Supplementary Information for:

Electrostatically Embedded Many-Body Method for Dipole Moments, Partial Atomic Charges, and Charge Transfer

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To be published in *Phys. Chem. Chem. Phys.*

This supporting information was updated on December 21, 2011
Length including this page: 32 pages

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Table S1. Dipole Moments and Errors for Forty-Four Configurations of $(NH_3)(H_2O)_{11}$

Step	Conventional Dipole Moment (D)	Error in EE-1B Dipole Moment (D)	Error in EE-PA Dipole Moment (D)	Error in EE-3B Dipole Moment (D)
1	13.967	-1.085	-0.132	0.091
2	13.819	-1.065	-0.126	0.079
3	14.079	-1.056	-0.111	0.074
4	14.107	-1.060	-0.112	0.072
5	14.105	-1.058	-0.114	0.079
6	14.550	-1.354	-0.105	0.085
7	14.177	-1.088	-0.112	0.072
8	14.197	-1.099	-0.113	0.074
9	14.158	-1.097	-0.114	0.072
10	13.704	-1.107	-0.108	0.086
11	13.711	-1.114	-0.105	0.080
12	13.703	-1.111	-0.106	0.084
13	13.988	-1.113	-0.108	0.090
14	13.985	-1.112	-0.107	0.085
15	13.935	-1.090	-0.098	0.082
16	13.975	-1.112	-0.107	0.090
17	13.878	-1.074	-0.093	0.084
18	14.093	-1.065	-0.091	0.081
19	13.811	-1.062	-0.092	0.086
20	14.049	-1.186	-0.090	0.083
21	14.130	-1.039	-0.097	0.076
22	13.881	-1.078	-0.093	0.081
23	13.875	-1.079	-0.092	0.078
24	13.840	-1.063	-0.091	0.089
25	13.695	-0.975	-0.081	0.062
26	13.745	-0.989	-0.085	0.072
27	13.708	-0.974	-0.086	0.079
28	13.742	-0.972	-0.085	0.078
29	13.393	-0.864	-0.089	0.081
30	13.738	-0.969	-0.084	0.073
31	13.152	-0.831	-0.083	0.062
32	13.790	-0.969	-0.082	0.071
33	13.778	-0.962	-0.084	0.078
34	13.850	-0.969	-0.084	0.077
35	13.833	-0.961	-0.087	0.076
36	13.807	-0.954	-0.085	0.074
37	13.798	-0.944	-0.085	0.070
38	13.908	-0.913	-0.088	0.079
39	13.912	-0.915	-0.086	0.078
40	14.082	-0.921	-0.086	0.080
41	13.910	-0.821	-0.092	0.083
42	14.186	-0.786	-0.096	0.084

43	13.820	-0.825	-0.091	0.081
44	13.752	-0.800	-0.094	0.070
MSE		-1.015	-0.097	0.079
MUE		1.015	0.097	0.079
RMSE		1.021	0.097	0.079
MUPE		7.3	0.7	0.6

Table S2. Dipole Moments and Errors for Forty-Four Configurations of $(NH_3)_2(H_2O)_{14}$

Step	Conventional Dipole Moment (D)	Error in EE-1B Dipole Moment (D)	Error in EE-PA Dipole Moment (D)	Error in EE-3B Dipole Moment (D)
1	18.354	-0.454	-0.205	0.081
2	18.372	-0.431	-0.206	0.080
3	18.345	-0.421	-0.208	0.095
4	18.423	-0.416	-0.211	0.093
5	18.355	-0.380	-0.228	0.091
6	18.375	-0.403	-0.208	0.070
7	18.354	-0.386	-0.220	0.090
8	17.902	-0.436	-0.198	0.084
9	17.951	-0.458	-0.194	0.089
10	18.095	-0.504	-0.181	0.075
11	18.333	-0.487	-0.189	0.082
12	18.163	-0.530	-0.191	0.056
13	18.085	-0.500	-0.181	0.061
14	18.148	-0.511	-0.176	0.068
15	18.131	-0.510	-0.179	0.089
16	18.501	-0.487	-0.180	0.081
17	18.132	-0.510	-0.176	0.066
18	18.147	-0.504	-0.177	0.081
19	18.208	-0.545	-0.186	0.088
20	18.043	-0.470	-0.192	0.090
21	17.999	-0.522	-0.183	0.063
22	18.008	-0.521	-0.184	0.061
23	18.071	-0.539	-0.182	0.068
24	17.949	-0.553	-0.185	0.086
25	18.124	-0.540	-0.187	0.079
26	18.240	-0.554	-0.186	0.059
27	18.254	-0.559	-0.186	0.072
28	18.188	-0.558	-0.186	0.075
29	18.403	-0.528	-0.193	0.070
30	17.729	-0.567	-0.178	0.092
31	17.733	-0.569	-0.176	0.081
32	17.514	-0.454	-0.181	0.096
33	17.774	-0.568	-0.174	0.065
34	17.633	-0.550	-0.171	0.069
35	17.534	-0.483	-0.159	0.060
36	16.801	-0.491	-0.168	0.069
37	17.542	-0.481	-0.161	0.075
38	17.540	-0.480	-0.160	0.075
39	17.499	-0.478	-0.162	0.058
40	17.678	-0.498	-0.147	0.058
41	17.333	-0.482	-0.162	0.067
42	17.617	-0.544	-0.163	0.086

43	17.444	-0.437	-0.170	0.073
44	17.542	-0.489	-0.158	0.064
MSE		-0.495	-0.183	0.076
MUE		0.495	0.183	0.076
RMSE		0.498	0.184	0.077
MUPE		2.8	1.0	0.4

Table S3a. Dipole Moments and EE-MB Errors for Six Configurations of $[Cl(H_2O)_6]^-$

System	Conventional μ (D)	Error in EE-1B (S1) μ (D)	Error in EE-1B (S2) μ (D)	Error in EE-PA (S1) μ (D)	Error in EE-PA (S2) μ (D)	Error in EE-3B (S1) μ (D)	Error in EE-3B (S2) μ (D)
int1	1.905	-0.289	-0.098	-0.247	-0.241	-0.182	-0.202
int2	1.654	-0.042	-0.198	-0.107	-0.066	-0.010	0.014
int3	8.242	-0.186	-0.075	0.015	-0.006	0.018	-0.006
surf1	8.153	-0.872	-0.724	-0.075	-0.102	-0.011	-0.020
surf2	7.870	-0.352	-0.110	0.088	0.009	-0.003	0.005
surf3	10.330	-0.808	-0.796	0.076	-0.017	0.013	0.016
MSE		-0.425	-0.333	-0.042	-0.070	-0.029	-0.032
MUE		0.425	0.333	0.102	0.073	0.039	0.044
RMSE		0.526	0.452	0.124	0.110	0.075	0.083
MUPE		7.2	6.0	3.7	3.0	1.8	2.0

Table S3b. Dipole Moments and MB Errors for Six Configurations of $[Cl(H_2O)_6]^-$

System	Conventional μ (D)	Error in 1B (S1) μ (D)	Error in 1B (S2) μ (D)	Error in PA (S1) μ (D)	Error in PA (S2) μ (D)	Error in 3B (S1) μ (D)	Error in 3B (S2) μ (D)
int1	1.905	-0.072	1.143	-0.256	-0.324	-0.251	-0.203
int2	1.654	0.503	-0.139	-0.257	-0.003	0.025	-0.007
int3	8.242	-1.163	-0.207	0.050	-0.170	-0.004	0.014
surf1	8.153	-2.346	-1.767	-0.212	-0.354	0.046	0.030
surf2	7.870	-2.113	-0.709	0.069	-0.130	0.063	0.019
surf3	10.330	-3.403	-2.790	0.191	-0.031	0.064	0.077
MSE		-1.432	-0.745	-0.069	-0.169	-0.010	-0.012
MUE		1.600	1.126	0.172	0.169	0.075	0.058
RMSE		1.965	1.460	0.191	0.215	0.111	0.090
MUPE		22.8	21.4	5.8	4.3	2.8	2.1

Table S4. M06-2X/cc-pV(T+d)+ Dipole Moments (D) of $(HF)_m$ Clusters and Average MB and EE-MB Errors

Cluster	Full	1B	PA	3B	EE-1B	EE-PA	EE-3B
hf3_fff	5.523	5.684	5.522	5.523	5.527	5.523	5.523
hf3_ffh	1.821	1.897	1.821	1.820	1.824	1.821	1.820
hf3_fhf	1.874	1.896	1.871	1.874	1.873	1.872	1.874
hf4_ffff	7.329	7.578	7.327	7.329	7.333	7.329	7.329
hf4_fffh	3.621	3.784	3.621	3.621	3.627	3.623	3.621
hf4_ffhf	3.686	3.789	3.682	3.687	3.688	3.685	3.686
hf4_ffhh	0.004	0.004	0.004	0.004	0.004	0.004	0.004
hf4_fhfh	0.004	0.004	0.004	0.004	0.004	0.004	0.004
hf4_fhhf	0.069	0.005	0.067	0.069	0.063	0.067	0.069
hf5_fffff	9.133	9.472	9.130	9.133	9.139	9.134	9.133
hf5_ffffh	5.435	5.685	5.433	5.435	5.441	5.436	5.435
hf5_fffhf	5.493	5.682	5.488	5.493	5.496	5.492	5.493
hf5_ffhff	5.496	5.683	5.492	5.497	5.501	5.497	5.496
hf5_fffhh	1.805	1.890	1.804	1.805	1.806	1.805	1.805
hf5_ffhfh	1.816	1.897	1.815	1.816	1.819	1.817	1.816
hf5_fhffh	1.797	1.896	1.795	1.797	1.801	1.797	1.797
hf5_fhfhf	1.871	1.895	1.867	1.872	1.869	1.869	1.871
hf5_fhhff	1.883	1.889	1.882	1.884	1.882	1.883	1.884
hf5_fhhhf	1.730	1.891	1.729	1.730	1.736	1.732	1.730
MSE[a] (D)		0.112	-0.002	0.000	0.002	0.000	0.000
MUE[b] (D)		0.119	0.002	0.000	0.003	0.001	0.000
RMSE[c] (D)		0.151	0.002	0.000	0.004	0.001	0.000
MUPE[d] (%)		8.4	0.3	0.1	0.7	0.3	0.1

[a]MSE = mean signed error over all $(HF)_m$ clusters for m = 3–5.

[b]MUE = mean unsigned error over all $(HF)_m$ clusters for m = 3–5.

[c]RMSE = root mean squared error over all $(HF)_m$ clusters for m = 3–5.

[d]MUPE = mean unsigned percent error over all $(HF)_m$ clusters for m = 3–5.

Table S5. M06-2X/cc-pV(T+d)+ Dipole Moments (D) of $(HF)_m(H_2O)_n$ Clusters and Average MB and EE-MB Errors

Cluster	Full	1B	PA	3B	EE-1B	EE-PA	EE-3B
whf2_BaCa	4.449	4.286	4.453	4.449	4.441	4.449	4.449
whf2_BaCr	3.838	3.609	3.834	3.838	3.820	3.838	3.838
whf2_BrCr	0.398	0.320	0.409	0.398	0.394	0.399	0.398
whf3_AaBaCa	6.663	6.183	6.649	6.663	6.601	6.663	6.663
whf3_AaBaCr	5.315	4.914	5.312	5.316	5.271	5.314	5.315
whf3_AaBrCr	1.748	1.577	1.741	1.748	1.723	1.746	1.748
whf3_ArBaCa	2.547	2.389	2.541	2.547	2.543	2.544	2.547
whf3_ArBaCr	3.271	3.016	3.263	3.271	3.253	3.271	3.271
whf3_ArBrCr	2.367	2.217	2.365	2.368	2.339	2.371	2.367
w2hf3_a	8.794	8.178	8.788	8.797	8.669	8.782	8.797
w2hf3_opt	11.392	8.717	11.254	11.425	10.382	11.342	11.409
MSE[a] (D)		-0.489	-0.016	0.003	-0.122	-0.006	0.002
MUE[b] (D)		0.489	0.018	0.004	0.122	0.007	0.002
RMSE[c] (D)		0.861	0.042	0.010	0.308	0.015	0.005
MUPE[d] (%)		9.5	0.5	0.0	1.5	0.1	0.0

[a]MSE = mean signed error over all $(HF)_m(H_2O)_n$ clusters shown in the table.

[b]MUE = mean unsigned error over all $(HF)_m(H_2O)_n$ clusters shown in the table.

[c]RMSE = root mean squared error over all $(HF)_m(H_2O)_n$ clusters shown in the table.

[d]MUPE = mean unsigned percent error over all $(HF)_m(H_2O)_n$ clusters shown in the table.

Table S6a. Conventional CHelpG Atomic Charges (in *e*) and EE-MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Int1

#	Atom	Conventional Charge	Error in EE-1B (S1)	Error in EE-1B (S2)	Error in EE-PA (S1)	Error in EE-PA (S2)	Error in EE-3B (S1)	Error in EE-3B (S2)
1	Cl	-0.563	-0.437	-0.424	-0.289	-0.276	-0.223	-0.123
2	O	-0.788	-0.019	-0.020	-0.075	-0.058	0.053	0.000
3	H	0.344	0.040	0.029	0.074	0.055	-0.033	0.016
4	H	0.419	0.003	0.015	0.020	0.021	-0.013	0.012
5	O	-0.795	-0.027	-0.017	-0.065	-0.052	0.036	0.009
6	H	0.337	0.089	0.081	0.080	0.077	-0.034	-0.010
7	H	0.412	-0.016	-0.019	-0.002	-0.008	-0.020	-0.005
8	O	-0.712	-0.106	-0.099	-0.042	-0.037	-0.062	-0.025
9	H	0.346	0.021	0.022	-0.033	-0.028	0.041	0.018
10	H	0.302	0.148	0.141	0.108	0.107	0.063	0.018
11	O	-0.768	-0.095	-0.136	-0.146	-0.069	-0.053	-0.061
12	H	0.384	0.005	-0.003	0.000	0.019	0.025	0.016
13	H	0.264	0.210	0.246	0.267	0.144	0.132	0.084
14	O	-0.764	-0.094	-0.083	-0.073	-0.055	0.032	0.040
15	H	0.378	0.015	0.014	-0.008	-0.016	-0.011	-0.020
16	H	0.266	0.199	0.189	0.126	0.118	0.018	-0.002
17	O	-0.810	-0.036	-0.025	-0.116	-0.098	-0.006	-0.001
18	H	0.377	0.009	0.008	0.027	0.025	0.021	-0.002
19	H	0.369	0.090	0.081	0.145	0.131	0.033	0.035
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.087	0.087	0.089	0.073	0.048	0.026
	RMSE		0.135	0.135	0.119	0.096	0.069	0.041
	MUPE		21.7	21.7	21.6	17.7	11.1	6.1

Table S6b. Conventional CHelpG Atomic Charges (in *e*) and MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Int1

#	Atom	Conventional Charge	Error in 1B (S1)	Error in 1B (S2)	Error in PA (S1)	Error in PA (S2)	Error in 3B (S1)	Error in 3B (S2)
1	Cl	-0.563	-0.437	-0.350	-0.004	-0.049	-0.138	-0.139
2	O	-0.788	0.115	0.115	-0.047	-0.054	0.055	0.025
3	H	0.344	-0.010	-0.010	0.033	0.025	-0.040	-0.004
4	H	0.419	-0.080	-0.080	-0.015	0.030	0.014	-0.002
5	O	-0.795	0.106	0.106	-0.072	-0.054	0.039	-0.004
6	H	0.337	0.008	0.008	0.061	0.068	-0.040	-0.017
7	H	0.412	-0.068	-0.068	0.008	-0.005	-0.011	0.022
8	O	-0.712	0.001	0.001	-0.015	-0.014	-0.040	-0.010
9	H	0.346	0.009	0.009	-0.037	-0.025	0.046	0.010
10	H	0.302	0.054	0.054	0.046	0.054	0.019	0.011
11	O	-0.768	0.081	-0.090	-0.097	-0.002	-0.001	-0.076
12	H	0.384	-0.041	-0.059	-0.015	0.006	0.015	0.011
13	H	0.264	0.080	0.182	0.166	0.027	0.028	0.127
14	O	-0.764	0.058	0.058	-0.065	-0.043	0.021	0.007
15	H	0.378	-0.024	-0.024	-0.024	-0.027	0.022	0.016
16	H	0.266	0.086	0.086	0.090	0.081	-0.016	-0.011
17	O	-0.810	0.113	0.113	-0.064	-0.029	0.018	-0.013
18	H	0.377	-0.029	-0.029	0.002	0.000	0.021	0.014
19	H	0.369	-0.021	-0.021	0.049	0.012	-0.013	0.035
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.075	0.077	0.048	0.032	0.032	0.029
	RMSE		0.119	0.110	0.062	0.039	0.043	0.049
	MUPE		15.4	16.9	11.9	7.8	7.0	7.0

Table S7a. Conventional CHelpG Atomic Charges (in *e*) and EE-MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Int2

#	Atom	Conventional Charge	Error in EE-1B (S1)	Error in EE-1B (S2)	Error in EE-PA (S1)	Error in EE-PA (S2)	Error in EE-3B (S1)	Error in EE-3B (S2)
1	Cl	-0.751	-0.249	-0.228	-0.061	0.001	-0.045	-0.102
2	O	-0.839	0.059	0.062	-0.023	-0.009	0.024	0.014
3	H	0.377	-0.008	-0.010	0.024	0.016	-0.010	-0.008
4	H	0.450	-0.038	-0.040	-0.007	-0.014	0.015	0.012
5	O	-0.831	-0.039	-0.032	-0.052	-0.021	-0.051	-0.080
6	H	0.368	0.113	0.105	0.097	0.068	0.076	0.089
7	H	0.400	-0.011	-0.010	0.000	-0.008	0.005	0.028
8	O	-0.840	0.005	-0.010	-0.010	0.066	0.034	-0.080
9	H	0.421	0.056	0.075	0.080	-0.066	-0.070	0.072
10	H	0.381	-0.023	-0.047	-0.046	-0.022	0.013	0.049
11	O	-0.816	-0.027	-0.013	-0.073	-0.055	0.061	0.038
12	H	0.319	0.122	0.113	0.054	0.049	-0.080	-0.065
13	H	0.379	0.022	0.017	0.024	0.013	0.003	0.013
14	O	-0.712	-0.105	-0.097	-0.024	0.001	0.026	0.019
15	H	0.389	0.062	0.053	0.004	-0.039	-0.022	0.003
16	H	0.335	0.032	0.032	-0.012	-0.008	-0.013	-0.020
17	O	-0.823	-0.010	0.001	-0.034	-0.019	-0.027	-0.027
18	H	0.363	0.006	0.004	-0.036	-0.037	0.030	0.030
19	H	0.432	0.033	0.024	0.096	0.084	0.029	0.018
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.054	0.051	0.040	0.031	0.033	0.040
	RMSE		0.079	0.074	0.050	0.040	0.041	0.050
	MUPE		10.9	10.5	8.4	6.9	6.9	8.1

Table S7b. Conventional CHelpG Atomic Charges (in *e*) and MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Int2

#	Atom	Conventional Charge	Error in 1B (S1)	Error in 1B (S2)	Error in PA (S1)	Error in PA (S2)	Error in 3B (S1)	Error in 3B (S2)
1	Cl	-0.751	-0.249	-0.171	0.129	0.097	-0.016	-0.040
2	O	-0.839	0.168	0.168	0.010	0.024	-0.007	-0.026
3	H	0.377	-0.041	-0.041	-0.008	-0.012	0.005	0.018
4	H	0.450	-0.114	-0.114	-0.032	-0.035	0.041	0.033
5	O	-0.831	0.132	0.132	-0.009	0.010	-0.017	-0.031
6	H	0.368	-0.019	-0.019	0.025	0.007	0.007	0.019
7	H	0.400	-0.050	-0.050	-0.020	-0.016	0.013	0.016
8	O	-0.840	0.129	-0.035	-0.018	0.063	0.045	-0.015
9	H	0.421	-0.065	0.034	0.008	-0.070	-0.069	0.022
10	H	0.381	-0.025	-0.038	-0.022	-0.010	0.011	0.000
11	O	-0.816	0.118	0.118	-0.096	-0.065	0.066	0.029
12	H	0.319	0.029	0.029	0.056	0.038	-0.070	-0.024
13	H	0.379	-0.029	-0.029	0.046	0.034	-0.006	-0.004
14	O	-0.712	0.017	0.017	-0.024	-0.006	0.033	0.017
15	H	0.389	-0.041	-0.041	0.008	-0.005	-0.047	-0.026
16	H	0.335	0.013	0.013	-0.023	-0.022	-0.006	-0.005
17	O	-0.823	0.122	0.122	-0.031	-0.003	0.013	-0.003
18	H	0.363	-0.012	-0.012	-0.014	-0.019	0.015	0.014
19	H	0.432	-0.081	-0.081	0.015	-0.008	-0.010	0.006
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.077	0.067	0.031	0.029	0.026	0.018
	RMSE		0.099	0.084	0.044	0.039	0.034	0.021
	MUPE		12.9	11.6	6.0	5.5	5.5	3.7

Table S8a. Conventional CHelpG Atomic Charges (in *e*) and EE-MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Int3

#	Atom	Conventional Charge	Error in EE-1B (S1)	Error in EE-1B (S2)	Error in EE-PA (S1)	Error in EE-PA (S2)	Error in EE-3B (S1)	Error in EE-3B (S2)
1	Cl	-0.714	-0.286	-0.256	-0.098	-0.057	0.025	0.037
2	O	-0.844	-0.037	-0.048	-0.116	-0.040	-0.018	-0.010
3	H	0.356	0.114	0.106	0.147	0.014	-0.013	-0.003
4	H	0.448	-0.037	-0.047	0.024	0.030	0.037	0.006
5	O	-0.793	-0.048	-0.044	-0.121	-0.111	0.064	0.028
6	H	0.403	0.017	0.025	0.056	0.074	-0.010	-0.009
7	H	0.363	0.057	0.046	0.088	0.067	-0.043	-0.004
8	O	-0.856	0.055	0.059	-0.020	-0.002	0.118	0.075
9	H	0.485	-0.047	-0.049	-0.009	-0.024	-0.083	-0.049
10	H	0.373	-0.009	-0.010	0.015	0.009	-0.070	-0.049
11	O	-0.876	0.033	0.056	-0.079	-0.026	0.015	0.011
12	H	0.388	0.084	0.068	0.048	0.027	-0.041	-0.014
13	H	0.428	-0.056	-0.064	0.020	0.001	0.012	0.004
14	O	-0.865	-0.031	-0.020	-0.068	-0.047	0.036	0.013
15	H	0.398	0.006	0.004	0.004	-0.004	0.017	0.010
16	H	0.401	0.091	0.082	0.115	0.097	-0.072	-0.046
17	O	-0.798	-0.012	-0.005	-0.087	-0.059	0.020	0.017
18	H	0.341	0.131	0.122	0.051	0.028	0.013	-0.021
19	H	0.366	-0.027	-0.025	0.031	0.023	-0.006	0.002
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.062	0.060	0.063	0.039	0.038	0.021
	RMSE		0.088	0.082	0.076	0.050	0.048	0.029
	MUPE		12.8	12.2	12.3	7.6	7.3	4.1

Table S8b. Conventional CHelpG Atomic Charges (in *e*) and MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Int3

#	Atom	Conventional Charge	Error in 1B (S1)	Error in 1B (S2)	Error in PA (S1)	Error in PA (S2)	Error in 3B (S1)	Error in 3B (S2)
1	Cl	-0.714	-0.286	-0.203	0.123	0.069	0.029	0.063
2	O	-0.844	0.146	0.015	-0.080	-0.015	0.000	-0.010
3	H	0.356	-0.007	0.073	0.082	0.014	0.003	0.008
4	H	0.448	-0.098	-0.131	0.006	0.026	0.039	-0.002
5	O	-0.793	0.100	0.100	-0.075	-0.062	0.109	0.050
6	H	0.403	-0.056	-0.056	0.004	0.030	-0.025	-0.016
7	H	0.363	-0.017	-0.017	0.042	0.021	-0.099	-0.041
8	O	-0.856	0.162	0.162	-0.021	0.003	0.124	0.055
9	H	0.485	-0.137	-0.137	-0.007	-0.026	-0.097	-0.042
10	H	0.373	-0.025	-0.025	0.009	0.005	-0.051	-0.026
11	O	-0.876	0.179	0.179	-0.065	0.008	0.006	0.005
12	H	0.388	-0.039	-0.039	-0.005	-0.066	-0.034	-0.017
13	H	0.428	-0.079	-0.079	0.011	-0.001	0.024	0.011
14	O	-0.865	0.163	0.163	-0.056	-0.035	0.092	0.049
15	H	0.398	-0.047	-0.047	-0.009	-0.002	-0.002	-0.005
16	H	0.401	-0.050	-0.050	0.087	0.063	-0.110	-0.072
17	O	-0.798	0.085	0.085	-0.048	-0.043	0.043	0.042
18	H	0.341	0.015	0.015	-0.003	-0.003	-0.052	-0.043
19	H	0.366	-0.008	-0.008	0.006	0.014	0.001	-0.009
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.089	0.083	0.039	0.027	0.049	0.030
	RMSE		0.115	0.103	0.053	0.035	0.064	0.037
	MUPE		14.5	14.4	6.9	5.2	9.7	5.8

Table S9a. Conventional CHelpG Atomic Charges (in *e*) and EE-MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Surf1

#	Atom	Conventional Charge	Error in EE-1B (S1)	Error in EE-1B (S2)	Error in EE-PA (S1)	Error in EE-PA (S2)	Error in EE-3B (S1)	Error in EE-3B (S2)
1	Cl	-0.738	-0.262	-0.169	-0.014	-0.039	-0.052	-0.034
2	O	-0.946	0.001	0.002	-0.016	0.000	0.096	0.020
3	H	0.439	0.027	0.014	0.084	0.054	-0.004	0.046
4	H	0.513	-0.034	-0.021	-0.030	-0.017	-0.049	0.020
5	O	-0.821	-0.067	-0.053	-0.095	-0.040	0.001	0.019
6	H	0.322	0.187	0.176	0.060	0.055	-0.006	-0.030
7	H	0.398	-0.018	-0.021	0.039	0.007	-0.005	-0.001
8	O	-0.870	-0.012	-0.001	-0.099	-0.046	0.057	-0.006
9	H	0.434	0.070	0.060	0.107	0.080	-0.073	-0.001
10	H	0.384	-0.005	-0.007	0.028	-0.003	0.004	0.016
11	O	-1.099	0.151	0.152	0.054	0.045	-0.024	0.025
12	H	0.477	-0.020	-0.021	-0.055	-0.055	0.035	-0.003
13	H	0.590	-0.099	-0.099	-0.049	-0.036	-0.027	-0.049
14	O	-0.868	-0.004	-0.002	0.030	0.139	0.050	-0.108
15	H	0.389	0.107	0.025	0.018	-0.058	-0.030	0.003
16	H	0.402	-0.026	-0.039	-0.035	-0.057	-0.003	0.066
17	O	-0.875	0.069	0.069	0.059	0.061	-0.044	-0.025
18	H	0.491	-0.043	-0.044	-0.070	-0.081	0.051	0.034
19	H	0.379	-0.021	-0.020	-0.018	-0.010	0.024	0.010
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.064	0.052	0.050	0.046	0.033	0.027
	RMSE		0.094	0.076	0.058	0.056	0.042	0.037
	MUPE		12.1	9.8	9.4	8.5	5.6	4.8

Table S9b. Conventional CHelpG Atomic Charges (in *e*) and MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Surf1

#	Atom	Conventional Charge	Error in 1B (S1)	Error in 1B (S2)	Error in PA (S1)	Error in PA (S2)	Error in 3B (S1)	Error in 3B (S2)
1	Cl	-0.738	-0.262	-0.168	0.085	0.051	-0.043	-0.008
2	O	-0.946	0.225	0.225	-0.017	-0.001	0.098	0.042
3	H	0.439	-0.079	-0.079	0.052	0.029	-0.035	0.009
4	H	0.513	-0.151	-0.151	-0.024	0.005	-0.029	-0.016
5	O	-0.821	0.072	0.072	-0.036	0.004	-0.029	-0.013
6	H	0.322	0.053	0.053	0.042	0.042	0.001	-0.027
7	H	0.398	-0.023	-0.023	-0.006	-0.023	0.016	0.013
8	O	-0.870	0.122	0.122	-0.030	0.007	0.044	-0.002
9	H	0.434	-0.060	-0.060	0.008	-0.031	-0.069	-0.001
10	H	0.384	-0.010	-0.010	-0.008	-0.012	0.007	0.003
11	O	-1.099	0.371	0.371	0.018	0.006	-0.025	0.007
12	H	0.477	-0.113	-0.113	-0.036	-0.028	0.037	0.004
13	H	0.590	-0.226	-0.226	-0.037	-0.022	-0.013	-0.032
14	O	-0.868	0.162	0.026	0.037	0.065	0.005	-0.023
15	H	0.389	-0.036	0.050	0.014	-0.065	-0.032	-0.007
16	H	0.402	-0.050	-0.093	-0.050	-0.022	0.025	0.031
17	O	-0.875	0.153	0.153	0.024	0.023	-0.022	0.001
18	H	0.491	-0.130	-0.130	-0.027	-0.023	0.041	0.010
19	H	0.379	-0.018	-0.018	-0.009	-0.004	0.023	0.009
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.122	0.113	0.029	0.024	0.031	0.014
	RMSE		0.153	0.143	0.035	0.031	0.038	0.018
	MUPE		18.6	17.8	5.4	4.9	5.5	2.6

Table S10a. Conventional CHelpG Atomic Charges (in *e*) and EE-MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Surf2

#	Atom	Conventional Charge	Error in EE-1B (S1)	Error in EE-1B (S2)	Error in EE-PA (S1)	Error in EE-PA (S2)	Error in EE-3B (S1)	Error in EE-3B (S2)
1	Cl	-0.712	-0.288	-0.205	-0.053	-0.015	-0.009	-0.005
2	O	-0.810	-0.021	-0.013	-0.116	-0.047	0.080	0.016
3	H	0.365	0.118	0.109	0.109	0.010	-0.024	0.025
4	H	0.363	-0.014	-0.013	0.036	0.025	-0.037	-0.016
5	O	-0.903	0.015	0.035	-0.092	-0.039	0.139	0.053
6	H	0.446	-0.047	-0.054	0.061	0.027	-0.082	-0.027
7	H	0.384	0.104	0.092	-0.001	-0.011	-0.078	-0.034
8	O	-0.911	0.034	0.041	-0.099	-0.108	-0.008	0.042
9	H	0.462	-0.047	-0.040	0.015	0.071	0.039	-0.019
10	H	0.457	0.005	-0.009	0.117	0.088	-0.001	-0.022
11	O	-0.958	0.061	0.063	-0.059	-0.063	0.021	0.011
12	H	0.438	0.005	-0.004	0.060	0.044	-0.040	-0.023
13	H	0.441	0.013	0.020	-0.001	0.029	-0.009	-0.003
14	O	-0.794	-0.102	-0.100	-0.120	-0.036	0.067	-0.006
15	H	0.446	-0.032	-0.049	0.019	0.046	-0.001	-0.001
16	H	0.263	0.218	0.150	0.140	-0.011	-0.067	0.016
17	O	-0.941	0.092	0.090	0.013	-0.001	-0.013	0.019
18	H	0.420	-0.034	-0.032	0.004	0.014	0.019	-0.012
19	H	0.545	-0.082	-0.082	-0.032	-0.021	0.005	-0.014
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.070	0.063	0.060	0.037	0.039	0.019
	RMSE		0.101	0.081	0.075	0.046	0.053	0.023
	MUPE		14.7	12.8	11.9	6.7	7.7	3.7

Table S10b. Conventional CHelpG Atomic Charges (in *e*) and MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Surf2

#	Atom	Conventional Charge	Error in 1B (S1)	Error in 1B (S2)	Error in PA (S1)	Error in PA (S2)	Error in 3B (S1)	Error in 3B (S2)
1	Cl	-0.712	-0.288	-0.202	0.079	0.058	-0.035	0.014
2	O	-0.810	0.094	0.094	-0.054	-0.044	0.046	0.036
3	H	0.365	-0.006	-0.006	-0.008	-0.009	0.016	0.004
4	H	0.363	-0.005	-0.005	0.016	0.024	-0.026	-0.024
5	O	-0.903	0.181	0.181	-0.082	-0.014	0.089	0.057
6	H	0.446	-0.086	-0.086	0.041	0.015	-0.045	-0.022
7	H	0.384	-0.023	-0.023	-0.011	-0.054	-0.030	-0.050
8	O	-0.911	0.192	0.192	-0.102	-0.063	0.080	0.052
9	H	0.462	-0.103	-0.103	0.016	0.017	-0.037	-0.028
10	H	0.457	-0.097	-0.097	0.061	0.016	-0.053	-0.029
11	O	-0.958	0.237	0.237	-0.138	-0.116	0.113	0.063
12	H	0.438	-0.077	-0.077	0.081	0.056	-0.079	-0.036
13	H	0.441	-0.081	-0.081	0.046	0.059	-0.048	-0.035
14	O	-0.794	0.088	-0.073	-0.104	0.006	0.102	-0.022
15	H	0.446	-0.093	-0.120	0.009	0.010	-0.036	0.011
16	H	0.263	0.090	0.192	0.137	0.020	-0.051	0.026
17	O	-0.941	0.197	0.197	-0.026	-0.032	0.041	0.041
18	H	0.420	-0.048	-0.048	0.018	0.023	-0.008	-0.016
19	H	0.545	-0.173	-0.173	0.020	0.028	-0.037	-0.041
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.114	0.115	0.055	0.035	0.051	0.032
	RMSE		0.136	0.135	0.069	0.044	0.058	0.036
	MUPE		18.7	20.4	10.2	6.2	9.1	5.8

Table S11a. Conventional CHelpG Atomic Charges (in *e*) and EE-MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Surf3

#	Atom	Conventional Charge	Error in EE-1B (S1)	Error in EE-1B (S2)	Error in EE-PA (S1)	Error in EE-PA (S2)	Error in EE-3B (S1)	Error in EE-3B (S2)
1	Cl	-0.710	-0.290	-0.195	0.007	0.049	0.015	-0.028
2	O	-0.904	-0.016	-0.013	0.003	0.017	0.050	-0.004
3	H	0.471	-0.008	-0.011	0.004	-0.016	-0.037	-0.019
4	H	0.473	-0.016	-0.017	0.024	0.026	-0.003	-0.003
5	O	-0.853	0.018	0.018	-0.120	-0.128	-0.029	0.034
6	H	0.400	-0.026	-0.017	0.013	0.048	0.041	-0.008
7	H	0.380	0.081	0.072	0.049	0.032	0.005	-0.011
8	O	-0.847	0.004	0.003	-0.052	-0.074	0.083	0.063
9	H	0.436	-0.023	-0.009	-0.023	0.031	-0.016	-0.021
10	H	0.393	0.037	0.025	0.090	0.073	-0.088	-0.067
11	O	-0.820	-0.049	-0.050	-0.049	-0.008	0.005	0.004
12	H	0.398	-0.023	-0.044	-0.031	0.045	0.053	-0.049
13	H	0.304	0.190	0.118	0.094	-0.068	-0.095	0.061
14	O	-0.875	-0.016	-0.005	-0.152	-0.085	0.078	0.070
15	H	0.405	-0.012	-0.013	0.076	0.048	-0.030	-0.032
16	H	0.390	0.108	0.098	0.087	0.022	-0.043	-0.013
17	O	-0.855	0.050	0.050	0.026	0.018	-0.016	-0.060
18	H	0.471	-0.023	-0.024	-0.023	-0.025	0.019	0.062
19	H	0.343	0.014	0.015	-0.020	-0.004	0.008	0.021
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.053	0.042	0.050	0.043	0.038	0.033
	RMSE		0.088	0.064	0.065	0.053	0.047	0.041
	MUPE		11.3	8.9	9.9	8.3	7.8	6.6

Table S11b. Conventional CHelpG Atomic Charges (in *e*) and MB Errors (in *e*) for $[Cl(H_2O)_6]^-$ Configuration Surf3

#	Atom	Conventional Charge	Error in 1B (S1)	Error in 1B (S2)	Error in PA (S1)	Error in PA (S2)	Error in 3B (S1)	Error in 3B (S2)
1	Cl	-0.710	-0.290	-0.194	0.070	0.061	-0.037	-0.034
2	O	-0.904	0.198	0.198	-0.009	-0.004	0.009	-0.025
3	H	0.471	-0.118	-0.118	0.015	0.004	0.000	0.021
4	H	0.473	-0.119	-0.119	0.020	0.033	-0.001	-0.002
5	O	-0.853	0.172	0.172	-0.040	-0.058	-0.025	0.011
6	H	0.400	-0.059	-0.059	-0.024	0.006	0.045	0.006
7	H	0.380	-0.039	-0.039	0.018	0.021	-0.009	-0.013
8	O	-0.847	0.165	0.165	-0.039	-0.013	0.034	0.001
9	H	0.436	-0.095	-0.095	-0.007	-0.003	-0.015	0.003
10	H	0.393	-0.052	-0.052	0.038	0.022	-0.037	-0.009
11	O	-0.820	0.127	-0.007	-0.022	0.025	0.036	-0.023
12	H	0.398	-0.051	-0.099	-0.046	0.032	0.032	-0.039
13	H	0.304	0.043	0.129	0.076	-0.078	-0.089	0.068
14	O	-0.875	0.185	0.185	-0.106	-0.064	0.078	0.033
15	H	0.405	-0.060	-0.060	0.038	0.020	-0.041	-0.015
16	H	0.390	-0.045	-0.045	0.029	0.002	0.001	0.001
17	O	-0.855	0.147	0.147	0.021	0.019	-0.031	-0.041
18	H	0.471	-0.117	-0.117	-0.019	-0.019	0.028	0.039
19	H	0.343	0.011	0.011	-0.014	-0.006	0.023	0.018
	MSE		0.000	0.000	0.000	0.000	0.000	0.000
	MUE		0.110	0.106	0.034	0.026	0.030	0.021
	RMSE		0.130	0.121	0.042	0.034	0.038	0.027
	MUPE		18.3	19.0	6.8	5.0	6.2	4.4

Table S12. CHelpG Charges (in *e*) on Atoms of $(HF)_5$ Configuration hf5_fhhhf

Atom[a]	Conventional	1B	PA	3B	EE-1B	EE-PA	EE-3B
H(A)	0.450	0.433	0.453	0.447	0.455	0.452	0.447
F(A)	-0.451	-0.433	-0.453	-0.446	-0.455	-0.452	-0.447
H(B)	0.441	0.433	0.441	0.438	0.444	0.442	0.438
F(B)	-0.438	-0.433	-0.441	-0.435	-0.444	-0.443	-0.435
F(C)	-0.420	-0.433	-0.419	-0.422	-0.420	-0.414	-0.421
H(C)	0.416	0.433	0.419	0.414	0.420	0.416	0.414
H(D)	0.441	0.433	0.441	0.438	0.444	0.441	0.439
F(D)	-0.438	-0.433	-0.441	-0.436	-0.444	-0.443	-0.436
H(E)	0.450	0.433	0.454	0.447	0.455	0.453	0.447
F(E)	-0.451	-0.433	-0.454	-0.446	-0.455	-0.452	-0.446
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.013	0.002	0.003	0.004	0.002	0.003
RMSE		0.014	0.003	0.003	0.004	0.003	0.003
MUPE		2.9	0.5	0.7	0.9	0.6	0.6

[a]See Figure 5 of the paper. For example, the atom listed as H(B) is the hydrogen atom of the HF molecule labeled "B" in Figure 5 of configuration hf5_fhhhf.

Table S13. CHelpG Charges (in *e*) on Atoms of $(HF)_3(H_2O)_2$ Configuration w2hf3_a

Atom[a]	Conventional	1B	PA	3B	EE-1B	EE-PA	EE-3B
O(A)	-0.746	-0.725	-0.792	-0.775	-0.757	-0.798	-0.774
H1(A)	0.361	0.363	0.390	0.376	0.379	0.394	0.375
H2(A)	0.364	0.362	0.393	0.366	0.378	0.397	0.366
H(B)	0.447	0.434	0.440	0.462	0.456	0.436	0.461
F(B)	-0.454	-0.434	-0.450	-0.461	-0.456	-0.446	-0.461
F(C)	-0.401	-0.434	-0.398	-0.402	-0.434	-0.398	-0.402
F(D)	-0.403	-0.434	-0.397	-0.396	-0.434	-0.398	-0.395
H(C)	0.418	0.434	0.412	0.420	0.434	0.410	0.421
H(D)	0.420	0.434	0.412	0.414	0.434	0.410	0.414
O(E)	-0.838	-0.725	-0.859	-0.833	-0.805	-0.870	-0.833
H1(E)	0.417	0.363	0.422	0.416	0.403	0.429	0.415
H2(E)	0.416	0.362	0.427	0.413	0.402	0.433	0.413
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.031	0.015	0.008	0.018	0.019	0.008
RMSE		0.043	0.019	0.011	0.020	0.024	0.011
MUPE		6.2	3.0	1.6	3.9	3.9	1.6

[a]See Figure 7 of the paper. For example, the atom listed as H2(A) is the hydrogen atom labeled "2" on the water molecule labeled "A" in Figure 7.

Table S14. CHelpG Charges (in *e*) on Atoms of $(HF)_3(H_2O)_2$ Configuration w2hf3_opt

Atom[a]	Conventional	1B	PA	3B	EE-1B	EE-PA	EE-3B
O(A)	-0.731	-0.721	-0.741	-0.728	-0.872	-0.735	-0.735
H1(A)	0.388	0.361	0.404	0.379	0.436	0.395	0.385
H2(A)	0.388	0.361	0.403	0.381	0.436	0.394	0.386
H(B)	0.418	0.433	0.396	0.435	0.491	0.387	0.435
F(B)	-0.501	-0.433	-0.485	-0.503	-0.491	-0.479	-0.504
F(C)	-0.398	-0.433	-0.422	-0.434	-0.473	-0.466	-0.413
F(D)	-0.401	-0.433	-0.427	-0.431	-0.474	-0.472	-0.408
H(C)	0.323	0.433	0.366	0.388	0.473	0.462	0.346
H(D)	0.326	0.433	0.373	0.384	0.474	0.471	0.340
O(E)	-0.592	-0.730	-0.679	-0.737	-0.927	-0.927	-0.631
H1(E)	0.388	0.365	0.405	0.431	0.464	0.487	0.398
H2(E)	0.391	0.365	0.408	0.436	0.464	0.481	0.400
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.052	0.028	0.038	0.104	0.085	0.012
RMSE		0.066	0.035	0.054	0.132	0.123	0.016
MUPE		12.7	6.8	9.2	23.9	20.3	2.9

[a]See Figure 7 of the paper. For example, the atom listed as H2(A) is the hydrogen atom labeled "2" on the water molecule labeled "A" in Figure 7.

Table S15a. Net Fragment Charges (in *e*) and Average Errors in EE-MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Int1

Fragment	Conventional	EE-1B (S1)	EE-1B (S2)	EE-PA (S1)	EE-PA (S2)	EE-3B (S1)	EE-3B (S2)
Cl	-0.563	-1.000	-0.987	-0.851	-0.838	-0.785	-0.686
A H_2O	-0.120	0.000	-0.013	0.002	-0.026	-0.016	-0.080
B H_2O	-0.120	0.000	0.000	-0.074	-0.073	-0.081	-0.102
C H_2O	-0.064	0.000	0.000	-0.007	-0.006	-0.016	-0.031
D H_2O	-0.064	0.000	0.000	-0.030	-0.022	-0.022	-0.054
E H_2O	-0.046	0.000	0.000	-0.033	-0.029	-0.063	-0.052
F H_2O	-0.025	0.000	0.000	-0.005	-0.006	-0.017	0.004
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.125	0.121	0.082	0.079	0.069	0.037
RMSE		0.182	0.176	0.122	0.115	0.097	0.052
MUPE		96.8	94.9	62.5	62.3	52.4	38.2

Table S15b. Net Fragment Charges (in *e*) and Average Errors in MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Int1

Fragment	Conventional	1B (S1)	1B (S2)	PA (S1)	PA (S2)	3B (S1)	3B (S2)
Cl	-0.563	-1.000	-0.913	-0.567	-0.612	-0.701	-0.702
A H_2O	-0.120	0.000	-0.087	-0.066	-0.089	-0.077	-0.059
B H_2O	-0.120	0.000	0.000	-0.118	-0.109	-0.092	-0.108
C H_2O	-0.064	0.000	0.000	-0.076	-0.081	-0.037	-0.028
D H_2O	-0.064	0.000	0.000	-0.070	-0.049	-0.039	-0.053
E H_2O	-0.046	0.000	0.000	-0.049	-0.036	-0.058	-0.045
F H_2O	-0.025	0.000	0.000	-0.054	-0.024	0.004	-0.006
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.125	0.100	0.016	0.019	0.043	0.040
RMSE		0.182	0.146	0.024	0.024	0.059	0.060
MUPE		96.8	84.2	28.9	17.0	43.8	34.0

Table S16a. Net Fragment Charges (in *e*) and Average Errors in EE-MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Int2

Fragment	Conventional	EE-1B (S1)	EE-1B (S2)	EE-PA (S1)	EE-PA (S2)	EE-3B (S1)	EE-3B (S2)
Cl	-0.751	-1.000	-0.979	-0.812	-0.750	-0.796	-0.854
A H_2O	-0.039	0.000	-0.021	-0.016	-0.061	-0.061	0.002
B H_2O	-0.028	0.000	0.000	-0.002	0.000	0.005	-0.007
C H_2O	0.011	0.000	0.000	-0.021	-0.035	0.002	0.013
D H_2O	-0.118	0.000	0.000	-0.113	-0.110	-0.134	-0.132
E H_2O	-0.063	0.000	0.000	-0.017	-0.024	-0.033	-0.027
F H_2O	-0.013	0.000	0.000	-0.019	-0.019	0.016	0.005
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.074	0.068	0.028	0.021	0.026	0.033
RMSE		0.108	0.101	0.034	0.027	0.028	0.045
MUPE		90.4	82.4	81.9	97.7	78.5	59.6

Table S16b. Net Fragment Charges (in *e*) and Average Errors in MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Int2

Fragment	Conventional	1B (S1)	1B (S2)	PA (S1)	PA (S2)	3B (S1)	3B (S2)
Cl	-0.751	-1.000	-0.922	-0.622	-0.654	-0.767	-0.791
A H_2O	-0.039	0.000	-0.078	-0.071	-0.057	-0.052	-0.032
B H_2O	-0.028	0.000	0.000	-0.058	-0.058	-0.011	-0.011
C H_2O	0.011	0.000	0.000	-0.028	-0.021	-0.009	-0.003
D H_2O	-0.118	0.000	0.000	-0.112	-0.111	-0.129	-0.118
E H_2O	-0.063	0.000	0.000	-0.067	-0.063	-0.059	-0.058
F H_2O	-0.013	0.000	0.000	-0.042	-0.036	0.027	0.013
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.074	0.063	0.038	0.030	0.017	0.015
RMSE		0.108	0.084	0.055	0.042	0.020	0.020
MUPE		90.4	89.1	114.3	92.9	86.1	59.6

Table S17a. Net Fragment Charges (in *e*) and Average Errors in EE-MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Int3

Fragment	Conventional	EE-1B (S1)	EE-1B (S2)	EE-PA (S1)	EE-PA (S2)	EE-3B (S1)	EE-3B (S2)
Cl	-0.714	-1.000	-0.970	-0.812	-0.771	-0.689	-0.677
A H_2O	-0.041	0.000	-0.030	0.015	-0.037	-0.034	-0.048
B H_2O	-0.092	0.000	0.000	-0.096	-0.099	-0.065	-0.093
C H_2O	-0.067	0.000	0.000	-0.016	-0.021	-0.086	-0.089
D H_2O	-0.061	0.000	0.000	-0.072	-0.060	-0.075	-0.060
E H_2O	-0.027	0.000	0.000	-0.004	0.003	-0.017	-0.012
F H_2O	0.001	0.000	0.000	-0.014	-0.015	-0.034	-0.021
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.082	0.073	0.037	0.023	0.019	0.015
RMSE		0.120	0.109	0.048	0.031	0.022	0.020
MUPE		91.4	80.5	261.4	261.8	524.4	333.1

Table S17b. Net Fragment Charges (in *e*) and Average Errors in MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Int3

Fragment	Conventional	1B (S1)	1B (S2)	PA (S1)	PA (S2)	3B (S1)	3B (S2)
Cl	-0.714	-1.000	-0.917	-0.591	-0.645	-0.685	-0.651
A H_2O	-0.041	0.000	-0.083	-0.032	-0.015	0.001	-0.045
B H_2O	-0.092	0.000	0.000	-0.137	-0.124	-0.101	-0.102
C H_2O	-0.067	0.000	0.000	-0.045	-0.040	-0.087	-0.095
D H_2O	-0.061	0.000	0.000	-0.120	-0.120	-0.065	-0.062
E H_2O	-0.027	0.000	0.000	-0.056	-0.038	-0.042	-0.033
F H_2O	0.001	0.000	0.000	-0.019	-0.017	-0.022	-0.013
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.082	0.070	0.044	0.034	0.020	0.018
RMSE		0.120	0.093	0.057	0.040	0.024	0.027
MUPE		91.4	90.3	326.5	292.7	364.0	214.1

Table S18a. Net Fragment Charges (in *e*) and Average Errors in EE-MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Surf1

Fragment	Conventional	EE-1B (S1)	EE-1B (S2)	EE-PA (S1)	EE-PA (S2)	EE-3B (S1)	EE-3B (S2)
Cl	-0.738	-1.000	-0.907	-0.752	-0.777	-0.790	-0.772
A H_2O	-0.077	0.000	-0.093	-0.063	-0.052	-0.060	-0.116
B H_2O	-0.102	0.000	0.000	-0.097	-0.080	-0.112	-0.114
C H_2O	-0.053	0.000	0.000	-0.016	-0.021	-0.065	-0.044
D H_2O	0.006	0.000	0.000	0.044	0.043	0.048	0.091
E H_2O	-0.032	0.000	0.000	-0.082	-0.078	-0.048	-0.059
F H_2O	-0.005	0.000	0.000	-0.033	-0.035	0.026	0.014
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.076	0.054	0.026	0.033	0.026	0.032
RMSE		0.112	0.078	0.030	0.034	0.030	0.040
MUPE		90.8	77.7	219.0	224.1	217.0	295.2

Table S18b. Net Fragment Charges (in *e*) and Average Errors in MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Surf1

Fragment	Conventional	1B (S1)	1B (S2)	PA (S1)	PA (S2)	3B (S1)	3B (S2)
Cl	-0.738	-1.000	-0.906	-0.653	-0.688	-0.781	-0.747
A H_2O	-0.077	0.000	-0.094	-0.076	-0.100	-0.078	-0.076
B H_2O	-0.102	0.000	0.000	-0.101	-0.079	-0.113	-0.128
C H_2O	-0.053	0.000	0.000	-0.083	-0.089	-0.070	-0.052
D H_2O	0.006	0.000	0.000	0.017	0.039	0.039	0.041
E H_2O	-0.032	0.000	0.000	-0.087	-0.075	-0.034	-0.053
F H_2O	-0.005	0.000	0.000	-0.016	-0.009	0.038	0.015
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.076	0.054	0.028	0.030	0.022	0.016
RMSE		0.112	0.078	0.040	0.034	0.027	0.020
MUPE		90.8	77.9	98.8	134.2	221.3	161.5

Table S19a. Net Fragment Charges (in *e*) and Average Errors in EE-MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Surf2

Fragment	Conventional	EE-1B (S1)	EE-1B (S2)	EE-PA (S1)	EE-PA (S2)	EE-3B (S1)	EE-3B (S2)
Cl	-0.712	-1.000	-0.916	-0.765	-0.727	-0.721	-0.717
A H_2O	-0.085	0.000	-0.084	-0.046	-0.085	-0.086	-0.076
B H_2O	-0.073	0.000	0.000	-0.105	-0.097	-0.093	-0.081
C H_2O	-0.083	0.000	0.000	-0.055	-0.096	-0.065	-0.058
D H_2O	0.008	0.000	0.000	0.041	0.059	0.038	0.008
E H_2O	-0.079	0.000	0.000	-0.079	-0.069	-0.107	-0.093
F H_2O	0.024	0.000	0.000	0.009	0.016	0.034	0.017
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.091	0.068	0.029	0.017	0.017	0.010
RMSE		0.125	0.093	0.033	0.023	0.019	0.012
MUPE		91.5	75.7	87.1	106.1	73.5	14.3

Table S19b. Net Fragment Charges (in *e*) and Average Errors in MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Surf2

Fragment	Conventional	1B (S1)	1B (S2)	PA (S1)	PA (S2)	3B (S1)	3B (S2)
Cl	-0.712	-1.000	-0.914	-0.633	-0.654	-0.747	-0.698
A H_2O	-0.085	0.000	-0.086	-0.043	-0.049	-0.070	-0.070
B H_2O	-0.073	0.000	0.000	-0.125	-0.126	-0.060	-0.089
C H_2O	-0.083	0.000	0.000	-0.128	-0.112	-0.048	-0.067
D H_2O	0.008	0.000	0.000	-0.017	-0.022	-0.003	0.002
E H_2O	-0.079	0.000	0.000	-0.090	-0.080	-0.093	-0.087
F H_2O	0.024	0.000	0.000	0.036	0.043	0.020	0.009
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.091	0.067	0.038	0.032	0.018	0.013
RMSE		0.125	0.093	0.044	0.037	0.021	0.013
MUPE		91.5	75.7	81.3	88.0	36.4	29.6

Table S20a. Net Fragment Charges (in *e*) and Average Errors in EE-MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Surf3

Fragment	Conventional	EE-1B (S1)	EE-1B (S2)	EE-PA (S1)	EE-PA (S2)	EE-3B (S1)	EE-3B (S2)
Cl	-0.710	-1.000	-0.905	-0.703	-0.661	-0.695	-0.738
A H_2O	-0.118	0.000	-0.095	-0.104	-0.149	-0.154	-0.102
B H_2O	-0.080	0.000	0.000	-0.069	-0.095	-0.075	-0.054
C H_2O	-0.073	0.000	0.000	-0.132	-0.122	-0.057	-0.058
D H_2O	-0.018	0.000	0.000	-0.004	0.012	-0.039	-0.043
E H_2O	0.040	0.000	0.000	0.071	0.067	0.051	0.014
F H_2O	-0.041	0.000	0.000	-0.059	-0.051	-0.030	-0.018
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.094	0.067	0.022	0.030	0.016	0.023
RMSE		0.127	0.088	0.027	0.033	0.019	0.023
MUPE		91.5	78.2	43.4	53.5	32.8	47.2

Table S20b. Net Fragment Charges (in *e*) and Average Errors in MB Approximations for $[Cl(H_2O)_6]^-$ Configuration Surf3

Fragment	Conventional	1B (S1)	1B (S2)	PA (S1)	PA (S2)	3B (S1)	3B (S2)
Cl	-0.710	-1.000	-0.905	-0.640	-0.649	-0.748	-0.745
A H_2O	-0.118	0.000	-0.095	-0.110	-0.140	-0.140	-0.112
B H_2O	-0.080	0.000	0.000	-0.118	-0.122	-0.042	-0.061
C H_2O	-0.073	0.000	0.000	-0.120	-0.103	-0.062	-0.069
D H_2O	-0.018	0.000	0.000	-0.026	-0.012	-0.036	-0.023
E H_2O	0.040	0.000	0.000	0.066	0.072	0.048	0.034
F H_2O	-0.041	0.000	0.000	-0.053	-0.047	-0.020	-0.025
MSE		0.000	0.000	0.000	0.000	0.000	0.000
MUE		0.094	0.067	0.030	0.028	0.022	0.013
RMSE		0.127	0.087	0.037	0.034	0.024	0.017
MUPE		91.5	78.1	37.8	35.4	36.4	17.4

Table S21. Net Charges[a] (in *e*) on Fragments of Two Configurations of $(HF)_3(H_2O)_2$ and on One Configuration of $(HF)_5$

Frag.[b]	Conventional	1B	PA	3B	EE-1B	EE-PA	EE-3B
hf5_fhhhf							
A	-0.001	0.000	0.000	0.001	0.000	0.000	0.001
B	0.003	0.000	0.000	0.003	0.000	-0.001	0.003
C	-0.004	0.000	0.000	-0.008	0.000	0.002	-0.007
D	0.003	0.000	0.000	0.003	0.000	-0.001	0.003
E	-0.001	0.000	0.000	0.001	0.000	0.000	0.001
w2hf3_a							
A	-0.021	0.000	-0.010	-0.033	0.000	-0.007	-0.033
B	-0.007	0.000	-0.009	0.001	0.000	-0.010	0.001
C	0.017	0.000	0.015	0.018	0.000	0.012	0.019
D	0.016	0.000	0.015	0.018	0.000	0.012	0.018
E	-0.005	0.000	-0.010	-0.004	0.000	-0.008	-0.004
w2hf3_opt							
A	0.046	0.000	0.066	0.032	0.000	0.055	0.036
B	-0.083	0.000	-0.089	-0.069	0.000	-0.091	-0.069
C	-0.076	0.000	-0.056	-0.046	0.000	-0.004	-0.066
D	-0.075	0.000	-0.054	-0.047	0.000	-0.001	-0.068
E	0.188	0.000	0.134	0.130	0.000	0.042	0.168
MSE[c]		0.000	0.000	0.000	0.000	0.000	0.000
MUE[c]		0.036	0.010	0.012	0.036	0.023	0.006
RMSE[c]		0.061	0.017	0.019	0.061	0.046	0.008
MUPE[c]		100.0	55.8	72.6	100.0	79.7	52.0

[a]The net charge on a fragment is defined as the sum of the CHelpG charges on the atoms that compose the given fragment.
[b]Frag. = Fragment. See Figures 5 and 7 of the paper in order to understand the fragment labels.
[c]MSE = mean signed error, MUE = mean unsigned error, RMSE = root mean squared error, MUPE = mean unsigned percent error. The averages are taken over all fragments of all three systems shown in the table (i.e., hf5_fhhhf, w2hf3_a, and w2hf3_opt).

Table S22. Net Charges[a] (in *e*) on Fragments of Six Configurations of $(HF)_3(H_2O)$

Frag.[b]	Conventional	1B	PA	3B	EE-1B	EE-PA	EE-3B
whf3_AaBaCa							
H_2O	0.036	0.000	0.028	0.037	0.000	0.032	0.037
A	-0.009	0.000	-0.003	-0.010	0.000	-0.004	-0.009
B	-0.013	0.000	-0.012	-0.014	0.000	-0.014	-0.014
C	-0.014	0.000	-0.012	-0.014	0.000	-0.014	-0.014
whf3_AaBaCr							
H_2O	0.033	0.000	0.024	0.033	0.000	0.026	0.033
A	-0.009	0.000	-0.004	-0.010	0.000	-0.004	-0.010
B	-0.013	0.000	-0.013	-0.012	0.000	-0.013	-0.013
C	-0.010	0.000	-0.007	-0.011	0.000	-0.009	-0.010
whf3_AaBrCr							
H_2O	0.029	0.000	0.019	0.032	0.000	0.022	0.033
A	-0.010	0.000	-0.005	-0.010	0.000	-0.004	-0.010
B	-0.009	0.000	-0.007	-0.011	0.000	-0.009	-0.011
C	-0.010	0.000	-0.007	-0.012	0.000	-0.009	-0.012
whf3_ArBaCa							
H_2O	0.035	0.000	0.031	0.036	0.000	0.031	0.036
A	-0.011	0.000	-0.008	-0.011	0.000	-0.009	-0.010
B	-0.013	0.000	-0.011	-0.013	0.000	-0.011	-0.013
C	-0.011	0.000	-0.011	-0.013	0.000	-0.011	-0.013
whf3_ArBaCr							
H_2O	0.028	0.000	0.027	0.030	0.000	0.025	0.030
A	-0.012	0.000	-0.009	-0.012	0.000	-0.009	-0.012
B	-0.010	0.000	-0.012	-0.011	0.000	-0.010	-0.011
C	-0.006	0.000	-0.006	-0.007	0.000	-0.005	-0.007
whf3_ArBrCr							
H_2O	0.023	0.000	0.022	0.028	0.000	0.019	0.028
A	-0.013	0.000	-0.009	-0.012	0.000	-0.009	-0.011
B	-0.005	0.000	-0.007	-0.007	0.000	-0.005	-0.008
C	-0.005	0.000	-0.007	-0.009	0.000	-0.005	-0.009
MSE[c]		0.000	0.000	0.000	0.000	0.000	0.000
MUE[c]		0.015	0.003	0.001	0.015	0.002	0.001
RMSE[c]		0.018	0.004	0.002	0.018	0.003	0.002
MUPE[c]		100.0	23.0	12.4	100.0	16.7	13.1

[a]See footnote *a* of Table S21.

[b]Frag. = Fragment. See Figure 6 of the paper in order to understand the fragment labels.

[c]MSE = mean signed error, MUE = mean unsigned error, RMSE = root mean squared error, MUPE = mean unsigned percent error. The averages are taken over all fragments of all six systems shown in the table.