552	-0.267237
H	1.374825	1.445672	0.087828	1.161823	1.146232	0.087317
H	-2.368279	2.015201	0.132629	-2.303449	1.790140	0.098051
H	1.214225	2.667514	0.993865	0.772114	2.208406	1.195070

Table S43 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating trans $(H_2O)_2(HCl)_2$*, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_2$ with $f1 = f3$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
Cl	2.353721	-0.144228	0.001047	-2.102647	0.119555	-0.000161	2.075724	-0.250623	0.020481
Cl	-2.353721	0.144228	-0.001047	2.102647	-0.119555	0.000161	-2.075724	0.250623	-0.020481
O	0.292046	2.013783	-0.095390	0.225282	1.888956	-0.101905	0.227460	1.872405	-0.138537
O	-0.292046	-2.013783	0.095390	-0.225282	-1.888956	0.101905	-0.227460	-1.872405	0.138537
H	0.585689	-1.595774	0.083914	1.057088	1.073046	-0.067001	-0.684842	1.328665	-0.115367
H	0.585689	-1.595774	0.083914	-1.057088	-1.073046	0.067001	0.684842	-1.328665	0.115367
H	1.475372	0.842494	-0.039206	-0.647209	1.371301	-0.090808	0.983501	1.127240	-0.098902
H	-1.475372	-0.842494	0.039206	0.647209	-1.371301	0.090808	-0.983501	-1.127240	0.098902
H	0.288924	2.622065	0.651316	0.260910	2.385240	0.728100	0.279960	2.375047	0.687663
H	-0.288924	-2.622065	-0.651316	-0.260910	-2.385240	-0.728100	-0.279960	-2.375047	-0.687663

*This structure does not undergo concerted proton transfer, but rather stepwise, and thus the product geometry corresponds to $(H_3O)_2^+(Cl)_2^-$

Table S44 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of alternating cis $(H_2O)_2(HCl)_2$*, i.e. $(H_2O\uparrow)_2(HCl)_2$ with $f1 = f3$

	Reactant			TS			Product		
	X	Y	Z	X	Y	Z	X	Y	Z
Cl	-1.603928	1.731714	-0.028885	-1.454012	1.519745	0.021928	1.534988	-1.324760	-0.109032
Cl	1.603928	-1.731714	-0.028885	1.454012	-1.519745	0.021928	-1.948002	-0.884673	0.096880
O	1.603928	1.255885	-0.023903	1.454012	1.228231	-0.115186	-0.948990	2.250577	-0.118834
O	-1.603928	-1.255885	-0.023903	-1.454012	-1.228231	-0.115186	1.693622	1.595839	0.135541
H	0.681277	1.561553	-0.042468	1.505428	0.065707	-0.062528	0.772180	1.924779	0.056858
H	-0.681277	-1.561553	-0.042468	-1.505428	-0.065707	-0.062528	-0.682493	-1.152597	0.013005
H	-1.652087	0.411661	-0.014597	0.463216	1.445373	-0.089773	-1.431263	1.411143	-0.076834
H	1.652087	-0.411661	-0.014597	-0.463216	-1.445373	-0.089773	1.655581	-0.000747	0.017735
H	1.997394	1.691712	0.739338	1.835035	1.581581	0.701014	-1.267809	2.681557	-0.917729
H	-1.997394	-1.691712	0.739338	-1.835035	-1.581581	0.701014	2.017983	1.924906	0.979906

*This structure does not undergo concerted proton transfer, but rather stepwise, and thus the product geometry corresponds to $(H_3O)_2^+(Cl)_2^-$

Table S45 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(H_2O)_1(HCl)_3$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
O	0.258591	-2.350154	0.281660	1.278912	-1.543145	0.000000
Cl	-0.094942	2.171150	0.168078	-0.258178	1.786714	0.000000
Cl	-2.458027	-0.520910	-0.178708	-0.258178	-0.465177	2.144935
Cl	2.413064	-0.304003	-0.197733	-0.258178	-0.465177	-2.144935
H	-0.617677	-1.955005	0.156906	0.735590	-1.232602	0.834229
H	0.885361	1.339577	0.023566	-0.321411	0.644734	-1.202164
H	-1.686847	0.506637	-0.066557	-0.321411	0.644734	1.202164
H	1.497837	-1.223956	0.018582	0.735590	-1.232602	-0.834229
H	0.230997	-2.752063	1.156381	2.107399	-1.037239	0.000000

Table S46 Cartesian coordinates (in Å) for the MP2/haTZ optimized structures of $(HCl)_4$

	Reactant/Product			TS		
	X	Y	Z	X	Y	Z
Cl	-1.735253	1.735253	0.516155	0.000000	2.104451	0.418518
Cl	-1.735253	-1.735253	-0.516155	0.000000	-2.104451	0.418518
Cl	1.735253	-1.735253	0.516155	-2.104451	0.000000	-0.418518
Cl	1.735253	1.735253	-0.516155	2.104451	0.000000	-0.418518
H	-0.503393	1.841239	0.155391	1.094128	1.094128	0.000000
H	-1.841239	-0.503393	-0.155391	-1.094128	-1.094128	0.000000
H	0.503393	-1.841239	0.155391	1.094128	-1.094128	0.000000
H	1.841239	0.503393	-0.155391	-1.094128	1.094128	0.000000

4 Harmonic Vibrational Frequencies

Table S47 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_{3h}}$ reactant and $\mathbf{D_{3h}}$ TS of $(HF)_3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a'	3714	0.0	a'_1	2085	0.0
a'	979	0.0	a'_1	726	0.0
a'	216	0.0	a'_2	$1695i$	0.0
e'	3834	710.6	e'	1787	3123.0
e'	604	352.8	e'	1541	430.5
e'	196	24.8	e'	562	0.9
a''	706	389.2	a''_2	1306	307.3
e''	508	0.0	e''	1043	0.0

Table S48 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_s}$ reactant and $\mathbf{C_{2v}}$ TS of $(HF)_2(HCl)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a'	3882	664.8	a_1	1929	769.1
a'	3812	310.2	a_1	1652	4048.4
a'	2898	247.4	a_1	1216	229.8
a'	809	109.6	a_1	627	20.6
a'	510	252.8	a_1	423	46.6
a'	420	148.0	a_2	876	0.0
a'	199	7.2	b_1	1168	163.3
a'	143	7.6	b_1	894	10.5
a'	127	15.7	b_2	1953	2363.5
a''	595	219.6	b_2	1329	573.0
a''	418	21.4	b_2	446	2.9
a''	320	3.0	b_2	$1478i$	6.9

Table S49 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_s}$ reactant and $\mathbf{C_{2v}}$ TS of $(HF)_1(HCl)_2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a′	3887	498.9	a_1	1860	2344.9
a′	2925	402.6	a_1	1551	852.4
a′	2892	156.4	a_1	1107	145.6
a′	644	76.9	a_1	497	20.8
a′	394	126.9	a_1	337	0.0
a′	352	111.0	a_2	838	0.0
a′	141	3.0	b_1	994	77.8
a′	126	7.9	b_1	733	0.6
a′	91	7.2	b_2	1320	5646.1
a″	453	129.2	b_2	1145	357.7
a″	314	2.6	b_2	406	38.0
a″	262	2.5	b_2	$1509i$	55.8

Table S50 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of $(HF)_2(H_2O)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3905	155.8	a′	3839	131.1
a	3782	655.5	a′	2402	1374.7
a	3749	74.3	a′	1820	637.3
a	3351	1076.9	a′	1567	337.0
a	1635	70.6	a′	1391	972.1
a	1121	112.6	a′	1184	64.3
a	892	200.5	a′	659	84.2
a	698	278.6	a′	546	200.2
a	615	68.5	a′	511	5.9
a	501	189.6	a″	2141	2578.5
a	346	72.6	a″	1604	213.2
a	291	13.2	a″	1277	287.8
a	224	83.6	a″	585	123.2
a	218	5.8	a″	544	39.3
a	126	16.4	a″	$1152i$	179.9

Table S51 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_2}$ TS of trans $(HF)_1(H_2O)_2$, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3915	126.6	a	3861	21.9
a	3896	119.7	a	2271	1814.3
a	3744	165.0	a	1873	1171.9
a	3622	478.4	a	1566	3.5
a	3416	918.5	a	1247	100.7
a	1647	17.1	a	739	19.9
a	1635	114.2	a	669	112.6
a	1069	118.1	a	547	45.6
a	886	164.2	a	498	90.0
a	674	202.2	b	3860	159.9
a	515	162.7	b	1980	967.8
a	383	77.3	b	1612	463.4
a	322	54.9	b	1593	462.6
a	293	84.4	b	1191	2137.2
a	278	1.8	b	603	304.0
a	211	12.4	b	592	3.1
a	190	142.7	b	445	46.9
a	138	10.0	b	$1326i$	235.6

Table S52 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of cis $(HF)_1(H_2O)_2$, i.e. $(HF)_1(H_2O{\uparrow})_2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3923	126.9	a′	3866	96.3
a	3900	123.6	a′	2270	1793.7
a	3749	161.0	a′	1921	1025.6
a	3650	391.7	a′	1628	88.4
a	3425	958.3	a′	1521	270.9
a	1646	55.5	a′	1215	66.6
a	1639	82.5	a′	674	77.0
a	1055	133.8	a′	599	128.8
a	879	163.6	a′	513	51.5
a	621	182.7	a′	471	29.3
a	464	140.6	a″	3864	76.5
a	387	33.4	a″	1971	944.9
a	343	103.2	a″	1561	894.1
a	279	9.3	a″	1170	2030.8
a	268	107.5	a″	773	71.7
a	205	6.3	a″	585	232.3
a	144	37.8	a″	496	8.4
a	102	103.7	a″	$1339i$	243.7

Table S53 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of $(HF)_1(H_2O)_1(HCl)_1$*

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3905	160.6	a	3811	161.1	a	3903	171.3
a	3768	76.1	a	2816	1730.3	a	3850	560.7
a	3471	1048.3	a	1989	2385.1	a	3748	50.1
a	2851	341.4	a	1804	647.9	a	2544	1080.9
a	1632	61.3	a	1608	115.7	a	1632	64.8
a	1019	151.9	a	1441	86.5	a	830	13.6
a	838	139.6	a	1243	594.2	a	640	122.8
a	484	74.2	a	997	539.1	a	542	206.7
a	426	177.2	a	964	24.9	a	469	104.5
a	388	22.8	a	618	80.1	a	444	141.4
a	321	79.9	a	553	47.0	a	286	47.9
a	274	4.4	a	447	35.8	a	216	105.7
a	171	67.0	a	414	101.3	a	186	8.5
a	142	12.9	a	349	171.4	a	153	2.8
a	89	11.9	a	$877i$	902.8	a	132	9.3

*The reactant and product of this structure are not equivalent

Table S54 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of $(H_2O)_3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3909	125.8	a′	3870	69.7
a	3909	73.2	a′	3866	55.9
a	3905	116.0	a′	2021	1.3
a	3654	484.8	a′	1701	95.2
a	3644	524.8	a′	1621	114.0
a	3582	11.5	a′	1404	353.3
a	1668	10.5	a′	1230	4238.4
a	1644	70.8	a′	739	0.3
a	1642	93.5	a′	668	0.0
a	860	9.9	a′	562	12.3
a	669	297.0	a′	497	4.3
a	574	153.4	a′	435	65.3
a	447	131.7	a″	3869	50.8
a	359	37.7	a″	1587	23.4
a	346	99.9	a″	1550	14.4
a	241	37.0	a″	1237	4629.5
a	219	6.0	a″	765	18.6
a	202	124.5	a″	686	1.2
a	189	21.3	a″	554	13.2
a	182	73.5	a″	444	31.5
a	174	66.6	a″	$1814i$	0.1

Table S55 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_2}$ TS of trans $(H_2O)_2(HCl)_1$, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3910	143.9	a	3829	46.6
a	3889	120.8	a	2702	2853.5
a	3760	104.4	a	1830	351.0
a	3609	352.4	a	1560	35.3
a	2512	1154.4	a	948	111.2
a	1643	25.3	a	716	7.3
a	1631	85.9	a	592	32.5
a	876	35.7	a	451	105.4
a	694	144.3	a	327	85.3
a	581	94.5	b	3827	207.5
a	433	117.1	b	2564	1046.8
a	355	108.8	b	1641	285.1
a	275	64.4	b	1574	93.6
a	247	81.3	b	1040	877.9
a	209	10.9	b	574	676.6
a	186	19.0	b	464	89.6
a	175	112.3	b	407	7.0
a	96	5.6	b	$643i$	561.7

Table S56 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of cis $(H_2O)_2(HCl)_1$, i.e. $(H_2O\uparrow)_2(HCl)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3918	145.2	a′	3834	147.5
a	3893	123.5	a′	2699	2865.7
a	3764	102.1	a′	1891	272.4
a	3638	301.6	a′	1629	5.3
a	2517	1156.8	a′	1444	209.7
a	1646	46.6	a′	925	106.0
a	1632	73.4	a′	610	13.0
a	845	38.6	a′	501	76.0
a	674	110.3	a′	443	70.6
a	550	124.6	a′	327	84.7
a	382	32.4	a″	3832	94.8
a	373	157.2	a″	2556	1045.6
a	270	99.0	a″	1605	294.7
a	236	87.9	a″	1028	824.4
a	203	4.2	a″	794	385.8
a	185	16.7	a″	473	339.4
a	110	95.7	a″	400	6.8
a	94	16.7	a″	$687i$	615.2

Table S57 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of $(H_2O)_1(HCl)_2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3902	157.1	a′	3780	180.1
a	3761	74.6	a′	2542	2146.3
a	2882	452.3	a′	1684	338.3
a	2611	856.1	a′	1300	328.4
a	1628	51.3	a′	1059	79.2
a	749	39.9	a′	785	6.2
a	591	58.3	a′	432	66.4
a	412	68.7	a′	406	102.0
a	369	150.9	a′	331	17.8
a	305	17.2	a″	2208	2429.1
a	257	63.5	a″	1581	47.4
a	182	32.1	a″	897	1107.2
a	166	53.0	a″	464	159.2
a	105	1.5	a″	382	368.2
a	92	8.1	a″	$690i$	1703.8

Table S58 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_{3h}}$ reactant and $\mathbf{D_{3h}}$ TS of $(HCl)_3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a'	2888	0.0	a'_1	1321	0.0
a'	515	0.0	a'_1	412	0.0
a'	102	0.0	a'_2	$1504i$	0.0
e'	2928	457.0	e'	1323	5028.1
e'	315	73.9	e'	992	310.6
e'	87	5.3	e'	313	1.7
a''	316	50.3	a''_2	820	21.1
e''	245	0.0	e''	702	0.0

Table S59 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_{4h}}$ reactant and $\mathbf{D_{4h}}$ TS of $(HF)_4$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a_g	3360	0.0	a_{1g}	1825	0.0
a_g	1151	0.0	a_{1g}	620	0.0
a_g	214	0.0	a_{2g}	$1441i$	0.0
b_g	3646	0.0	b_{1g}	1217	0.0
b_g	696	0.0	b_{1g}	613	0.0
b_g	302	0.0	b_{2g}	2137	0.0
b_g	97	0.0	b_{2g}	163	0.0
e_g	713	0.0	e_g	1139	0.0
a_u	818	488.2	a_{2u}	1244	415.4
b_u	669	0.0	b_{1u}	71	0.0
b_u	44	0.0	b_{2u}	1090	0.0
e_u	3566	1881.6	e_u	1739	5548.3
e_u	898	335.6	e_u	1478	1.7
e_u	284	51.4	e_u	639	0.6

Table S60 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_s}$ reactant and $\mathbf{C_{2v}}$ TS of $(HF)_3(HCl)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a′	3726	317.2	a_1	2137	37.7
a′	3684	1791.5	a_1	1721	490.5
a′	3564	568.9	a_1	1649	6449.5
a′	2757	583.0	a_1	1191	188.3
a′	993	98.1	a_1	603	8.3
a′	770	265.0	a_1	437	82.3
a′	705	114.5	a_1	137	0.1
a′	522	14.5	a_2	1100	0.0
a′	274	15.8	a_2	918	0.0
a′	240	31.1	b_1	1167	243.7
a′	179	19.0	b_1	942	35.6
a′	157	8.0	b_1	53	0.0
a′	73	0.1	b_2	1886	4872.7
a″	721	297.7	b_2	1417	143.0
a″	646	0.5	b_2	1043	108.6
a″	547	41.8	b_2	645	0.1
a″	441	7.3	b_2	450	29.5
a″	30	0.1	b_2	$1243i$	0.8

Table S61 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of $(HF)_3(H_2O)_1$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3891	139.6	a′	3845	137.7
a	3665	424.0	a′	2387	541.0
a	3605	984.7	a′	1969	3086.5
a	3428	1130.9	a′	1802	1365.7
a	2941	1603.5	a′	1523	28.3
a	1653	49.6	a′	1357	383.3
a	1260	89.8	a′	1204	127.6
a	1026	179.9	a′	609	3.0
a	965	255.6	a′	507	232.8
a	815	198.3	a′	473	31.0
a	800	130.1	a′	146	0.5
a	712	36.7	a′	65	5.6
a	637	60.5	a″	2197	4003.4
a	432	71.5	a″	1647	111.2
a	361	22.1	a″	1370	41.6
a	297	106.6	a″	1155	1.6
a	290	39.2	a″	1048	236.5
a	248	20.2	a″	760	206.6
a	196	5.2	a″	627	104.2
a	94	0.4	a″	557	110.9
a	44	3.7	a″	$850i$	270.6

Table S62 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_s}$ reactant and $\mathbf{C_{2v}}$ TS of non-alternating $(HF)_2(HCl)_2$, i.e. $f1 = f2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a′	3781	672.6	a_1	1775	6200.1
a′	3683	991.3	a_1	1611	259.1
a′	2831	658.7	a_1	1122	22.9
a′	2778	508.5	a_1	911	67.8
a′	869	132.2	a_1	625	0.2
a′	650	130.8	a_1	417	72.8
a′	568	75.1	a_1	348	3.3
a′	429	3.8	a_2	916	0.0
a′	244	13.5	a_2	35	0.0
a′	174	24.7	b_1	1123	128.8
a′	147	6.9	b_1	930	51.4
a′	115	7.1	b_1	770	2.9
a′	57	0.2	b_2	2087	536.1
a″	648	175.4	b_2	1308	4955.8
a″	517	43.5	b_2	1174	1943.6
a″	418	15.6	b_2	473	31.5
a″	354	5.8	b_2	112	0.0
a″	19	0.1	b_2	$1281i$	126.0

Table S63 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_{2h}}$ reactant and $\mathbf{D_{2h}}$ TS of alternating $(HF)_2(HCl)_2$, i.e. $f1 = f3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a_g	3753	0.0	a_g	1901	0.0
a_g	2811	0.0	a_g	1501	0.0
a_g	776	0.0	a_g	443	0.0
a_g	428	0.0	a_g	114	0.0
a_g	179	0.0	b_{1g}	939	0.0
a_g	134	0.0	b_{2g}	906	0.0
a_g	53	0.0	b_{3g}	953	0.0
b_g	504	0.0	b_{3g}	478	0.0
b_g	399	0.0	b_{3g}	$1363i$	0.0
a_u	538	209.7	a_u	896	0.0
a_u	401	10.3	b_{1u}	1320	8023.5
a_u	18	0.4	b_{1u}	1047	1607.7
b_u	3776	1736.9	b_{1u}	469	171.4
b_u	2838	1050.5	b_{2u}	1772	4776.7
b_u	647	204.4	b_{2u}	1318	177.5
b_u	533	102.3	b_{2u}	431	28.8
b_u	183	20.1	b_{3u}	978	145.2
b_u	149	26.9	b_{3u}	35	0.2

Table S64 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant, $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of non-alternating $(HF)_2(H_2O)_1(HCl)_1$*, i.e. $f1 = f2$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3885	181.4	a	3824	154.6	a	3883	134.5
a	3682	414.9	a	2807	2118.3	a	3720	563.9
a	3581	839.4	a	2018	1718.9	a	3651	904.6
a	3113	1792.6	a	1771	211.7	a	3555	830.1
a	2758	464.1	a	1681	1771.5	a	2182	1942.3
a	1642	35.2	a	1525	3092.3	a	1644	37.8
a	1178	140.4	a	1476	534.5	a	1006	13.0
a	966	146.2	a	1319	388.6	a	863	194.8
a	848	169.6	a	1166	80.0	a	760	138.0
a	744	86.7	a	1136	26.0	a	708	177.6
a	619	75.8	a	960	18.2	a	687	110.5
a	505	52.4	a	900	152.8	a	588	18.0
a	458	18.3	a	636	22.1	a	571	27.6
a	392	82.7	a	605	225.5	a	379	60.4
a	340	12.8	a	575	7.7	a	273	110.9
a	263	42.1	a	473	0.4	a	257	23.1
a	230	64.8	a	405	83.0	a	228	15.6
a	160	18.6	a	326	152.3	a	205	33.3
a	142	7.8	a	123	0.2	a	164	4.3
a	71	0.8	a	51	5.2	a	74	0.4
a	30	2.4	a	$1055i$	1195.9	a	31	2.3

*The reactant and product of this structure are not equivalent

Table S65 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of alternating $(HF)_2(H_2O)_1(HCl)_1$, i.e. $f1 = f3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3897	142.6	a′	3828	162.6
a	3744	785.8	a′	2608	178.4
a	3672	555.4	a′	2255	5234.9
a	3189	1387.7	a′	1795	231.9
a	2651	923.4	a′	1352	345.8
a	1651	54.9	a′	1128	5.1
a	1139	96.1	a′	928	71.6
a	936	141.8	a′	458	87.3
a	751	123.9	a′	443	83.0
a	641	152.1	a′	365	102.6
a	559	100.6	a′	112	2.3
a	532	21.2	a′	38	6.1
a	503	1.5	a″	2514	3877.4
a	399	67.4	a″	1785	60.4
a	327	23.7	a″	1600	50.8
a	265	92.7	a″	1114	295.8
a	201	24.1	a″	918	9.1
a	181	27.9	a″	894	37.1
a	158	2.2	a″	589	42.7
a	71	0.2	a″	408	68.9
a	30	5.2	a″	$107i$	3.4

Table S66 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_2}$ TS of non-alternating trans $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_1(H_2O\downarrow)_1$ with $f1 = f2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3904	122.7	a	3861	50.8
a	3887	112.4	a	2427	3878.8
a	3680	329.3	a	1829	146.8
a	3541	1192.8	a	1590	17.7
a	3412	684.6	a	1442	76.2
a	2900	1786.7	a	1073	115.2
a	1670	19.4	a	719	26.5
a	1645	78.9	a	641	0.6
a	1262	118.3	a	615	6.6
a	1043	152.3	a	512	146.3
a	894	262.5	a	455	142.9
a	863	49.1	a	62	2.6
a	773	96.6	b	3860	159.9
a	609	85.5	b	2438	122.6
a	484	62.5	b	1710	436.5
a	391	19.1	b	1579	144.3
a	360	95.5	b	1461	4975.3
a	344	66.1	b	1248	508.4
a	279	55.7	b	1205	244.8
a	250	50.4	b	669	153.2
a	227	79.9	b	584	34.4
a	188	5.1	b	413	56.1
a	91	1.1	b	137	0.6
a	44	1.9	b	$926i$	117.8

Table S67 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of non-alternating cis $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_2$ with $f1 = f2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3913	123.6	a′	3868	136.9
a	3890	112.5	a′	2419	3938.6
a	3684	332.2	a′	1886	100.8
a	3548	1220.3	a′	1695	17.2
a	3451	562.9	a′	1453	90.8
a	2920	1790.7	a′	1393	267.0
a	1672	32.6	a′	1220	61.9
a	1654	63.2	a′	1038	80.9
a	1253	128.8	a′	646	17.2
a	1028	164.5	a′	630	14.6
a	875	195.1	a′	592	88.8
a	801	100.6	a′	456	165.8
a	767	88.1	a′	438	63.8
a	572	52.0	a″	3865	61.9
a	505	68.5	a″	2426	97.5
a	396	117.3	a″	1689	439.3
a	365	55.5	a″	1455	4995.0
a	313	68.0	a″	1209	605.4
a	275	34.0	a″	818	68.5
a	243	23.1	a″	606	117.2
a	189	13.0	a″	453	20.7
a	172	88.6	a″	136	0.1
a	86	3.0	a″	52	3.0
a	35	3.6	a″	$953i$	131.0

Table S68 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_I}$ reactant and $\mathbf{C_{2h}}$ TS of alternating trans $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O{\uparrow})_1(H_2O{\downarrow})_1$ with $f1 = f3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a_g	3895	0.0	a_g	3865	0.0
a_g	3605	0.0	a_g	2148	0.0
a_g	3098	0.0	a_g	1830	0.0
a_g	1660	0.0	a_g	1388	0.0
a_g	1195	0.0	a_g	568	0.0
a_g	945	0.0	a_g	488	0.0
a_g	650	0.0	a_g	152	0.0
a_g	425	0.0	b_g	1678	0.0
a_g	327	0.0	b_g	1200	0.0
a_g	291	0.0	b_g	726	0.0
a_g	198	0.0	b_g	653	0.0
a_g	90	0.0	b_g	$976i$	0.0
a_u	3895	247.6	a_u	1989	4519.0
a_u	3609	894.0	a_u	1594	331.0
a_u	3203	3139.5	a_u	1186	22.4
a_u	1657	110.2	a_u	651	53.5
a_u	1102	275.1	a_u	551	215.0
a_u	964	275.4	b_u	3864	209.5
a_u	721	201.2	b_u	1822	3389.4
a_u	434	119.7	b_u	1677	1818.3
a_u	332	62.6	b_u	1387	903.9
a_u	294	181.6	b_u	564	425.5
a_u	228	43.0	b_u	485	78.2
a_u	43	14.4	b_u	74	23.4

Table S69 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_2}$ reactant and $\mathbf{C_{2v}}$ TS of alternating cis $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O{\uparrow})_2$ with $f1 = f3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3897	58.4	a_1	3868	89.2
a	3607	0.0	a_1	2148	0.1
a	3104	0.3	a_1	1839	16.9
a	1663	46.0	a_1	1425	263.4
a	1191	1.1	a_1	568	0.0
a	973	277.2	a_1	498	1.9
a	644	31.5	a_1	152	0.5
a	414	27.3	a_1	78	18.3
a	329	1.5	a_2	1671	0.0
a	294	8.1	a_2	1190	0.0
a	197	0.2	a_2	723	0.0
a	90	0.8	a_2	638	0.0
a	46	9.5	a_2	$978i$	0.0
b	3897	188.2	b_1	1992	4451.7
b	3611	885.5	b_1	1605	383.3
b	3209	3129.3	b_1	1176	22.3
b	1655	64.4	b_1	672	49.8
b	1099	241.6	b_1	550	217.0
b	925	42.6	b_2	3866	117.1
b	708	167.0	b_2	1824	3363.1
b	445	85.6	b_2	1663	1939.3
b	330	51.4	b_2	1342	548.5
b	279	187.4	b_2	564	423.8
b	227	36.5	b_2	468	81.3

Table S70 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_s}$ reactant and $\mathbf{C_{2v}}$ TS of $(HF)_1(HCl)_3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a′	3804	799.6	a_1	1884	1472.7
a′	2874	537.4	a_1	1426	41.8
a′	2854	806.8	a_1	1255	5469.7
a′	2810	262.8	a_1	1072	0.3
a′	700	62.5	a_1	418	23.9
a′	521	61.6	a_1	359	0.7
a′	484	68.2	a_1	90	0.0
a′	359	0.2	a_2	900	0.0
a′	176	8.4	a_2	754	0.0
a′	135	14.4	b_1	943	79.1
a′	114	7.5	b_1	776	10.1
a′	104	3.2	b_1	14	0.0
a′	43	0.1	b_2	1259	8198.4
a″	497	108.5	b_2	1040	830.2
a″	384	16.9	b_2	826	146.0
a″	339	14.4	b_2	486	134.0
a″	327	0.1	b_2	342	5.7
a″	9	0.1	b_2	$1396i$	96.0

Table S71 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant, $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of non-alternating $(HF)_1(H_2O)_1(HCl)_2$*, i.e. $f3 = f4$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3890	183.6	a	3809	171.5	a	3891	133.8
a	3709	279.6	a	2797	2014.3	a	3780	774.6
a	3295	1432.0	a	2250	2493.7	a	3688	354.8
a	2818	716.9	a	1746	1009.9	a	2741	870.1
a	2719	638.8	a	1717	2265.4	a	2361	1529.1
a	1641	38.6	a	1614	1742.7	a	1644	42.6
a	1077	124.5	a	1352	593.7	a	884	14.5
a	902	130.4	a	1141	125.9	a	717	103.4
a	610	26.1	a	1029	333.7	a	673	100.2
a	557	99.5	a	941	48.3	a	573	113.8
a	481	24.3	a	849	950.1	a	523	76.8
a	422	28.3	a	809	201.3	a	463	9.4
a	370	61.6	a	752	5.8	a	395	6.9
a	356	28.7	a	557	33.0	a	348	59.6
a	310	9.1	a	476	18.8	a	247	111.5
a	215	71.1	a	393	78.7	a	212	6.5
a	169	34.6	a	345	137.6	a	188	21.5
a	133	5.0	a	291	68.2	a	155	11.4
a	113	5.6	a	90	1.1	a	122	8.1
a	55	0.6	a	28	4.7	a	57	0.2
a	20	4.2	a	$378i$	319.0	a	20	2.8

*The reactant and product of this structure are not equivalent

Table S72 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of alternating $(HF)_1(H_2O)_1(HCl)_2$, i.e. $f2 = f4$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3881	179.1	a′	3787	171.4
a	3709	1262.7	a′	2500	1740.3
a	3691	4.8	a′	1740	2610.4
a	2826	607.0	a′	1685	37.1
a	2366	1510.1	a′	1356	9.6
a	1635	30.4	a′	1238	255.2
a	888	32.2	a′	970	58.6
a	726	52.7	a′	440	4.4
a	654	136.3	a′	410	63.5
a	564	76.7	a′	346	85.9
a	562	79.6	a′	103	0.3
a	438	36.2	a′	37	5.8
a	415	13.5	a″	2240	4915.4
a	326	66.6	a″	1617	23.5
a	223	68.0	a″	1031	78.6
a	202	36.6	a″	929	0.2
a	191	10.8	a″	808	148.2
a	146	15.2	a″	505	71.8
a	130	3.0	a″	489	2.6
a	53	0.5	a″	381	537.0
a	18	1.1	a″	$918i$	2823.3

Table S73 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant, $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of non-alternating trans $(HF)_1(H_2O)_2(HCl)_1$*, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$ with $f2 = f3$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3897	161.3	a	3858	115.9	a	3904	129.5
a	3890	115.2	a	3839	142.4	a	3872	111.0
a	3710	294.5	a	3117	1551.5	a	3714	400.9
a	3476	759.6	a	2262	1439.2	a	3646	1066.5
a	3113	1544.2	a	1991	4295.1	a	3413	646.0
a	2672	888.4	a	1777	191.1	a	2008	2372.8
a	1664	24.9	a	1668	528.0	a	1661	52.2
a	1637	57.6	a	1621	22.3	a	1640	49.5
a	1168	109.0	a	1447	298.9	a	1062	18.6
a	985	145.0	a	1320	456.1	a	875	94.8
a	828	110.9	a	1073	20.0	a	788	103.9
a	630	52.0	a	1023	1012.6	a	726	129.4
a	517	56.4	a	982	30.3	a	604	106.0
a	499	17.9	a	848	139.5	a	554	42.7
a	448	70.8	a	671	31.7	a	451	49.4
a	358	79.8	a	538	33.9	a	362	12.6
a	327	0.2	a	494	114.1	a	333	159.5
a	303	121.7	a	451	136.5	a	278	21.9
a	246	43.4	a	430	72.3	a	222	148.5
a	203	82.0	a	353	76.4	a	212	26.5
a	169	24.9	a	297	116.2	a	201	20.5
a	134	4.9	a	107	3.2	a	159	5.1
a	70	0.7	a	41	3.4	a	72	1.0
a	32	1.9	a	$338i$	288.4	a	33	1.5

*The reactant and product of this structure are not equivalent

Table S74 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant, $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of non-alternating cis $(HF)_1(H_2O)_2(HCl)_1$*, i.e. $(HF)_1(H_2O{\uparrow})_2(HCl)_1$ with $f2 = f3$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3906	163.5	a	3864	120.2	a	3916	130.2
a	3893	115.2	a	3840	127.1	a	3876	111.5
a	3713	300.1	a	3086	1629.9	a	3721	410.4
a	3511	688.3	a	2320	1493.6	a	3654	1053.6
a	3126	1537.0	a	1977	4338.6	a	3464	554.9
a	2678	897.2	a	1819	473.2	a	2043	2312.8
a	1671	36.9	a	1693	192.2	a	1661	10.2
a	1642	43.7	a	1630	311.1	a	1646	86.7
a	1163	116.4	a	1394	57.8	a	1036	27.8
a	967	143.1	a	1330	871.2	a	842	76.5
a	748	112.9	a	1095	478.3	a	752	158.6
a	619	30.6	a	1054	26.3	a	700	56.8
a	507	33.0	a	975	29.3	a	598	113.1
a	492	19.7	a	820	131.4	a	520	26.9
a	451	104.4	a	703	55.0	a	460	49.9
a	343	140.0	a	537	122.4	a	371	111.4
a	337	19.1	a	481	14.6	a	306	100.1
a	282	51.5	a	442	95.1	a	266	6.6
a	239	26.9	a	425	81.5	a	214	84.5
a	168	24.5	a	345	116.5	a	201	10.8
a	148	87.7	a	301	85.7	a	161	6.4
a	132	5.7	a	107	3.0	a	132	95.4
a	66	1.1	a	28	4.9	a	65	6.5
a	19	3.9	a	$289i$	145.0	a	24	5.5

*The reactant and product of this structure are not equivalent

Table S75 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_2}$ TS of alternating trans $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O{\uparrow})_1(H_2O{\downarrow})_1(HCl)_1$ with $f2 = f4$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3886	158.9	a	3833	4.7
a	3885	125.2	a	2569	2285.2
a	3654	505.5	a	1938	3016.1
a	3619	337.2	a	1762	42.4
a	3235	1532.1	a	1596	153.5
a	2264	1678.6	a	1350	5.4
a	1651	33.4	a	975	18.4
a	1644	43.7	a	594	20.2
a	1110	113.1	a	572	72.9
a	938	92.5	a	430	15.2
a	898	111.2	a	347	112.0
a	745	72.4	a	124	0.2
a	642	126.2	b	3832	260.2
a	561	23.4	b	2434	3124.3
a	394	99.4	b	1664	121.2
a	383	27.2	b	1646	83.1
a	316	10.8	b	1340	259.9
a	276	116.3	b	1021	715.4
a	243	85.5	b	731	56.6
a	231	7.9	b	596	58.5
a	188	33.4	b	431	358.4
a	149	6.2	b	414	181.8
a	71	0.3	b	62	21.9
a	32	10.3	b	$552i$	644.8

Table S76 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of alternating cis $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O\uparrow)_2(HCl)_1$ with $f2 = f4$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3888	155.3	a′	3835	116.4
a	3886	128.1	a′	2571	2283.6
a	3656	501.8	a′	1940	2949.3
a	3621	333.0	a′	1770	75.5
a	3242	1525.0	a′	1601	182.9
a	2272	1668.3	a′	1365	183.2
a	1652	40.1	a′	966	24.3
a	1643	36.1	a′	608	22.8
a	1109	102.6	a′	572	70.2
a	931	103.6	a′	435	17.9
a	895	125.4	a′	347	110.9
a	737	61.1	a′	125	0.5
a	634	109.7	a′	65	17.8
a	556	45.9	a″	3834	145.6
a	400	72.9	a″	2437	3126.5
a	375	45.5	a″	1658	130.7
a	315	8.9	a″	1643	55.7
a	272	84.9	a″	1312	90.4
a	238	120.5	a″	1018	711.9
a	228	4.9	a″	729	53.7
a	188	33.0	a″	586	63.0
a	149	5.6	a″	425	506.5
a	71	1.0	a″	409	36.7
a	34	6.4	a″	$554i$	650.2

Table S77 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of the isomer of $(HF)_1(H_2O)_3$ with alternating relative orientations of dangling hydrogen atoms, i.e. $f2 = f4 = H_2O\uparrow$ and $f3 = H_2O\downarrow$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3907	108.9	a′	3878	69.1
a	3897	95.2	a′	3858	91.2
a	3892	106.7	a′	2271	1486.9
a	3652	372.4	a′	1845	27.7
a	3506	781.4	a′	1660	721.8
a	3396	977.2	a′	1564	127.9
a	3117	1375.3	a′	1502	3188.7
a	1680	11.2	a′	1255	54.4
a	1658	56.7	a′	683	12.1
a	1647	81.1	a′	589	73.5
a	1170	89.4	a′	542	55.2
a	992	147.3	a′	501	168.6
a	890	148.1	a′	399	41.1
a	805	126.8	a′	139	1.2
a	635	110.6	a′	71	4.1
a	484	41.7	a″	3878	82.5
a	435	33.8	a″	1914	4040.5
a	379	39.6	a″	1716	538.2
a	351	101.0	a″	1598	145.9
a	324	6.3	a″	1459	68.6
a	271	141.9	a″	1121	478.2
a	256	58.0	a″	741	96.9
a	238	35.9	a″	731	231.2
a	211	88.4	a″	599	11.4
a	194	6.7	a″	521	387.3
a	86	2.2	a″	428	57.5
a	47	2.8	a″	$1100i$	465.3

Table S78 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant, $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of the isomer of $(HF)_1(H_2O)_3$* with adjacent dangling hydrogen atoms on the same side of the ring, i.e. $f2 = f3 = H_2O\uparrow$ and $f4 = H_2O\downarrow$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3912	111.4	a	3881	66.7	a	3904	103.5
a	3901	98.4	a	3876	87.2	a	3902	107.7
a	3891	103.6	a	3863	82.7	a	3895	97.9
a	3653	376.0	a	2272	1507.8	a	3653	371.7
a	3531	723.7	a	1920	3814.0	a	3503	782.9
a	3404	934.3	a	1869	225.2	a	3420	923.9
a	3116	1421.8	a	1737	234.1	a	3128	1372.9
a	1680	20.2	a	1678	760.8	a	1682	25.0
a	1661	31.9	a	1614	318.5	a	1670	44.4
a	1654	98.0	a	1550	75.3	a	1650	76.8
a	1167	101.5	a	1492	3156.5	a	1164	101.3
a	992	150.9	a	1361	388.7	a	975	163.6
a	876	124.8	a	1235	39.6	a	864	133.3
a	755	156.4	a	1092	337.7	a	750	114.1
a	595	31.5	a	825	183.5	a	636	69.3
a	505	112.7	a	726	43.0	a	545	88.8
a	453	3.1	a	662	151.2	a	421	78.6
a	386	42.6	a	614	69.6	a	378	55.3
a	347	168.3	a	579	31.6	a	334	69.5
a	324	2.8	a	525	309.3	a	299	57.7
a	263	70.4	a	505	168.2	a	266	75.0
a	232	13.6	a	497	83.1	a	257	31.3
a	229	111.4	a	435	26.1	a	237	35.9
a	194	8.0	a	402	65.5	a	213	93.6
a	175	75.7	a	138	0.4	a	193	9.7
a	81	1.6	a	58	9.9	a	83	0.7
a	36	10.3	a	$1108i$	478.2	a	36	7.7

*The reactant and product of this structure are not equivalent

Table S79 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{S_4}$ reactant and $\mathbf{D_{2d}}$ TS of $(H_2O)_4$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3901	0.0	a_1	3872	0.0
a	3401	0.0	a_1	1830	0.0
a	1689	0.0	a_1	622	0.0
a	984	0.0	a_1	571	0.0
a	408	0.0	a_1	81	0.0
a	289	0.0	a_2	1634	0.0
a	208	0.0	a_2	576	0.0
a	50	0.0	a_2	$1653i$	0.0
b	3900	114.3	b_1	1387	0.0
b	3535	18.9	b_1	743	0.0
b	1647	83.8	b_1	603	0.0
b	754	179.7	b_2	3873	110.0
b	436	18.5	b_2	1581	207.3
b	260	0.7	b_2	1506	0.1
b	214	56.0	b_2	394	34.8
b	80	2.3	b_2	145	2.7
e	3900	124.8	e	3872	61.5
e	3496	1385.1	e	1633	557.7
e	1661	52.0	e	1534	87.4
e	820	168.9	e	1105	6393.0
e	451	49.2	e	684	186.1
e	256	221.6	e	634	16.7
e	239	28.4	e	426	20.4

Table S80 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of the isomer of $(H_2O)_3(HCl)_1$ with alternating relative orientations of dangling hydrogen atoms, i.e. $f1 = f3 = H_2O\uparrow$ and $f2 = H_2O\downarrow$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3898	138.9	a′	3856	98.4
a	3897	107.9	a′	3844	126.8
a	3879	102.7	a′	2851	1971.3
a	3687	356.8	a′	1865	2763.8
a	3531	679.3	a′	1776	314.2
a	3391	768.8	a′	1598	23.7
a	2166	2035.6	a′	1524	165.4
a	1672	24.5	a′	964	31.1
a	1649	30.0	a′	622	11.6
a	1639	63.7	a′	511	141.3
a	1017	27.5	a′	466	66.3
a	854	88.8	a′	363	20.5
a	799	165.5	a′	312	84.4
a	731	27.9	a′	105	2.9
a	538	100.7	a′	51	2.6
a	454	22.5	a″	3856	102.5
a	418	37.0	a″	2750	2465.9
a	327	118.7	a″	1742	381.8
a	313	26.9	a″	1611	0.1
a	280	74.5	a″	1371	378.3
a	251	111.2	a″	1111	963.5
a	240	42.7	a″	907	180.7
a	197	76.7	a″	699	54.6
a	192	37.3	a″	515	24.2
a	141	4.3	a″	401	375.1
a	69	1.0	a″	350	55.5
a	37	1.1	a″	$344i$	293.0

Table S81 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant, $\mathbf{C_1}$ TS, and $\mathbf{C_1}$ product of the isomer of $(H_2O)_3(HCl)_1$* with adjacent dangling hydrogen atoms on the same side of the ring, i.e. $f1 = f2 = H_2O\uparrow$ and $f3 = H_2O\downarrow$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3904	148.6	a	3858	41.2	a	3901	99.9
a	3900	103.1	a	3857	170.9	a	3896	147.5
a	3877	102.7	a	3845	110.1	a	3882	100.2
a	3688	363.1	a	2886	1953.2	a	3690	349.9
a	3556	616.8	a	2732	2440.0	a	3529	696.3
a	3397	769.5	a	1899	2690.2	a	3420	699.3
a	2160	2059.8	a	1823	59.5	a	2187	1990.7
a	1675	30.3	a	1728	364.2	a	1673	33.4
a	1651	23.6	a	1649	117.5	a	1664	23.9
a	1644	65.4	a	1608	54.7	a	1640	57.4
a	1013	35.5	a	1475	297.3	a	980	20.0
a	850	97.1	a	1303	525.9	a	838	168.8
a	756	110.8	a	1123	848.5	a	774	53.9
a	709	76.0	a	946	5.4	a	680	49.5
a	501	16.4	a	872	208.6	a	544	65.7
a	470	113.4	a	762	7.0	a	524	107.3
a	430	20.2	a	604	57.0	a	399	69.6
a	335	73.2	a	533	64.2	a	311	73.6
a	318	120.2	a	496	53.4	a	286	82.2
a	278	38.6	a	453	82.2	a	262	50.8
a	235	35.0	a	386	292.9	a	255	69.1
a	221	108.5	a	372	78.5	a	239	37.7
a	192	38.0	a	345	33.2	a	194	80.2
a	155	75.3	a	311	89.4	a	191	30.2
a	140	4.0	a	104	3.2	a	141	5.3
a	65	1.2	a	34	9.2	a	66	0.1
a	24	7.9	a	$343i$	299.2	a	25	5.6

*The reactant and product of this structure are not equivalent

Table S82 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_2}$ TS of non-alternating trans $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_2$ with $f1 = f2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3899	166.8	a	3830	58.3
a	3879	113.1	a	2854	3502.8
a	3726	240.7	a	1721	42.0
a	3488	692.3	a	1532	120.6
a	2760	804.4	a	978	2.3
a	2216	1902.5	a	830	82.7
a	1657	26.9	a	698	0.0
a	1634	46.5	a	617	0.0
a	966	40.2	a	424	128.8
a	807	103.4	a	353	2.9
a	720	36.7	a	296	83.3
a	554	63.9	a	30	3.5
a	459	42.4	b	3829	221.7
a	409	46.4	b	2799	213.3
a	401	15.2	b	1713	390.0
a	318	74.5	b	1597	100.8
a	289	127.9	b	1100	6578.6
a	261	7.5	b	1001	724.4
a	197	38.9	b	807	8.8
a	194	94.2	b	514	33.0
a	132	7.5	b	443	188.4
a	118	6.2	b	371	24.8
a	56	0.5	b	79	0.4
a	23	1.3	b	$612i$	384.8

Table S83 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_2}$ TS of non-alternating cis $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_2(HCl)_2$ with $f1 = f2$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3901	158.8	a	3842	147.9
a	3885	114.1	a	3828	118.7
a	3727	245.6	a	2846	3388.0
a	3514	630.9	a	2776	386.2
a	2770	777.4	a	1812	49.6
a	2246	1844.4	a	1681	38.4
a	1665	29.0	a	1652	440.1
a	1643	41.4	a	1381	303.8
a	936	31.9	a	1093	6969.2
a	757	97.5	a	1025	28.4
a	643	60.5	a	942	37.3
a	563	12.6	a	843	132.4
a	504	88.4	a	802	4.5
a	410	81.3	a	708	321.0
a	390	37.3	a	621	20.6
a	304	55.7	a	534	30.9
a	269	87.2	a	435	102.2
a	237	36.9	a	382	61.7
a	194	38.4	a	368	45.6
a	162	58.4	a	348	17.2
a	130	8.6	a	296	86.4
a	117	5.4	a	80	0.3
a	53	0.1	a	20	3.3
a	9	3.7	a	$646i$	258.4

Table S84 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_i}$ reactant, $\mathbf{C_i}$ TS, and $\mathbf{C_i}$ product of alternating trans $(H_2O)_2(HCl)_2$*, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_2$ with $f1 = f3$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a_g	3880	0.0	a_g	3808	0.0	a_g	3797	0.0
a_g	3664	0.0	a_g	2913	0.0	a_g	2407	0.0
a_g	2371	0.0	a_g	1666	0.0	a_g	1766	0.0
a_g	1638	0.0	a_g	1545	0.0	a_g	1684	0.0
a_g	878	0.0	a_g	1222	0.0	a_g	1567	0.0
a_g	682	0.0	a_g	857	0.0	a_g	1259	0.0
a_g	484	0.0	a_g	588	0.0	a_g	770	0.0
a_g	327	0.0	a_g	511	0.0	a_g	514	0.0
a_g	228	0.0	a_g	406	0.0	a_g	420	0.0
a_g	201	0.0	a_g	386	0.0	a_g	361	0.0
a_g	131	0.0	a_g	97	0.0	a_g	155	0.0
a_g	53	0.0	a_g	$336i$	0.0	a_g	103	0.0
a_u	3880	320.8	a_u	3807	297.7	a_u	3796	308.9
a_u	3676	729.6	a_u	2969	3402.7	a_u	2332	4232.
a_u	2434	2986.3	a_u	1658	574.4	a_u	2233	6996.
a_u	1638	60.9	a_u	1516	250.1	a_u	1631	38.7
a_u	811	80.7	a_u	1275	4664.4	a_u	1611	13.6
a_u	679	102.6	a_u	1179	2736.8	a_u	1243	379.4
a_u	552	140.1	a_u	838	65.1	a_u	863	6.1
a_u	335	127.1	a_u	512	5.0	a_u	514	33.2
a_u	227	170.3	a_u	463	137.0	a_u	416	133.6
a_u	206	34.1	a_u	384	139.9	a_u	363	238.4
a_u	151	23.7	a_u	281	123.4	a_u	349	158.9
a_u	18	6.4	a_u	44	18.5	a_u	49	22.3

*This structure does not undergo concerted proton transfer, but rather stepwise, and thus the frequencies reported correspond to the proton transfer process connecting the reactant, $(H_2O)_2(HCl)_2$, and the product, $(H_3O)_2^+(Cl)_2^-$

Table S85 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_2}$ reactant, $\mathbf{C_2}$ TS, and $\mathbf{C_2}$ product of alternating cis $(H_2O)_2(HCl)_2$*, i.e. $(H_2O\uparrow)_2(HCl)_2$ with $f1 = f3$

Reactant			TS			Product		
Irrep	ω	IR	Irrep	ω	IR	Irrep	ω	IR
a	3882	71.9	a	3810	122.3	a	3882	72.0
a	3666	0.0	a	2912	0.1	a	3666	0.0
a	2380	2.6	a	1671	13.8	a	2380	2.6
a	1640	28.6	a	1548	0.1	a	1640	28.6
a	872	0.2	a	1227	90.0	a	872	0.2
a	694	94.0	a	860	10.5	a	694	94.0
a	482	24.5	a	590	0.0	a	482	24.5
a	321	33.0	a	506	2.6	a	321	33.0
a	229	0.6	a	406	0.0	a	229	0.6
a	200	1.7	a	388	0.7	a	200	1.7
a	131	0.0	a	97	0.2	a	131	0.0
a	53	0.4	a	46	16.0	a	53	0.4
a	22	3.1	a	$333i$	0.2	a	22	3.1
b	3883	246.8	b	3808	173.1	b	3882	246.7
b	3677	723.3	b	2968	3407.1	b	3677	723.3
b	2442	2950.5	b	1657	589.0	b	2442	2950.6
b	1635	31.0	b	1516	236.8	b	1635	31.1
b	803	70.6	b	1276	5026.7	b	803	70.6
b	660	24.7	b	1169	2262.3	b	660	24.7
b	546	121.8	b	829	54.6	b	546	121.8
b	333	84.0	b	518	3.2	b	333	84.0
b	223	146.1	b	462	139.4	b	223	146.1
b	200	51.7	b	376	141.1	b	200	51.7
b	150	23.7	b	281	122.1	b	150	23.7

*This structure does not undergo concerted proton transfer, but rather stepwise, and thus the frequencies reported correspond to the proton transfer process connecting the reactant, $(H_2O)_2(HCl)_2$, and the product, $(H_3O)_2^+(Cl)_2^-$

Table S86 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{C_1}$ reactant and $\mathbf{C_s}$ TS of $(H_2O)_1(HCl)_3$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	3888	175.6	a′	3769	168.6
a	3720	244.8	a′	2611	1452.7
a	2855	583.3	a′	1656	16.4
a	2790	760.7	a′	1424	3903.1
a	2480	1225.2	a′	1270	426.3
a	1633	33.4	a′	951	67.1
a	799	34.7	a′	789	22.1
a	659	42.1	a′	403	49.7
a	535	19.5	a′	323	116.9
a	493	99.7	a′	310	29.4
a	379	21.1	a′	67	1.9
a	364	23.5	a′	7	2.4
a	338	10.7	a″	2383	4016.7
a	298	59.6	a″	1645	4.8
a	210	60.1	a″	965	141.4
a	189	30.2	a″	753	2.7
a	130	16.2	a″	744	15.3
a	118	5.9	a″	585	1621.8
a	105	2.4	a″	475	6.5
a	42	0.3	a″	305	101.1
a	12	1.7	a″	$536i$	1810.4

Table S87 MP2/haTZ harmonic vibrational frequencies (ω in cm^{-1}) and infrared intensities (IR in km mol^{-1}) for the $\mathbf{S_4}$ reactant and $\mathbf{D_{2d}}$ TS of $(HCl)_4$

Reactant/Product			TS		
Irrep	ω	IR	Irrep	ω	IR
a	2831	0.0	a_1	1191	0.0
a	556	0.0	a_1	361	0.0
a	296	0.0	a_1	25	0.0
a	96	0.0	a_2	738	0.0
a	8	0.0	a_2	$1467i$	0.0
b	2897	121.6	b_1	766	0.0
b	365	55.3	b_1	335	0.0
b	297	0.2	b_2	1435	876.8
b	107	1.1	b_2	822	21.5
b	30	0.1	b_2	68	0.1
e	2877	911.3	e	1112	8486.6
e	440	33.9	e	996	4.6
e	304	17.3	e	755	1.8
e	108	10.1	e	354	1.0

5 IRC Relative Energies and Reaction Coordinates

Table S88 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_3$

Reaction Coordinate	Energy
0.00000	18.1
0.10163	17.7
0.20322	16.7
0.30481	15.3
0.40637	13.6
0.50780	11.9
0.60885	10.6
0.70978	9.6
0.81111	8.7
0.91263	7.9
1.01421	7.1
1.11581	6.4
1.21743	5.8
1.31904	5.2
1.42066	4.7
1.52228	4.1
1.62390	3.7
1.72552	3.3
1.82714	2.8
1.92876	2.5
2.03038	2.2
2.13200	1.9
2.23362	1.6
2.33524	1.3
2.43686	1.1
2.53848	0.9
2.64010	0.7
2.74172	0.6
2.84334	0.5
2.94496	0.3
3.04658	0.3
3.14820	0.2
3.24983	0.1
3.35145	0.1
3.45308	0.0
3.55471	0.0
3.65636	0.0

Table S89 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_2(HCl)_1$

Reaction Coordinate	Energy
0.00000	19.9
0.10126	19.6
0.20246	18.8
0.30372	17.7
0.40496	16.2
0.50620	14.6
0.60740	13.1
0.70837	11.8
0.80895	10.8
0.90980	10.0
1.01097	9.3
1.11222	8.6
1.21351	8.0
1.31480	7.4
1.41610	6.8
1.51741	6.3
1.61871	5.8
1.72002	5.3
1.82132	4.9
1.92263	4.5
2.02394	4.1
2.12524	3.7
2.22655	3.4
2.32786	3.1
2.42917	2.8
2.53047	2.5
2.63178	2.3
2.73309	2.0
2.83439	1.8
2.93570	1.6
3.03701	1.4
3.13832	1.2
3.23962	1.1
3.34093	0.9
3.44224	0.8
3.54354	0.7
3.64485	0.6
3.74616	0.5
3.84746	0.4
3.94876	0.3
4.05007	0.3
4.15137	0.2
4.25267	0.2
4.35397	0.1
4.45526	0.1
4.55656	0.0
4.65784	0.0
4.75913	0.0
4.86040	0.0

Table S90 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_1(HCl)_2$

Reaction Coordinate	Energy
0.00000	22.3
0.10104	22.0
0.20205	21.2
0.30309	20.0
0.40413	18.5
0.50516	16.8
0.60615	15.2
0.70690	13.9
0.80713	12.9
0.90761	12.1
1.00852	11.4
1.10952	10.7
1.21055	10.1
1.31160	9.5
1.41266	8.9
1.51372	8.4
1.61479	7.9
1.71586	7.4
1.81692	7.0
1.91799	6.6
2.01906	6.1
2.12013	5.7
2.22120	5.4
2.32227	5.0
2.42334	4.7
2.52441	4.4
2.62548	4.1
2.72655	3.8
2.82762	3.5
2.92869	3.2
3.02976	3.0
3.13083	2.8
3.23190	2.5
3.33297	2.3
3.43404	2.1
3.53510	2.0
3.63617	1.8
3.73724	1.6
3.83831	1.5
3.93938	1.3
4.04045	1.2
4.14152	1.1
4.24259	1.0
4.34366	0.8
4.44473	0.7
4.54580	0.7
4.64687	0.6
4.74794	0.5
4.84901	0.4
4.95008	0.4
5.05115	0.3
5.15221	0.3
5.25328	0.2
5.35434	0.2
5.45541	0.1
5.55647	0.1
5.65752	0.1
5.75858	0.1
5.85962	0.0
5.96066	0.0

Table S91 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_2(H_2O)_1$

Reaction Coordinate	Energy
0.00000	16.2
0.10467	16.0
0.20920	15.5
0.31388	14.7
0.41854	13.6
0.52324	12.3
0.62793	10.9
0.73247	9.6
0.83647	8.5
0.94051	7.7
1.04508	7.0
1.14978	6.3
1.25452	5.7
1.35926	5.1
1.46400	4.5
1.56875	4.1
1.67350	3.6
1.77825	3.2
1.88300	2.8
1.98775	2.5
2.09250	2.1
2.19724	1.8
2.30199	1.6
2.40674	1.4
2.51149	1.1
2.61623	1.0
2.72098	0.8
2.82572	0.6
2.93046	0.5
3.03520	0.4
3.13993	0.3
3.24466	0.2
3.34938	0.2
3.45409	0.1
3.55878	0.1
3.66345	0.1
3.76810	0.0
3.87273	0.0
3.97737	0.0

Table S92 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for trans $(HF)_1(H_2O)_2$, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1$

Reaction Coordinate	Energy
0.00000	19.4
0.10350	19.2
0.20690	18.6
0.31039	17.5
0.41386	16.2
0.51735	14.7
0.62084	13.0
0.72424	11.5
0.82716	10.2
0.92989	9.3
1.03323	8.4
1.13674	7.6
1.24028	6.9
1.34384	6.3
1.44739	5.6
1.55095	5.1
1.65451	4.5
1.75807	4.1
1.86163	3.6
1.96519	3.2
2.06875	2.8
2.17231	2.4
2.27587	2.1
2.37943	1.8
2.48299	1.6
2.58655	1.3
2.69011	1.1
2.79366	0.9
2.89722	0.8
3.00077	0.6
3.10433	0.5
3.20788	0.4
3.31143	0.3
3.41497	0.2
3.51851	0.2
3.62203	0.1
3.72554	0.1
3.82901	0.0
3.93242	0.0
4.03571	0.0

Table S93 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for cis $(HF)_1(H_2O)_2$, i.e. $(HF)_1(H_2O{\uparrow})_2$

Reaction Coordinate	Energy
0.00000	20.0
0.10333	19.7
0.20660	19.1
0.30995	18.0
0.41327	16.7
0.51662	15.1
0.61997	13.5
0.72324	11.9
0.82607	10.6
0.92864	9.6
1.03183	8.8
1.13519	8.0
1.23859	7.3
1.34200	6.6
1.44542	5.9
1.54883	5.4
1.65225	4.8
1.75567	4.3
1.85909	3.8
1.96250	3.4
2.06592	3.0
2.16934	2.6
2.27276	2.3
2.37618	2.0
2.47959	1.7
2.58301	1.5
2.68643	1.3
2.78984	1.1
2.89326	0.9
2.99667	0.7
3.10008	0.6
3.20350	0.5
3.30691	0.4
3.41031	0.3
3.51371	0.2
3.61711	0.1
3.72049	0.1
3.82386	0.1
3.92720	0.0
4.03049	0.0
4.13367	0.0

Table S94 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_1(H_2O)_1(HCl)_1$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−4.74414	0.0	0.00000	14.2
−4.63873	0.0	+0.10514	14.1
−4.53329	0.0	+0.20989	13.9
−4.42782	0.0	+0.31528	13.7
−4.32234	0.1	+0.42065	13.4
−4.21686	0.1	+0.52612	13.2
−4.11137	0.1	+0.63159	12.9
−4.00589	0.2	+0.73707	12.6
−3.90039	0.2	+0.84253	12.2
−3.79490	0.3	+0.94800	11.8
−3.68941	0.3	+1.05340	11.4
−3.58392	0.4	+1.15879	10.9
−3.47843	0.5	+1.26418	10.3
−3.37293	0.6	+1.36959	9.6
−3.26744	0.7	+1.47502	8.9
−3.16195	0.8	+1.58031	8.2
−3.05646	0.9	+1.68514	7.6
−2.95096	1.0	+1.79001	7.1
−2.84547	1.2	+1.89536	6.6
−2.73997	1.3	+2.00083	6.2
−2.63448	1.5	+2.10632	5.9
−2.52899	1.7	+2.21182	5.5
−2.42349	1.9	+2.31731	5.2
−2.31800	2.1	+2.42281	4.9
−2.21250	2.3	+2.52831	4.6
−2.10701	2.6	+2.63381	4.3
−2.00151	2.9	+2.73931	4.1
−1.89602	3.1	+2.84481	3.8
−1.79053	3.5	+2.95031	3.6
−1.68503	3.8	+3.05580	3.4
−1.57954	4.2	+3.16130	3.3
−1.47405	4.6	+3.26680	3.1
−1.36855	5.0	+3.37230	3.0
−1.26306	5.4	+3.47780	2.8
−1.15758	5.9	+3.58330	2.7
−1.05210	6.4	+3.68880	2.6
−0.94666	7.0	+3.79430	2.5
−0.84138	7.6	+3.89980	2.4
−0.73706	8.3	+4.00530	2.4
−0.63244	9.2	+4.11080	2.3
−0.52713	10.5	+4.21630	2.2
−0.42168	11.7	+4.32180	2.2
−0.31622	12.8	+4.42729	2.2
−0.21076	13.6	+4.53278	2.2
−0.10541	14.0	+4.63825	2.1
0.00000	14.2	+4.74365	2.1

Table S95 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(H_2O)_3$

Reaction Coordinate	Energy
0.00000	26.5
0.10131	26.1
0.20259	25.0
0.30387	23.2
0.40514	21.1
0.50639	18.7
0.60755	16.6
0.70834	14.9
0.80884	13.6
0.90980	12.4
1.01099	11.4
1.11225	10.5
1.21353	9.6
1.31482	8.8
1.41612	8.0
1.51741	7.3
1.61871	6.6
1.72001	6.0
1.82130	5.4
1.92260	4.8
2.02390	4.3
2.12519	3.9
2.22649	3.4
2.32779	3.0
2.42908	2.6
2.53038	2.3
2.63168	2.0
2.73298	1.7
2.83427	1.4
2.93557	1.2
3.03687	1.0
3.13816	0.8
3.23946	0.7
3.34076	0.5
3.44206	0.4
3.54335	0.3
3.64465	0.2
3.74595	0.1
3.84725	0.1
3.94854	0.0
4.04984	0.0
4.15109	0.0

Table S96 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for trans $(H_2O)_2(HCl)_1$, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$

Reaction Coordinate	Energy
0.00000	10.5
0.11202	10.5
0.22355	10.3
0.33558	10.1
0.44755	9.8
0.55969	9.6
0.67178	9.2
0.78390	8.9
0.89593	8.4
1.00795	7.9
1.11999	7.3
1.23207	6.6
1.34408	5.8
1.45558	5.2
1.56681	4.7
1.67881	4.2
1.79095	3.8
1.90311	3.4
2.01527	3.1
2.12743	2.7
2.23959	2.4
2.35176	2.1
2.46392	1.9
2.57608	1.7
2.68825	1.4
2.80041	1.3
2.91257	1.1
3.02473	0.9
3.13690	0.8
3.24905	0.6
3.36121	0.5
3.47337	0.4
3.58552	0.4
3.69766	0.3
3.80980	0.2
3.92192	0.2
4.03404	0.1
4.14613	0.1
4.25821	0.1
4.37028	0.0
4.48236	0.0
4.59447	0.0
4.70661	0.0

Table S97 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for cis $(H_2O)_2(HCl)_1$, i.e. $(H_2O\uparrow)_2(HCl)_1$

Reaction Coordinate	Energy
0.00000	11.0
0.10958	11.0
0.21894	10.8
0.32867	10.6
0.43843	10.3
0.54834	10.0
0.65821	9.7
0.76810	9.3
0.87792	8.9
0.98773	8.3
1.09755	7.7
1.20741	7.0
1.31723	6.2
1.42671	5.5
1.53567	5.0
1.64532	4.5
1.75522	4.1
1.86515	3.7
1.97508	3.3
2.08501	3.0
2.19495	2.7
2.30488	2.4
2.41482	2.1
2.52475	1.9
2.63469	1.6
2.74462	1.4
2.85456	1.2
2.96449	1.1
3.07442	0.9
3.18436	0.8
3.29429	0.7
3.40422	0.6
3.51415	0.5
3.62407	0.4
3.73399	0.3
3.84391	0.2
3.95382	0.2
4.06371	0.1
4.17360	0.1
4.28347	0.1
4.39332	0.0
4.50317	0.0
4.61304	0.0
4.72291	0.0

Table S98 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(H_2O)_1(HCl)_2$

Reaction Coordinate	Energy
0.00000	12.5
0.10585	12.5
0.21148	12.3
0.31723	12.0
0.42285	11.7
0.52865	11.3
0.63437	10.9
0.74015	10.3
0.84594	9.7
0.95175	8.9
1.05748	8.2
1.16275	7.5
1.26771	7.0
1.37336	6.6
1.47918	6.2
1.58503	5.8
1.69089	5.4
1.79675	5.0
1.90261	4.7
2.00848	4.4
2.11435	4.1
2.22022	3.8
2.32608	3.5
2.43195	3.2
2.53782	3.0
2.64369	2.7
2.74956	2.5
2.85543	2.3
2.96130	2.1
3.06716	1.9
3.17303	1.7
3.27890	1.6
3.38477	1.4
3.49064	1.3
3.59651	1.2
3.70237	1.0
3.80824	0.9
3.91411	0.8
4.01998	0.7
4.12585	0.6
4.23171	0.5
4.33758	0.5
4.44345	0.4
4.54931	0.3
4.65518	0.3
4.76104	0.2
4.86691	0.2
4.97277	0.2
5.07864	0.1
5.18450	0.1
5.29036	0.1
5.39623	0.0
5.50209	0.0
5.60796	0.0
5.71383	0.0

Table S99 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HCl)_3$

Reaction Coordinate	Energy
0.00000	23.5
0.10095	23.3
0.20186	22.5
0.30279	21.2
0.40371	19.7
0.50462	18.0
0.60549	16.5
0.70613	15.2
0.80603	14.2
0.90619	13.5
1.00697	12.9
1.10784	12.3
1.20873	11.7
1.30964	11.2
1.41056	10.6
1.51149	10.1
1.61242	9.7
1.71335	9.2
1.81428	8.8
1.91521	8.3
2.01615	7.9
2.11708	7.5
2.21801	7.1
2.31895	6.8
2.41988	6.4
2.52081	6.1
2.62175	5.8
2.72268	5.4
2.82361	5.1
2.92455	4.9
3.02548	4.6
3.12642	4.3
3.22735	4.1
3.32828	3.8
3.42922	3.6
3.53015	3.4
3.63109	3.1
3.73202	2.9
3.83295	2.7
3.93389	2.6
4.03482	2.4
4.13576	2.2
4.23669	2.0
4.33762	1.9
4.43856	1.8
4.53949	1.6
4.64043	1.5
4.74136	1.4
4.84230	1.2
4.94323	1.1
5.04416	1.0
5.14510	0.9
5.24603	0.8
5.34697	0.8
5.44790	0.7
5.54884	0.6
5.64977	0.5
5.75071	0.5
5.85164	0.4
5.95258	0.4
6.05351	0.3
6.15445	0.3
6.25538	0.2
6.35632	0.2
6.45725	0.1
6.55819	0.1
6.65912	0.1
6.76006	0.1
6.86099	0.0
6.96193	0.0
7.06287	0.0
7.16381	0.0

Table S100 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_4$

Reaction Coordinate	Energy
0.00000	11.8
0.10190	11.6
0.20374	10.9
0.30559	9.8
0.40737	8.7
0.50875	7.8
0.60937	7.0
0.71087	6.4
0.81269	5.9
0.91457	5.4
1.01645	4.9
1.11834	4.4
1.22023	4.0
1.32212	3.6
1.42401	3.2
1.52589	2.8
1.62778	2.5
1.72967	2.2
1.83156	1.9
1.93345	1.7
2.03534	1.4
2.13723	1.2
2.23911	1.0
2.34100	0.8
2.44289	0.7
2.54478	0.6
2.64667	0.4
2.74856	0.3
2.85045	0.2
2.95234	0.2
3.05423	0.1
3.15612	0.1
3.25802	0.0
3.35992	0.0
3.46185	0.0

Table S101 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·$amu^{1/2}$) for each point on the IRC calculation for $(HF)_3(HCl)_1$

Reaction Coordinate	Energy
0.00000	14.5
0.10175	14.3
0.20339	13.8
0.30514	13.0
0.40686	11.9
0.50858	10.8
0.61020	9.8
0.71131	9.0
0.81210	8.4
0.91370	7.8
1.01549	7.3
1.11730	6.8
1.21911	6.3
1.32092	5.9
1.42274	5.5
1.52455	5.0
1.62637	4.7
1.72818	4.3
1.83000	4.0
1.93182	3.6
2.03363	3.3
2.13545	3.0
2.23726	2.8
2.33908	2.5
2.44090	2.3
2.54271	2.1
2.64453	1.8
2.74635	1.6
2.84816	1.5
2.94998	1.3
3.05180	1.1
3.15361	1.0
3.25543	0.9
3.35725	0.7
3.45906	0.6
3.56088	0.5
3.66270	0.5
3.76451	0.4
3.86632	0.3
3.96814	0.2
4.06994	0.2
4.17175	0.1
4.27354	0.1
4.37532	0.1
4.47705	0.0
4.57871	0.0
4.68022	0.0
4.78159	0.0

Table S102 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for $(HF)_3(H_2O)_1$

Reaction Coordinate	Energy
0.00000	9.6
0.11212	9.5
0.22402	9.2
0.33615	8.7
0.44819	8.0
0.56036	7.2
0.67245	6.4
0.78402	5.7
0.89536	5.1
1.00748	4.6
1.11971	4.1
1.23196	3.7
1.34422	3.3
1.45647	2.9
1.56873	2.5
1.68098	2.2
1.79324	1.9
1.90550	1.6
2.01775	1.4
2.13001	1.2
2.24227	1.0
2.35453	0.8
2.46678	0.6
2.57904	0.5
2.69130	0.4
2.80355	0.3
2.91581	0.2
3.02807	0.1
3.14032	0.1
3.25257	0.0
3.36478	0.0
3.47635	0.0

Table S103 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating $(HF)_2(HCl)_2$, i.e. $f1 = f2$

Reaction Coordinate	Energy
0.00000	18.0
0.10141	17.8
0.20274	17.2
0.30414	16.3
0.40553	15.2
0.50693	13.9
0.60828	12.7
0.70936	11.7
0.80954	11.0
0.91035	10.4
1.01172	9.9
1.11315	9.4
1.21459	8.9
1.31604	8.4
1.41749	8.0
1.51893	7.5
1.62038	7.1
1.72183	6.7
1.82328	6.3
1.92472	5.9
2.02617	5.6
2.12762	5.3
2.22907	4.9
2.33052	4.6
2.43197	4.3
2.53342	4.0
2.63486	3.8
2.73631	3.5
2.83776	3.3
2.93921	3.0
3.04066	2.8
3.14211	2.6
3.24356	2.4
3.34501	2.2
3.44646	2.0
3.54790	1.9
3.64935	1.7
3.75080	1.5
3.85225	1.4
3.95370	1.3
4.05515	1.1
4.15660	1.0
4.25805	0.9
4.35950	0.8
4.46095	0.7
4.56240	0.6
4.66385	0.5
4.76530	0.5
4.86675	0.4
4.96819	0.3
5.06964	0.3
5.17109	0.2
5.27254	0.2
5.37399	0.1
5.47544	0.1
5.57688	0.1
5.67833	0.1
5.77977	0.0
5.88121	0.0
5.98264	0.0
6.08404	0.0

Table S104 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating $(HF)_2(HCl)_2$, i.e. $f1 = f3$

Reaction Coordinate	Energy
0.00000	19.4
0.10127	19.1
0.20252	18.5
0.30382	17.4
0.40511	16.2
0.50640	14.8
0.60763	13.6
0.70847	12.6
0.80843	11.8
0.90927	11.2
1.01054	10.7
1.11186	10.2
1.21318	9.6
1.31451	9.1
1.41584	8.7
1.51718	8.2
1.61851	7.8
1.71984	7.3
1.82117	6.9
1.92250	6.5
2.02384	6.2
2.12517	5.8
2.22650	5.4
2.32783	5.1
2.42917	4.8
2.53050	4.5
2.63183	4.2
2.73316	3.9
2.83449	3.7
2.93583	3.4
3.03716	3.2
3.13849	2.9
3.23982	2.7
3.34116	2.5
3.44249	2.3
3.54382	2.2
3.64515	2.0
3.74649	1.8
3.84782	1.7
3.94915	1.5
4.05048	1.4
4.15182	1.3
4.25315	1.1
4.35448	1.0
4.45581	0.9
4.55714	0.8
4.65847	0.7
4.75980	0.7
4.86113	0.6
4.96246	0.5
5.06379	0.5
5.16512	0.4
5.26644	0.3
5.36776	0.3
5.46907	0.3
5.57037	0.2
5.67166	0.2
5.77294	0.2
5.87421	0.1
5.97545	0.1
6.07669	0.1
6.17794	0.1
6.27919	0.1
6.38046	0.1
6.48175	0.0
6.58306	0.0
6.68438	0.0
6.78570	0.0
6.88703	0.0

Table S105 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating $(HF)_2(H_2O)_1(HCl)_1$, i.e. $f1 = f2$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−4.43668	0.0	0.00000	10.5
−4.33379	0.0	+0.10323	10.4
−4.23079	0.0	+0.20611	10.1
−4.12767	0.0	+0.30878	9.7
−4.02449	0.1	+0.41131	9.4
−3.92128	0.1	+0.51446	9.1
−3.81804	0.1	+0.61768	8.8
−3.71479	0.2	+0.72092	8.6
−3.61154	0.2	+0.82417	8.3
−3.50829	0.3	+0.92743	8.0
−3.40503	0.3	+1.03068	7.8
−3.30177	0.4	+1.13394	7.5
−3.19851	0.5	+1.23702	7.2
−3.09525	0.6	+1.34046	7.0
−2.99199	0.7	+1.44371	6.7
−2.88873	0.8	+1.54695	6.5
−2.78547	0.9	+1.65018	6.2
−2.68221	1.1	+1.75340	6.0
−2.57895	1.2	+1.85660	5.7
−2.47568	1.4	+1.95977	5.5
−2.37242	1.5	+2.06290	5.2
−2.26916	1.7	+2.16594	5.0
−2.16590	1.9	+2.26903	4.8
−2.06264	2.1	+2.37223	4.5
−1.95938	2.4	+2.47547	4.3
−1.85612	2.6	+2.57872	4.1
−1.75286	2.9	+2.68197	4.0
−1.64959	3.1	+2.78523	3.8
−1.54633	3.4	+2.88848	3.6
−1.44307	3.7	+2.99174	3.5
−1.33981	4.0	+3.09500	3.4
−1.23655	4.4	+3.19826	3.2
−1.13329	4.8	+3.30152	3.1
−1.03003	5.1	+3.40478	3.0
−0.92678	5.5	+3.50805	2.9
−0.82353	6.0	+3.61131	2.8
−0.72039	6.4	+3.71457	2.7
−0.61802	6.9	+3.81783	2.7
−0.51582	7.5	+3.92110	2.6
−0.41281	8.3	+4.02436	2.6
−0.30964	9.2	+4.12762	2.5
−0.20642	9.9	+4.23087	2.5
−0.10325	10.3	+4.33412	2.5
0.00000	10.5	+4.43733	2.4
		+4.54041	2.4
		+4.64281	2.4

Table S106 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating $(HF)_2(H_2O)_1(HCl)_1$, i.e. $f1 = f3$

Reaction Coordinate	Energy
0.00000	8.4
0.20676	8.3
0.41297	8.2
0.61718	7.9
0.82491	7.1
1.03238	5.8
1.23119	4.9
1.43946	4.2
1.64792	3.6
1.85638	3.0
2.06485	2.5
2.27333	2.0
2.48180	1.6
2.69027	1.3
2.89874	1.0
3.10720	0.8
3.31566	0.6
3.52410	0.4
3.73251	0.3
3.94081	0.2
4.14881	0.1
4.35596	0.1
4.56222	0.0
4.76948	0.0

Table S107 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating trans $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_1(H_2O\downarrow)_1$ with $f1 = f2$

Reaction Coordinate	Energy
0.00000	11.1
0.10830	11.0
0.21634	10.7
0.32456	10.2
0.43265	9.6
0.54093	8.9
0.64921	8.1
0.75749	7.2
0.86553	6.5
0.97303	5.8
1.08104	5.3
1.18935	4.8
1.29769	4.3
1.40604	3.8
1.51439	3.4
1.62274	3.0
1.73109	2.7
1.83944	2.4
1.94779	2.1
2.05614	1.8
2.16449	1.5
2.27285	1.3
2.38120	1.1
2.48955	0.9
2.59790	0.8
2.70625	0.6
2.81461	0.5
2.92296	0.4
3.03131	0.3
3.13966	0.2
3.24801	0.1
3.35635	0.1
3.46469	0.0
3.57300	0.0
3.68108	0.0

Table S108 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating cis $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_2$ with $f1 = f2$

Reaction Coordinate	Energy
0.00000	11.6
0.10751	11.5
0.21488	11.2
0.32237	10.7
0.42974	10.0
0.53729	9.3
0.64484	8.5
0.75240	7.6
0.85977	6.8
0.96658	6.2
1.07381	5.6
1.18139	5.1
1.28901	4.6
1.39663	4.1
1.50426	3.7
1.61188	3.3
1.71951	2.9
1.82713	2.6
1.93476	2.3
2.04239	2.0
2.15002	1.7
2.25765	1.5
2.36528	1.3
2.47291	1.1
2.58053	0.9
2.68816	0.7
2.79579	0.6
2.90342	0.5
3.01105	0.4
3.11867	0.3
3.22630	0.2
3.33393	0.1
3.44155	0.1
3.54917	0.0
3.65675	0.0
3.76412	0.0

Table S109 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating trans $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O\uparrow)_1(H_2O\downarrow)_1$ with $f1 = f3$

Reaction Coordinate	Energy
0.00000	11.8
0.10993	11.8
0.21971	11.4
0.32972	10.7
0.43970	9.8
0.54967	8.8
0.65942	7.8
0.76845	7.1
0.87791	6.4
0.98788	5.8
1.09791	5.3
1.20795	4.8
1.31800	4.3
1.42805	3.8
1.53809	3.4
1.64814	3.0
1.75819	2.7
1.86824	2.4
1.97829	2.1
2.08834	1.8
2.19839	1.5
2.30843	1.3
2.41848	1.1
2.52853	0.9
2.63858	0.7
2.74863	0.6
2.85868	0.5
2.96872	0.3
3.07877	0.3
3.18882	0.2
3.29886	0.1
3.40890	0.1
3.51892	0.0
3.62886	0.0
3.73759	0.0

Table S110 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating cis $(HF)_2(H_2O)_2$, i.e. $(HF)_2(H_2O{\uparrow})_2$ with $f1 = f3$

Reaction Coordinate	Energy
0.00000	12.1
0.10993	11.8
0.21971	11.4
0.32972	10.7
0.43970	9.8
0.54967	8.8
0.65942	7.8
0.76845	7.1
0.87791	6.4
0.98788	5.8
1.09791	5.3
1.20795	4.8
1.31800	4.3
1.42805	3.8
1.53809	3.4
1.64814	3.0
1.75819	2.7
1.86824	2.4
1.97829	2.1
2.08834	1.8
2.19839	1.5
2.30843	1.3
2.41848	1.1
2.52853	0.9
2.63858	0.7
2.74863	0.6
2.85868	0.5
2.96872	0.3
3.07877	0.3
3.18882	0.2
3.29886	0.1
3.40890	0.1
3.51892	0.0
3.62886	0.0
3.73759	0.0

Table S111 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for $(HF)_1(HCl)_3$

Reaction Coordinate	Energy
0.00000	22.5
0.10118	22.2
0.20234	21.5
0.30353	20.5
0.40471	19.1
0.50589	17.6
0.60705	16.1
0.70805	14.9
0.80816	14.1
0.90800	13.5
1.00906	12.9
1.11025	12.4
1.21146	11.9
1.31266	11.4
1.41387	10.9
1.51508	10.4
1.61629	10.0
1.71750	9.5
1.81871	9.1
1.91991	8.7
2.02112	8.3
2.12233	7.9
2.22354	7.6
2.32475	7.2
2.42596	6.9
2.52717	6.5
2.62838	6.2
2.72958	5.9
2.83079	5.6
2.93200	5.3
3.03321	5.0
3.13442	4.8
3.23563	4.5
3.33684	4.2
3.43805	4.0
3.53926	3.8
3.64046	3.6
3.74167	3.3
3.84288	3.1
3.94409	3.0
4.04530	2.8
4.14651	2.6
4.24772	2.4
4.34893	2.2
4.45014	2.1
4.55135	1.9
4.65255	1.8
4.75376	1.7
4.85497	1.5
4.95618	1.4
5.05739	1.3
5.15860	1.2
5.25981	1.1
5.36102	1.0
5.46223	0.9
5.56344	0.8
5.66465	0.7
5.76586	0.7
5.86707	0.6
5.96827	0.5
6.06948	0.5
6.17069	0.4
6.27190	0.4
6.37311	0.3
6.47432	0.3
6.57553	0.2
6.67673	0.2
6.77794	0.1
6.87914	0.1
6.98035	0.1
7.08154	0.1
7.18273	0.1
7.28391	0.0
7.38507	0.0
7.48620	0.0
7.58727	0.0

Table S112 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating $(HF)_1(H_2O)_1(HCl)_2$, i.e. $f1 = f2$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−5.46288	0.0	0.00000	11.2
−5.31122	0.0	+0.15183	11.1
−5.15932	0.0	+0.30323	11.0
−5.00735	0.1	+0.45507	10.7
−4.85536	0.1	+0.60682	10.4
−4.70336	0.2	+0.75831	10.1
−4.55135	0.2	+0.90974	9.8
−4.39934	0.3	+1.06165	9.4
−4.24732	0.4	+1.21355	9.0
−4.09531	0.5	+1.36550	8.7
−3.94330	0.6	+1.51731	8.3
−3.79128	0.8	+1.66911	7.8
−3.63926	0.9	+1.82084	7.4
−3.48725	1.1	+1.97207	6.9
−3.33523	1.3	+2.12326	6.5
−3.18322	1.5	+2.27517	6.1
−3.03120	1.7	+2.42715	5.8
−2.87919	1.9	+2.57916	5.4
−2.72717	2.2	+2.73117	5.1
−2.57516	2.5	+2.88318	4.8
−2.42314	2.8	+3.03519	4.5
−2.27113	3.1	+3.18721	4.3
−2.11911	3.5	+3.33922	4.0
−1.96710	3.8	+3.49124	3.8
−1.81508	4.2	+3.64326	3.6
−1.66307	4.7	+3.79527	3.4
−1.51106	5.1	+3.94729	3.3
−1.35905	5.6	+4.09931	3.1
−1.20705	6.2	+4.25132	3.0
−1.05513	6.7	+4.40334	2.8
−0.90658	7.3	+4.55535	2.7
−0.75669	8.3	+4.70737	2.6
−0.60490	9.5	+4.85938	2.5
−0.45309	10.4	+5.01139	2.5
−0.30180	10.9	+5.16338	2.4
−0.15184	11.1	+5.31537	2.4
0.00000	11.2	+5.46730	2.3
		+5.61913	2.3
		+5.77061	2.3
		+5.92138	2.3

Table S113 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating $(HF)_1(H_2O)_1(HCl)_2$, i.e. $f1 = f3$

Reaction Coordinate	Energy
0.00000	10.7
0.10290	10.6
0.20560	10.3
0.30837	9.9
0.41068	9.5
0.51311	9.2
0.61592	8.9
0.71886	8.5
0.82180	8.2
0.92475	7.8
1.02767	7.4
1.13058	7.0
1.23349	6.6
1.33638	6.2
1.43914	5.8
1.54184	5.5
1.64468	5.2
1.74762	4.9
1.85058	4.6
1.95354	4.3
2.05650	4.0
2.15946	3.7
2.26243	3.5
2.36539	3.2
2.46836	3.0
2.57132	2.8
2.67429	2.6
2.77725	2.4
2.88022	2.2
2.98318	2.0
3.08615	1.9
3.18911	1.7
3.29208	1.5
3.39504	1.4
3.49801	1.3
3.60097	1.1
3.70394	1.0
3.80690	0.9
3.90987	0.8
4.01283	0.7
4.11580	0.6
4.21876	0.6
4.32173	0.5
4.42469	0.4
4.52765	0.4
4.63061	0.3
4.73357	0.3
4.83652	0.2
4.93947	0.2
5.04240	0.1
5.14533	0.1
5.24823	0.1
5.35110	0.1
5.45394	0.1
5.55676	0.0
5.65958	0.0
5.76243	0.0
5.86532	0.0
5.96824	0.0

Table S114 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating trans $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$ with $f2 = f3$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−5.04144	2.0	0.00000	8.0
−4.89041	2.1	+0.15275	8.0
−4.73834	2.1	+0.30334	7.8
−4.58561	2.1	+0.45590	7.3
−4.43269	2.2	+0.60864	6.4
−4.27972	2.2	+0.76087	5.5
−4.12673	2.3	+0.90918	4.9
−3.97373	2.4	+1.06200	4.3
−3.82074	2.5	+1.21498	3.8
−3.66774	2.7	+1.36798	3.4
−3.51476	2.8	+1.52098	3.0
−3.36177	3.0	+1.67399	2.6
−3.20885	3.2	+1.82699	2.2
−3.05594	3.4	+1.97999	1.9
−2.90330	3.6	+2.13300	1.6
−2.75067	3.8	+2.28600	1.4
−2.59793	4.0	+2.43900	1.1
−2.44507	4.2	+2.59200	0.9
−2.29219	4.5	+2.74500	0.8
−2.13922	4.7	+2.89800	0.6
−1.98625	5.0	+3.05099	0.5
−1.83326	5.2	+3.20397	0.4
−1.68027	5.5	+3.35694	0.3
−1.52726	5.8	+3.50989	0.2
−1.37429	6.1	+3.66280	0.1
−1.22130	6.5	+3.81563	0.1
−1.06850	6.8	+3.96829	0.1
−0.91593	7.1	+4.12072	0.0
−0.76351	7.4	+4.27301	0.0
−0.61074	7.6	+4.42547	0.0
−0.45832	7.8		
−0.30542	7.9		
−0.15265	8.0		
0.00000	8.0		

Table S115 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating cis $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O{\uparrow})_2(HCl)_1$ with $f2 = f3$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−5.16589	2.1	0.00000	8.4
−5.00578	2.1	+0.16124	8.4
−4.84589	2.1	+0.32062	8.2
−4.68482	2.2	+0.48135	7.8
−4.52326	2.2	+0.64276	7.0
−4.36157	2.3	+0.80399	6.0
−4.19984	2.3	+0.96118	5.2
−4.03809	2.4	+1.12227	4.6
−3.87634	2.6	+1.28398	4.1
−3.71460	2.7	+1.44573	3.6
−3.55284	2.9	+1.60749	3.1
−3.39112	3.0	+1.76924	2.7
−3.22939	3.2	+1.93100	2.3
−3.06773	3.5	+2.09275	2.0
−2.90612	3.7	+2.25451	1.7
−2.74493	3.9	+2.41626	1.4
−2.58359	4.2	+2.57802	1.2
−2.42211	4.5	+2.73977	1.0
−2.26048	4.8	+2.90152	0.8
−2.09883	5.0	+3.06326	0.6
−1.93709	5.3	+3.22500	0.5
−1.77537	5.6	+3.38673	0.4
−1.61362	6.0	+3.54843	0.3
−1.45188	6.3	+3.71010	0.2
−1.29014	6.6	+3.87170	0.2
−1.12856	7.0	+4.03319	0.1
−0.96703	7.3	+4.19446	0.1
−0.80652	7.7	+4.35560	0.1
−0.64518	8.0	+4.51681	0.0
−0.48428	8.2	+4.67823	0.0
−0.32286	8.3	+4.83982	0.0
−0.16135	8.4		
0.00000	8.4		

Table S116 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating trans $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_1$ with $f2 = f4$

Reaction Coordinate	Energy
0.00000	6.4
0.12228	6.3
0.24462	6.1
0.36698	5.9
0.48924	5.7
0.61189	5.5
0.73455	5.2
0.85726	4.9
0.97993	4.6
1.10260	4.4
1.22522	4.0
1.34782	3.7
1.47035	3.4
1.59266	3.0
1.71506	2.7
1.83772	2.5
1.96042	2.2
2.08313	2.0
2.20585	1.7
2.32857	1.5
2.45129	1.3
2.57401	1.2
2.69674	1.0
2.81946	0.8
2.94219	0.7
3.06491	0.6
3.18764	0.5
3.31036	0.4
3.43309	0.3
3.55580	0.2
3.67852	0.2
3.80122	0.1
3.92389	0.1
4.04650	0.0
4.16897	0.0
4.29115	0.0
4.41310	0.0

Table S117 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating cis $(HF)_1(H_2O)_2(HCl)_1$, i.e. $(HF)_1(H_2O\uparrow)_2(HCl)_1$ with $f2 = f4$

Reaction Coordinate	Energy
0.00000	6.6
0.12240	6.4
0.24441	6.2
0.36665	6.0
0.48875	5.8
0.61123	5.5
0.73370	5.3
0.85624	5.0
0.97873	4.7
1.10123	4.4
1.22366	4.1
1.34609	3.8
1.46845	3.4
1.59059	3.1
1.71279	2.8
1.83527	2.5
1.95778	2.3
2.08032	2.0
2.20286	1.8
2.32540	1.6
2.44794	1.4
2.57049	1.2
2.69303	1.0
2.81558	0.9
2.93813	0.7
3.06067	0.6
3.18322	0.5
3.30577	0.4
3.42831	0.3
3.55085	0.2
3.67339	0.2
3.79591	0.1
3.91841	0.1
4.04087	0.1
4.16320	0.0
4.28530	0.0
4.40712	0.0

Table S118 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for the isomer of $(HF)_1(H_2O)_3$ with alternating relative orientations of dangling hydrogen atoms, i.e. $f2 = f4 = H_2O\uparrow$ and $f3 = H_2O\downarrow$

Reaction Coordinate	Energy
0.00000	15.7
0.10552	15.5
0.21093	15.0
0.31651	14.3
0.42204	13.3
0.52756	12.1
0.63306	10.9
0.73853	9.7
0.84360	8.7
0.94820	8.0
1.05361	7.3
1.15923	6.7
1.26487	6.1
1.37052	5.6
1.47616	5.1
1.58180	4.6
1.68745	4.2
1.79309	3.7
1.89873	3.3
2.00438	3.0
2.11002	2.6
2.21567	2.3
2.32131	2.0
2.42696	1.8
2.53260	1.5
2.63825	1.3
2.74389	1.1
2.84954	0.9
2.95518	0.8
3.06083	0.6
3.16647	0.5
3.27212	0.4
3.37776	0.3
3.48340	0.2
3.58904	0.1
3.69468	0.1
3.80030	0.1
3.90587	0.0
4.01113	0.0
4.11388	0.0

Table S119 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for the isomer of $(HF)_1(H_2O)_3$ with adjacent dangling hydrogen atoms on the same side of the ring, i.e. $f2 = f3 = H_2O\uparrow$ and $f4 = H_2O\downarrow$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−4.10999	0.0	0.00000	16.1
−4.00529	0.0	+0.10525	15.9
−3.89995	0.0	+0.21055	15.4
−3.79450	0.1	+0.31597	14.6
−3.68903	0.1	+0.42135	13.6
−3.58355	0.2	+0.52670	12.4
−3.47807	0.3	+0.63204	11.1
−3.37258	0.3	+0.73734	10.0
−3.26710	0.4	+0.84225	9.0
−3.16161	0.6	+0.94675	8.2
−3.05612	0.7	+1.05202	7.6
−2.95064	0.9	+1.15748	6.9
−2.84515	1.0	+1.26296	6.3
−2.73967	1.2	+1.36844	5.8
−2.63418	1.4	+1.47392	5.3
−2.52869	1.7	+1.57941	4.8
−2.42321	1.9	+1.68489	4.3
−2.31772	2.2	+1.79038	3.9
−2.21223	2.5	+1.89586	3.5
−2.10675	2.8	+2.00135	3.1
−2.00126	3.1	+2.10683	2.8
−1.89577	3.5	+2.21232	2.5
−1.79029	3.9	+2.31781	2.2
−1.68480	4.4	+2.42329	1.9
−1.57932	4.8	+2.52878	1.7
−1.47383	5.3	+2.63427	1.4
−1.36835	5.8	+2.73975	1.2
−1.26287	6.4	+2.84524	1.1
−1.15739	7.0	+2.95073	0.9
−1.05193	7.6	+3.05621	0.7
−0.94675	8.3	+3.16170	0.6
−0.84236	9.1	+3.26719	0.5
−0.73733	10.1	+3.37267	0.4
−0.63200	11.2	+3.47816	0.3
−0.52666	12.5	+3.58364	0.2
−0.42130	13.6	+3.68912	0.2
−0.31593	14.6	+3.79459	0.1
−0.21051	15.4	+3.90004	0.1
−0.10524	15.9	+4.00536	0.1
0.00000	16.1	+4.10934	0.1

Table S120 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for $(H_2O)_4$

Reaction Coordinate	Energy
0.00000	22.9
0.10158	22.5
0.20311	21.6
0.30466	20.1
0.40620	18.3
0.50771	16.4
0.60911	14.7
0.70991	13.4
0.81035	12.4
0.91165	11.6
1.01317	10.8
1.11473	10.0
1.21628	9.3
1.31784	8.6
1.41940	7.9
1.52096	7.3
1.62252	6.7
1.72409	6.2
1.82565	5.7
1.92721	5.2
2.02877	4.7
2.13033	4.3
2.23189	3.9
2.33345	3.5
2.43501	3.1
2.53657	2.8
2.63813	2.5
2.73969	2.2
2.84125	1.9
2.94282	1.7
3.04438	1.4
3.14594	1.2
3.24750	1.0
3.34906	0.9
3.45062	0.7
3.55218	0.6
3.65375	0.5
3.75531	0.4
3.85687	0.3
3.95843	0.2
4.05999	0.1
4.16155	0.1
4.26310	0.0
4.36462	0.0
4.46577	0.0
4.56171	0.0

Table S121 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for the isomer of $(H_2O)_3(HCl)_1$ with alternating relative orientations of dangling hydrogen atoms, i.e. $f1 = f3 = H_2O\uparrow$ and $f2 = H_2O\downarrow$

Reaction Coordinate	Energy
0.00000	6.5
0.14564	6.4
0.29054	6.3
0.43588	6.1
0.58104	5.8
0.72610	5.5
0.87154	5.2
1.01726	4.8
1.16297	4.5
1.30872	4.2
1.45440	3.9
1.60009	3.6
1.74565	3.2
1.89117	2.9
2.03642	2.6
2.18155	2.2
2.32709	2.0
2.47280	1.7
2.61852	1.5
2.76426	1.3
2.91000	1.1
3.05575	0.9
3.20150	0.7
3.34725	0.6
3.49300	0.5
3.63875	0.4
3.78449	0.3
3.93021	0.2
4.07590	0.1
4.22152	0.1
4.36700	0.1
4.51224	0.0
4.65722	0.0
4.80233	0.0

Table S122 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for the isomer of $(H_2O)_3(HCl)_1$ with adjacent dangling hydrogen atoms on the same side of the ring, i.e. $f1 = f2 = H_2O\uparrow$ and $f3 = H_2O\downarrow$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−4.79897	0.0	0.00000	6.7
−4.65377	0.0	+0.14509	6.7
−4.50882	0.0	+0.29031	6.6
−4.36376	0.1	+0.43556	6.4
−4.21844	0.1	+0.58075	6.2
−4.07294	0.1	+0.72578	5.8
−3.92735	0.2	+0.87080	5.5
−3.78171	0.2	+1.01641	5.2
−3.63605	0.3	+1.16203	4.8
−3.49039	0.4	+1.30770	4.5
−3.34471	0.6	+1.45334	4.2
−3.19904	0.7	+1.59900	3.9
−3.05336	0.8	+1.74456	3.6
−2.90768	1.0	+1.89010	3.2
−2.76201	1.2	+2.03555	2.9
−2.61634	1.4	+2.18076	2.5
−2.47068	1.7	+2.32574	2.2
−2.32503	1.9	+2.47127	2.0
−2.17943	2.2	+2.61689	1.7
−2.03396	2.5	+2.76255	1.5
−1.88912	2.8	+2.90821	1.2
−1.74386	3.2	+3.05388	1.0
−1.59840	3.6	+3.19955	0.9
−1.45285	4.0	+3.34523	0.7
−1.30729	4.3	+3.49091	0.6
−1.16163	4.6	+3.63658	0.5
−1.016 00	5.0	+3.78225	0.3
−0.87034	5.3	+3.92791	0.3
−0.72493	5.6	+4.07355	0.2
−0.57983	6.0	+4.21915	0.1
−0.43505	6.3	+4.36468	0.1
−0.28979	6.5	+4.51008	0.0
−0.14525	6.7	+4.65527	0.0
0.00000	6.7	+4.80036	0.0
		+4.94557	0.0
		+5.09100	0.0

Table S123 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating trans $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_2$ with $f1 = f2$

Reaction Coordinate	Energy
0.00000	6.7
0.10882	6.6
0.21713	6.4
0.32570	6.3
0.43424	6.1
0.54302	5.9
0.65183	5.7
0.76068	5.5
0.86951	5.3
0.97836	5.1
1.08720	4.9
1.19604	4.7
1.30488	4.5
1.41372	4.3
1.52254	4.1
1.63137	3.9
1.74018	3.8
1.84897	3.6
1.95774	3.4
2.06649	3.2
2.17519	3.0
2.28389	2.8
2.39266	2.6
2.50148	2.4
2.61031	2.2
2.71916	2.0
2.82800	1.9
2.93685	1.7
3.04569	1.6
3.15454	1.4
3.26339	1.3
3.37224	1.1
3.48109	1.0
3.58994	0.9
3.69879	0.8
3.80764	0.7
3.91649	0.6
4.02534	0.5
4.13419	0.5
4.24304	0.4
4.35188	0.3
4.46073	0.3
4.56958	0.2
4.67842	0.2
4.78727	0.1
4.89611	0.1
5.00495	0.1
5.11377	0.0
5.22258	0.0
5.33133	0.0
5.43991	0.0

Table S124 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for non-alternating cis $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_2(HCl)_2$ with $f1 = f2$

Reaction Coordinate	Energy
0.00000	7.4
0.10787	7.3
0.21557	7.2
0.32324	7.0
0.43088	6.8
0.53880	6.6
0.64678	6.3
0.75479	6.1
0.86280	5.9
0.97082	5.7
1.07883	5.5
1.18685	5.3
1.29486	5.0
1.40288	4.8
1.51088	4.6
1.61888	4.4
1.72686	4.2
1.83482	4.0
1.94276	3.8
2.05068	3.5
2.15853	3.3
2.26638	3.1
2.37432	2.9
2.48232	2.7
2.59033	2.5
2.69835	2.3
2.80636	2.1
2.91438	1.9
3.02240	1.8
3.13043	1.6
3.23845	1.5
3.34647	1.3
3.45450	1.2
3.56252	1.1
3.67054	1.0
3.77857	0.8
3.88659	0.7
3.99461	0.6
4.10264	0.6
4.21066	0.5
4.31868	0.4
4.42671	0.3
4.53473	0.3
4.64275	0.2
4.75078	0.2
4.85880	0.1
4.96682	0.1
5.07484	0.1
5.18286	0.0
5.29088	0.0
5.39890	0.0
5.50692	0.0
5.61491	0.0

Table S125 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating trans $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_1(H_2O\downarrow)_1(HCl)_2$ with $f1 = f3$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−4.32350	0.0	0.00000	4.3
−4.18841	0.0	+0.13358	4.3
−4.05344	0.0	+0.26872	4.2
−3.91852	0.0	+0.40392	4.2
−3.78353	0.1	+0.53918	4.1
−3.64844	0.1	+0.67444	4.1
−3.51327	0.1	+0.80971	4.1
−3.37806	0.2	+0.94498	4.0
−3.24282	0.2	+1.08023	4.0
−3.10756	0.3	+1.21533	4.0
−2.97230	0.4		
−2.83703	0.4		
−2.70175	0.5		
−2.56648	0.6		
−2.43120	0.7		
−2.29593	0.9		
−2.16065	1.0		
−2.02537	1.1		
−1.89009	1.3		
−1.75481	1.5		
−1.61953	1.7		
−1.48425	1.9		
−1.34897	2.1		
−1.21370	2.3		
−1.07842	2.5		
−0.94315	2.8		
−0.80788	3.1		
−0.67267	3.3		
−0.53798	3.6		
−0.40360	3.9		
−0.26865	4.1		
−0.13378	4.3		
0.00000	4.3		

Table S126 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for alternating cis $(H_2O)_2(HCl)_2$, i.e. $(H_2O\uparrow)_2(HCl)_2$ with $f1 = f3$

Reaction Coordinate	Energy	Reaction Coordinate	Energy
−1.22316	4.1	0.00000	4.4
−1.08725	4.1	+0.13589	4.3
−0.95119	4.1	+0.27084	4.2
−0.81508	4.1	+0.40667	3.9
−0.67900	4.2	+0.54184	3.7
−0.54289	4.2	+0.67725	3.4
−0.40689	4.3	+0.81320	3.1
−0.27078	4.3	+0.94930	2.8
−0.13516	4.3	+1.08540	2.6
0.00000	4.4	+1.22151	2.3
		+1.35762	2.1
		+1.49373	1.9
		+1.62984	1.7
		+1.76595	1.5
		+1.90206	1.3
		+2.03818	1.2
		+2.17429	1.0
		+2.31040	0.9
		+2.44651	0.7
		+2.58262	0.6
		+2.71873	0.5
		+2.85483	0.4
		+2.99094	0.4
		+3.12703	0.3
		+3.26312	0.2
		+3.39920	0.2
		+3.53524	0.1
		+3.67124	0.1
		+3.80716	0.1
		+3.94299	0.1
		+4.07875	0.0
		+4.21455	0.0
		+4.35047	0.0

Table S127 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for $(H_2O)_1(HCl)_3$

Reaction Coordinate	Energy
0.00000	12.2
0.12089	12.0
0.24178	11.8
0.36298	11.6
0.48404	11.2
0.60499	10.8
0.72579	10.4
0.84696	10.0
0.96811	9.6
1.08928	9.1
1.21044	8.6
1.33157	8.0
1.45227	7.5
1.57269	7.0
1.69379	6.6
1.81505	6.3
1.93632	5.9
2.05760	5.5
2.17888	5.2
2.30016	4.9
2.42144	4.6
2.54273	4.3
2.66401	4.0
2.78529	3.7
2.90657	3.4
3.02786	3.2
3.14914	3.0
3.27042	2.7
3.39171	2.5
3.51299	2.3
3.63427	2.1
3.75556	1.9
3.87684	1.8
3.99812	1.6
4.11940	1.4
4.24069	1.3
4.36197	1.2
4.48326	1.0
4.60454	0.9
4.72582	0.8
4.84711	0.7
4.96839	0.6
5.08967	0.5
5.21096	0.5
5.33224	0.4
5.45352	0.3
5.57480	0.3
5.69608	0.2
5.81736	0.2
5.93864	0.1
6.05992	0.1
6.18118	0.1
6.30244	0.0
6.42366	0.0
6.54481	0.0
6.66574	0.0

Table S128 MP2/haTZ energies (in kcal mol^{-1}) and reaction coordinates (in bohr·amu$^{1/2}$) for each point on the IRC calculation for $(HCl)_4$

Reaction Coordinate	Energy
0.00000	26.2
0.10109	25.9
0.20214	25.1
0.30321	23.9
0.40427	22.4
0.50533	20.8
0.60638	19.1
0.70735	17.7
0.80785	16.6
0.90673	15.9
1.00738	15.4
1.10843	14.8
1.20949	14.3
1.31056	13.8
1.41163	13.3
1.51270	12.8
1.61378	12.3
1.71485	11.9
1.81592	11.4
1.91699	11.0
2.01806	10.6
2.11913	10.2
2.22021	9.8
2.32128	9.4
2.42235	9.0
2.52342	8.6
2.62449	8.3
2.72557	7.9
2.82664	7.6
2.92771	7.3
3.02878	6.9
3.12985	6.6
3.23092	6.4
3.33200	6.1
3.43307	5.8
3.53414	5.5
3.63521	5.3
3.73628	5.0
3.83736	4.8
3.93843	4.5
4.03950	4.3
4.14057	4.1
4.24164	3.9
4.34272	3.7
4.44379	3.5
4.54486	3.3
4.64593	3.1
4.74700	2.9
4.84808	2.8
4.94915	2.6
5.05022	2.4
5.15129	2.3
5.25237	2.1
5.35344	2.0
5.45451	1.9
5.55558	1.7
5.65666	1.6
5.75773	1.5
5.85880	1.4
5.95987	1.3
6.06094	1.2
6.16202	1.1
6.26309	1.0
6.36416	0.9
6.46523	0.8
6.56631	0.8
6.66738	0.7
6.76845	0.6
6.86953	0.6
6.97060	0.5
7.07167	0.4
7.17274	0.4
7.27382	0.3
7.37489	0.3
7.47596	0.3
7.57704	0.2
7.67811	0.2
7.77919	0.2
7.88026	0.1
7.98133	0.1
8.08241	0.1
8.18348	0.1
8.28456	0.0
8.38563	0.0
8.48671	0.0
8.58778	0.0

6 Correlation Analysis

Reference 44 attempted to establish correlations between the barrier height and other properties of the homogeneous trimers, tetramers and pentamers. Although some interesting relationships were identified, the sample size was too limited to draw any definitive conclusions. With the present extension to heterogenous clusters, we also analyzed a wide range of relationships between various data types. Following the suggestion of a reviewer, we also employed the molecular tailoring approach (MTA) at the MP2/haTZ level of theory to estimate the individual hydrogen bond strengths.[S1,S2] The MTA hydrogen bond energies are obtained using a fragmentation scheme outlined in references S1 and S2. To estimate a hydrogen bond energy in a cyclic tetramer system, for example, two trimer fragments would be created, one of which (F1) is absent the hydrogen bond donor monomer fragment, and the other of which (F2) is absent the hydrogen bond acceptor monomer fragment. Single-point MP2/haTZ energies are computed for both of these trimer fragments (E_{F1} and E_{F2}), but the sum of E_{F1} and E_{F2} double counts the dimer fragment not involved in the hydrogen bonding (F3). Subtracting the energy of this dimer fragment (E_{F3}) from the sum of the trimer fragment energies recovers the energy of the parent tetramer (E_m) minus the energy of the hydrogen bond. Thus, each individual hydrogen bond energy is obtained as $(E_{F1} + E_{F2} - E_{F3}) - E_m$.[S1,S2] This procedure is repeated four times to obtain each individual hydrogen bond strength for our cyclic tetramers, and an analogous procedure must be repeated three times for a cyclic trimer and five times for a cyclic pentamer to find all individual hydrogen bond energies.

We first examined homogeneous clusters to check if the MTA hydrogen bond strengths could reproduce the strong correlations identified in our previous study (Figure 5 in Ref. 44) between the dissociation energy per fragment (D_e/n) and properties of the CPT transition state (such as the magnitude of the imaginary vibrational frequency ($|\omega_i|$) and the barrier height per fragment ($\Delta E^{\ddagger}/n$)). For C_1 systems like $(H_2O)_3$, $(H_2O)_5$, and $(HCl)_5$, the individual hydrogen bond strengths obtained via MTA are similar, but not equivalent, for each hydrogen bond. In these cases, the individual hydrogen bond energies in each system have been added together and divided by the number of fragments in order to obtain an average MTA hydrogen bond energy. Both measures of the hydrogen bond strength yield very strong correlations with those TS properties ($R^2 > 0.98$) for $(HF)_n$ and $(H_2O)_n$, where $n = 3$, 4, 5, but not for $(HCl)_n$, where R^2 was below 0.27 (as shown in Figure S1).

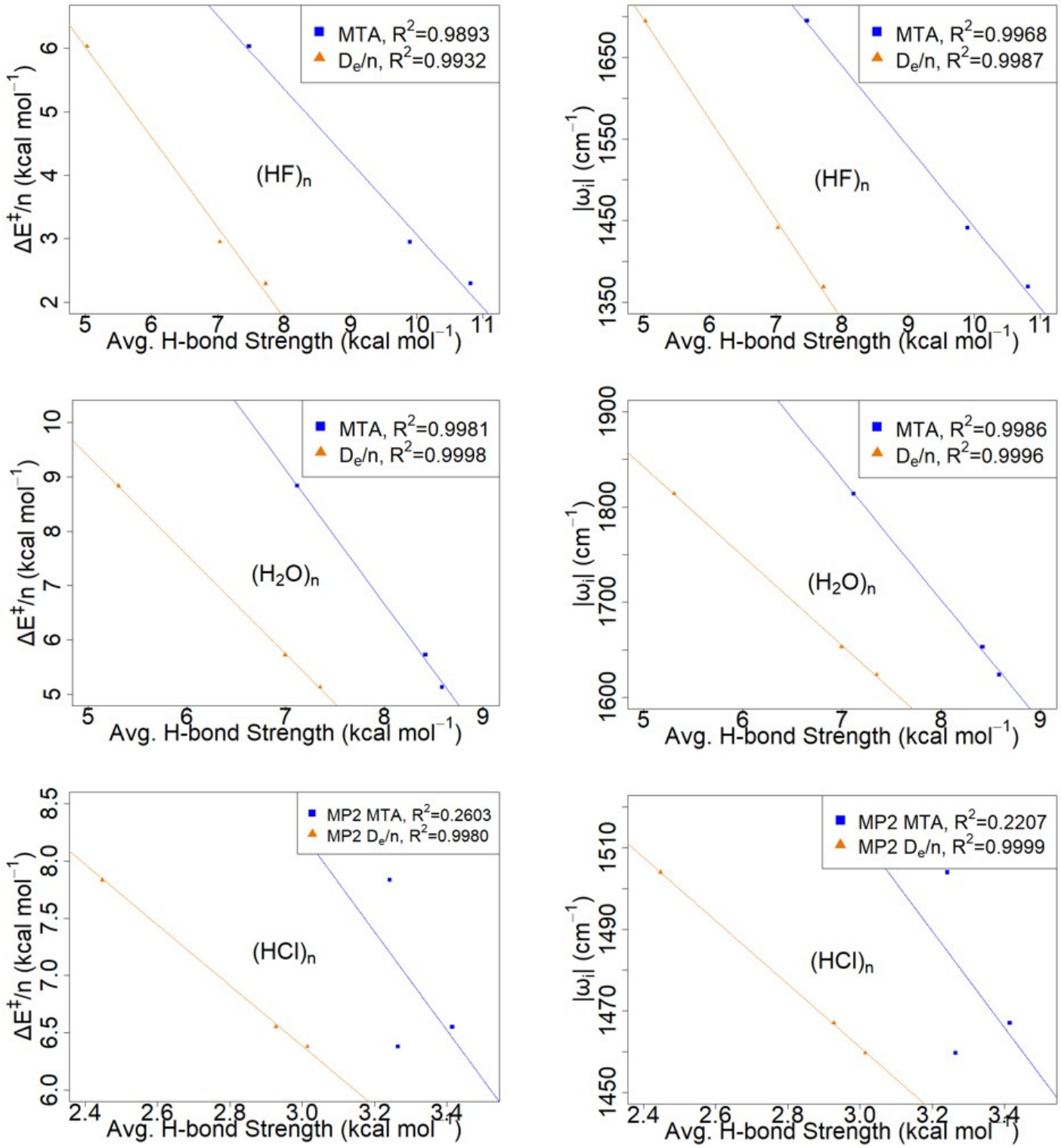

Figure S1 The orange triangle data points show examples of correlations with average hydrogen bond strengths reported in the previous study (Ref. 44) for the homogeneous $(HF)_n$ clusters (top row), $(H_2O)_n$ clusters (middle row), and $(HCl)_n$ clusters (bottom row), as measured by D_e/n for $n = 3$, 4 and 5, whereas the blue square data points show the same relationships with the average MTA hydrogen bond strengths. All data was obtained at the MP2/haTZ level of theory.

We next examined relationships among the data for all 30 systems. However, the strong correlations for $(HF)_n$ and $(H_2O)_n$ do NOT extend to the heterogeneous systems, and R^2 drops below 0.5 for both relationships when they are included. Furthermore, no reasonable general correlations were found for related energetic or structural properties (e.g., interaction energy (E_{int}), relaxation/distortion energy of monomers (E_{rlx}), covalent bond length change of donors (ΔR)) in these 30 $(HF)_x(H_2O)_y(HCl)_z$ systems, as can be seen in Table S129.

Table S129 R^2 values for various parameters related to hydrogen bond strengths, including dissociation energy (D_e), interaction energy (E_{int}), relaxation energy (E_{rlx}), and bond length distortion (ΔR), correlated with barrier height ($\Delta E^{\ddagger}$), barrier height divided by the number of fragments ($\Delta E^{\ddagger}/n$), and imaginary frequencies ($|\omega_i|$)

R^2 (N=30)	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}/n$	$\lvert\omega_i\rvert$
D_e	0.3278	0.4527	0.1147
E_{int}	0.3527	0.4789	0.1361
D_e/n	0.2837	0.3188	0.0755
E_{int}/n	0.3154	0.3499	0.0985
Sum of E_{rlx}	0.4739	0.5871	0.2275
Average E_{rlx}	0.4707	0.4874	0.2688
Sum of ΔR	0.5166	0.6048	0.1943
Average ΔR	0.5084	0.5347	0.1735

We also examined the same relationships for subsets of hydrogen bond types as suggested by a reviewer. Although no good correlations were identified for the 8 OH$\cdots$F interactions, the 9 OH$\cdots$O interactions or the 12 FH$\cdots$O interactions ($R^2 < 0.5$ for each), we observed a good correlation between the 9 FH$\cdots$F interactions and the barrier height ($R^2 > 0.9$ for both $\Delta E^{\ddagger}$ and $\Delta E^{\ddagger}/n$) but not the magnitude of the imaginary frequency ($R^2 < 0.6$ for $|\omega_i|$). These results are summarized in Table S130. With such a small sample size for a selective subset of interactions, any conclusions about the underlying chemical physics drawn from the two strongest correlations would be highly speculative, and a recent article in Science[S3] discussed the pitfalls associated with drawing conclusions from selectively chosen data.

Table S130 R^2 values for various types of hydrogen bond strengths correlated with barrier height ($\Delta E^{\ddagger}$, barrier height divided by the number of fragments ($\Delta E^{\ddagger}/n$), and imaginary frequencies ($|\omega_i|$)

R^2	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}/n$	$\lvert\omega_i\rvert$
OH$\cdots$F (N=8)	0.1509	0.1904	0.3668
OH$\cdots$O (N=9)	0.2280	0.4053	0.1675
FH$\cdots$O (N=12)	0.3216	0.4940	0.4860
FH$\cdots$F (N=9)	0.9540	0.9070	0.5178

Lastly, we attempted to use the MTA hydrogen bond strengths to gain some insight into the non-zero relative energies. The difference in energy between the reactants and products for the CPT process are compared between CCSD(T), MP2, and using the sum of hydrogen bond energies via the MTA method. For example, the sum of the MTA hydrogen bond energies for the $(HF)_1(H_2O)_2(HCl)_1$ reactant is 34.5 kcal mol^{-1}, and for the product the sum is 34.6 kcal mol^{-1}. The difference in the reactant and product is therefore -0.1 kcal mol^{-1}, which can be seen in the last row of Table S131. However, the sum of the hydrogen bond energies qualitatively fails to reproduce the relative energy for one of these 4 systems as shown in Table S131.

Table S131 Differences in energy between CPT reactants and products in systems where this ΔE value is not 0, compared between CCSD(T) energetics, MP2 energetics, and the sum of hydrogen bond strengths by MTA (all in kcal mol^{-1})

ΔE (kcal mol^{-1})	CCSD(T)	MP2	Hydrogen Bond Sum (MP2)
$(HF)_1(H_2O)_1(HCl)_1$	+2.3	+2.1	+2.0
$(HF)_2(H_2O)_1(HCl)_1$	+2.7	+2.4	+1.6
$(HF)_1(H_2O)_1(HCl)_2$	+2.5	+2.2	+2.0
$(HF)_1(H_2O)_2(HCl)_1$	+2.4	+2.0	-0.1

References

[S1] D. Patkar, M. B. Ahirwar, S. R. Gadre and M. M. Deshmukh, *J. Phys. Chem. A*, 2021, **125**, 8836-8845.

[S2] D. Patkar, M. B. Ahirwar, S. P. Shrivastava and M. M. Deshmukh, *New J. Chem.*, 2022, **46**, 2368-2379.

[S3] O'Grady C., *Science*, 2025, **390**, 222-223.