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Electronic supplementary information for *PCCP*

Number of atoms with this many neighbours during the simulation on average

Cl\* refers to CID chlorine atoms (defined by having a D within 1.55Å)

Cl- refers to the rest of Cl atoms, i.e. chloride ions (defined by not having a D within 1.55Å)

	\Sigma	average coordinati on #	0	1	2	3	4	5	6	7	8	9	cut off for coordination number definition
10:22 330K													10:22 330K
n(O)	21.992	1.924	1.329	6.623	7.891	4.697	1.437	0.015	0.000	0.000	0.000	0.000	OO R < 3.0Å
n(O)	21.991	1.513	4.212	6.366	7.588	3.548	0.276	0.001	0.000	0.000	0.000	0.000	OCI R < 3.5Å
n(Cl)	9.995	3.329	0.089	0.998	1.791	2.263	2.761	1.711	0.354	0.025	0.003	0.000	CIO R < 3.5Å
n(Cl)	9.997	3.853	0.014	0.269	0.963	2.278	3.593	2.225	0.588	0.061	0.006	0.000	CIX R < 3.5Å
n(Cl)	9.996	0.523	5.595	3.590	0.792	0.019	0.000	0.000	0.000	0.000	0.000	0.000	CICI R < 3.5Å
n(O)	21.992	3.351	0.000	0.000	0.000	14.258	7.712	0.022	0.000	0.000	0.000	0.000	OD R < 2.5Å
n(Cl)	9.999	3.415	0.000	0.802	1.476	2.159	3.918	1.618	0.026	0.000	0.000	0.000	CID R < 2.75Å
n(CID)	2.991	2.000	0.000	0.801	1.427	0.724	0.039	0.000	0.000	0.000	0.000	0.000	Cl*D R < 2.75
n(Cl-)	7.008	4.162	0.000	0.001	0.049	1.435	3.879	1.618	0.026	0.000	0.000	0.000	Cl-D R < 2.75
10:22 470K													10:22 470K
n(O)	21.997	1.942	0.934	6.260	8.873	5.053	0.831	0.046	0.000	0.000	0.000	0.000	OO R < 3.0Å
n(O)	21.999	1.465	3.406	8.676	6.815	2.517	0.558	0.023	0.004	0.000	0.000	0.000	OCI R < 3.5Å
n(Cl)	9.999	0.729	4.063	4.647	1.224	0.065	0.000	0.000	0.000	0.000	0.000	0.000	CIO R < 3.5Å
n(Cl)	9.999	3.952	0.050	0.215	0.916	2.396	3.115	2.271	0.821	0.189	0.020	0.006	CIX R < 3.5Å
n(Cl)	9.999	0.729	4.063	4.647	1.224	0.065	0.000	0.000	0.000	0.000	0.000	0.000	CICI R < 3.5Å
n(O)	21.998	3.446	0.000	0.000	0.139	12.582	8.616	0.649	0.012	0.000	0.000	0.000	OD R < 2.5Å
n(Cl)	9.999	3.107	0.000	0.955	2.509	2.667	2.491	1.153	0.198	0.026	0.000	0.000	CID R < 2.75Å
n(CID)	4.916	2.266	0.000	0.951	2.206	1.312	0.398	0.046	0.003	0.000	0.000	0.000	Cl*D R < 2.75
n(Cl-)	5.083	0.000	0.000	0.004	0.303	1.355	2.093	1.107	0.195	0.026	0.000	0.000	Cl-D R < 2.75
10:22 909K													10:22 909K
n(O)	21.998	1.853	1.550	6.558	8.689	4.120	0.977	0.065	0.034	0.005	0.000	0.000	OO R < 3.0Å
n(O)	21.995	1.463	3.420	8.530	6.852	2.854	0.304	0.029	0.006	0.000	0.000	0.000	OCI R < 3.5Å
n(Cl)	9.998	3.219	0.145	0.757	2.029	3.039	2.336	1.286	0.354	0.052	0.000	0.000	CIO R < 3.5Å
n(Cl)	9.999	4.211	0.022	0.176	0.765	1.864	3.052	2.502	1.271	0.309	0.038	0.000	CIX R < 3.5Å
n(Cl)	9.998	0.991	3.003	4.617	1.903	0.410	0.065	0.000	0.000	0.000	0.000	0.000	CICI R < 3.5Å
n(O)	21.995	3.546	0.000	0.000	1.063	10.413	8.242	2.008	0.250	0.019	0.000	0.000	OD R < 2.5Å
n(Cl)	9.997	3.003	0.000	0.771	2.608	3.472	2.242	0.776	0.118	0.010	0.000	0.000	CID R < 2.75Å
n(CID)	6.861	2.697	0.000	0.762	2.264	2.454	1.084	0.266	0.031	0.000	0.000	0.000	Cl*D R < 2.75
n(Cl-)	3.136	0.000	0.000	0.009	0.344	1.018	1.158	0.510	0.087	0.010	0.000	0.000	Cl-D R < 2.75

Electronic supplementary information for *PCCP*

7:25 340K

n(O)	24.999	2.291	0.040	4.856	9.816	8.383	1.883	0.021	0.000	0.000	0.000	0.000	7:25 340K
n(O)	24.998	1.029	5.678	13.549	5.149	0.613	0.009	0.000	0.000	0.000	0.000	0.000	OO R < 3.0Å
n(Cl)	6.998	3.675	0.096	0.426	0.780	1.697	1.934	1.531	0.488	0.046	0.000	0.000	OCI R < 3.5Å
n(Cl)	6.998	4.139	0.023	0.148	0.526	1.185	2.255	2.062	0.718	0.077	0.004	0.000	CIO R < 3.5Å
n(Cl)	7.000	0.464	3.880	2.995	0.121	0.004	0.000	0.000	0.000	0.000	0.000	0.000	CIX R < 3.5Å
n(O)	24.998	3.480	0.000	0.000	0.014	13.201	11.540	0.243	0.000	0.000	0.000	0.000	CICI R < 3.5Å
n(Cl)	7.000	3.716	0.000	0.666	1.098	0.932	1.642	2.204	0.439	0.019	0.000	0.000	OD R < 2.5Å
n(CID)	1.981	1.824	0.000	0.657	1.039	0.263	0.020	0.002	0.000	0.000	0.000	0.000	CID R < 2.75Å
n(Cl-)	5.019	0.000	0.000	0.009	0.059	0.669	1.622	2.202	0.439	0.019	0.000	0.000	Cl*D R < 2.75
													Cl-D R < 2.75

4:28 290K

n(O)	27.999	2.466	0.128	3.482	10.534	11.007	2.773	0.066	0.009	0.000	0.000	0.000	4:28 290K
n(O)	27.997	0.686	11.015	14.780	2.178	0.024	0.000	0.000	0.000	0.000	0.000	0.000	OO R < 3.0Å
n(Cl)	4.000	4.802	0.000	0.000	0.001	0.225	1.280	1.646	0.760	0.082	0.006	0.000	OCI R < 3.5Å
n(Cl)	4.000	4.802	0.000	0.000	0.001	0.225	1.280	1.646	0.760	0.082	0.006	0.000	CIO R < 3.5Å
n(Cl)	4.000	0.000	4.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	CIX R < 3.5Å
n(O)	27.997	3.583	0.000	0.000	0.011	12.455	14.741	0.782	0.008	0.000	0.000	0.000	CICI R < 3.5Å
n(Cl)	3.999	4.562	0.000	0.000	0.010	0.238	1.772	1.453	0.526	0.000	0.000	0.000	OD R < 2.5Å
n(CID)	0.000	no CID -molecules											CID R < 2.75Å
n(Cl-)	3.999	0.000	0.000	0.000	0.010	0.238	1.772	1.453	0.526	0.000	0.000	0.000	Cl*D R < 2.75
													Cl-D R < 2.75

Pair correlation functions of each simulation.

system 4:28 DCI:D2O, RDF

r [Å]	g(O,O)	g(O,Cl)	g(O,D)	g(Cl,Cl)	g(Cl,D)	g(D,D)
0.043	0.000	0.000	0.000	0.000	0.000	0.000
0.086	0.000	0.000	0.000	0.000	0.000	0.000
0.129	0.000	0.000	0.000	0.000	0.000	0.000
0.172	0.000	0.000	0.000	0.000	0.000	0.000
0.214	0.000	0.000	0.000	0.000	0.000	0.000
0.257	0.000	0.000	0.000	0.000	0.000	0.000
0.300	0.000	0.000	0.000	0.000	0.000	0.000
0.343	0.000	0.000	0.000	0.000	0.000	0.000
0.386	0.000	0.000	0.000	0.000	0.000	0.000
0.429	0.000	0.000	0.000	0.000	0.000	0.000
0.472	0.000	0.000	0.000	0.000	0.000	0.000
0.515	0.000	0.000	0.000	0.000	0.000	0.000
0.557	0.000	0.000	0.000	0.000	0.000	0.000
0.600	0.000	0.000	0.000	0.000	0.000	0.000
0.643	0.000	0.000	0.000	0.000	0.000	0.000
0.686	0.000	0.000	0.000	0.000	0.000	0.000
0.729	0.000	0.000	0.000	0.000	0.000	0.000
0.772	0.000	0.000	0.000	0.000	0.000	0.000
0.815	0.000	0.000	0.000	0.000	0.000	0.000
0.857	0.000	0.000	0.000	0.000	0.000	0.000
0.900	0.000	0.000	0.008	0.000	0.000	0.000
0.943	0.000	0.000	2.218	0.000	0.000	0.000

Electronic supplementary information for *PCCP*

0.986	0.000	0.000	23.971	0.000	0.000	0.000
1.029	0.000	0.000	26.493	0.000	0.000	0.000
1.072	0.000	0.000	8.025	0.000	0.000	0.000
1.115	0.000	0.000	2.200	0.000	0.000	0.000
1.158	0.000	0.000	0.956	0.000	0.000	0.000
1.200	0.000	0.000	0.619	0.000	0.000	0.000
1.243	0.000	0.000	0.501	0.000	0.030	0.000
1.286	0.000	0.000	0.440	0.000	0.024	0.000
1.329	0.000	0.000	0.468	0.000	0.020	0.000
1.372	0.000	0.000	0.511	0.000	0.025	0.000
1.415	0.000	0.000	0.554	0.000	0.037	0.008
1.458	0.000	0.000	0.595	0.000	0.013	0.083
1.501	0.000	0.000	0.662	0.000	0.005	0.443
1.543	0.000	0.000	0.719	0.000	0.009	1.325
1.586	0.000	0.000	0.812	0.000	0.022	2.409
1.629	0.000	0.000	0.852	0.000	0.026	2.717
1.672	0.000	0.000	0.909	0.000	0.047	2.152
1.715	0.000	0.000	0.910	0.000	0.104	1.446
1.758	0.000	0.000	0.877	0.000	0.183	1.011
1.801	0.000	0.000	0.833	0.000	0.296	0.828
1.844	0.000	0.000	0.766	0.000	0.508	0.734
1.886	0.000	0.000	0.669	0.000	0.835	0.710
1.929	0.000	0.000	0.582	0.000	1.147	0.714
1.972	0.000	0.000	0.493	0.000	1.510	0.742
2.015	0.000	0.000	0.434	0.000	1.845	0.825
2.058	0.000	0.000	0.370	0.000	2.069	0.888
2.101	0.000	0.000	0.309	0.000	2.139	0.961
2.144	0.000	0.000	0.248	0.000	2.201	1.030
2.187	0.000	0.000	0.210	0.000	2.099	1.081
2.229	0.000	0.000	0.178	0.000	2.002	1.103
2.272	0.001	0.000	0.146	0.000	1.787	1.090
2.315	0.013	0.000	0.137	0.000	1.589	1.062
2.358	0.117	0.000	0.128	0.000	1.325	1.023
2.401	0.456	0.000	0.124	0.000	1.141	0.976
2.444	0.937	0.000	0.122	0.000	0.984	0.894
2.487	1.340	0.000	0.122	0.000	0.777	0.828
2.530	1.507	0.000	0.129	0.000	0.643	0.776
2.572	1.608	0.000	0.140	0.000	0.594	0.733
2.615	1.756	0.000	0.162	0.000	0.459	0.687
2.658	1.882	0.000	0.195	0.000	0.409	0.652
2.701	1.967	0.013	0.242	0.000	0.385	0.618
2.744	1.873	0.038	0.315	0.000	0.369	0.610
2.787	1.805	0.159	0.413	0.000	0.335	0.606
2.830	1.660	0.336	0.546	0.000	0.335	0.604
2.872	1.500	0.669	0.686	0.000	0.332	0.612
2.915	1.286	1.120	0.862	0.000	0.330	0.634
2.958	1.183	1.666	1.027	0.000	0.370	0.667
3.001	1.060	2.144	1.197	0.000	0.388	0.702
3.044	0.947	2.600	1.349	0.000	0.433	0.730
3.087	0.883	2.696	1.451	0.000	0.496	0.764
3.130	0.836	2.687	1.552	0.000	0.572	0.813
3.173	0.792	2.671	1.588	0.000	0.664	0.848
3.215	0.773	2.498	1.594	0.000	0.759	0.890
3.258	0.761	2.292	1.556	0.000	0.874	0.924
3.301	0.792	2.002	1.525	0.000	1.031	0.958

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Electronic supplementary information for *PCCP*

3.344	0.849	1.669	1.490	0.000	1.183	1.004
3.387	0.848	1.560	1.453	0.000	1.355	1.048
3.430	0.871	1.425	1.398	0.000	1.457	1.076
3.473	0.879	1.292	1.348	0.054	1.528	1.126
3.516	0.907	1.236	1.290	0.056	1.632	1.156
3.558	0.949	1.244	1.266	0.065	1.717	1.191
3.601	0.983	1.171	1.244	0.188	1.765	1.238
3.644	1.038	1.221	1.216	0.080	1.723	1.266
3.687	1.036	1.250	1.195	0.123	1.750	1.310
3.730	1.093	1.235	1.177	0.267	1.695	1.323
3.773	1.160	1.247	1.157	0.252	1.682	1.322
3.816	1.161	1.226	1.153	0.374	1.608	1.328
3.859	1.193	1.235	1.134	0.347	1.552	1.309
3.901	1.214	1.317	1.126	0.471	1.429	1.277
3.944	1.219	1.359	1.113	0.536	1.342	1.250
3.987	1.231	1.427	1.105	0.391	1.294	1.223
4.030	1.246	1.332	1.099	0.551	1.249	1.202
4.073	1.260	1.342	1.086	0.500	1.231	1.173
4.116	1.240	1.357	1.070	0.470	1.189	1.148
4.159	1.229	1.358	1.068	0.700	1.220	1.124
4.202	1.253	1.333	1.063	0.613	1.180	1.111
4.244	1.242	1.339	1.040	0.655	1.161	1.095
4.287	1.236	1.349	1.037	0.634	1.153	1.081
4.330	1.213	1.365	1.024	0.680	1.123	1.066
4.373	1.197	1.324	1.009	0.668	1.101	1.063
4.416	1.159	1.349	0.992	0.785	1.095	1.042
4.459	1.165	1.329	0.990	0.801	1.097	1.038
4.502	1.137	1.274	0.989	0.893	1.080	1.034
4.544	1.141	1.289	0.993	0.951	1.062	1.024
4.587	1.116	1.274	0.990	0.993	1.052	1.020
4.630	1.083	1.231	0.987	0.748	1.038	1.010
4.673	1.080	1.170	0.983	0.686	1.012	1.005
4.716	1.060	1.187	0.983	0.615	1.017	1.003
4.759	1.023	1.234	0.982	0.612	1.008	0.996
4.802	0.996	1.188	0.986	0.647	1.008	0.992
4.845	0.969	1.134	0.984	0.712	1.010	0.979
4.887	0.929	1.098	0.979	0.682	1.010	0.968
4.930	0.937	1.076	0.977	0.707	1.007	0.967
4.973	0.891	1.059	0.975	0.801	0.988	0.951
5.016	0.841	1.036	0.959	0.925	0.968	0.933
5.059	0.833	1.009	0.958	0.813	0.963	0.927
5.102	0.813	0.904	0.949	0.700	0.974	0.917
5.145	0.774	0.876	0.935	0.804	0.979	0.908
5.188	0.773	0.916	0.921	0.672	0.964	0.908
5.230	0.772	0.867	0.919	0.508	0.937	0.909
5.273	0.770	0.889	0.915	0.770	0.932	0.898
5.316	0.787	0.898	0.912	0.915	0.934	0.911
5.359	0.796	0.851	0.908	1.130	0.957	0.914
5.402	0.782	0.760	0.903	0.811	0.937	0.916
5.445	0.809	0.789	0.906	0.778	0.898	0.916
5.488	0.831	0.745	0.910	0.904	0.882	0.916
5.531	0.816	0.758	0.908	1.248	0.892	0.928
5.573	0.825	0.735	0.909	0.989	0.902	0.930
5.616	0.825	0.758	0.916	0.858	0.875	0.937
5.659	0.818	0.733	0.907	1.102	0.873	0.937

Electronic supplementary information for *PCCP*

5.702	0.840	0.752	0.912	0.943	0.872	0.947
5.745	0.859	0.745	0.923	1.029	0.872	0.956
5.788	0.886	0.739	0.921	1.036	0.860	0.960
5.831	0.913	0.771	0.926	0.855	0.829	0.963
5.874	0.940	0.736	0.934	0.825	0.867	0.975
5.916	0.903	0.752	0.943	0.835	0.881	0.976
5.959	0.919	0.806	0.950	0.880	0.854	0.987
6.002	0.962	0.777	0.970	0.870	0.839	0.985
6.045	0.998	0.774	0.974	0.986	0.844	0.988
6.088	1.010	0.793	0.978	0.937	0.830	0.996
6.131	1.017	0.832	0.989	1.123	0.857	1.004
6.174	1.045	0.874	1.001	1.007	0.839	1.005
6.217	1.035	0.815	1.021	1.231	0.861	0.998
6.259	1.087	0.792	1.026	0.990	0.838	1.002
6.302	1.107	0.849	1.032	1.230	0.823	1.012
6.345	1.130	0.799	1.048	1.270	0.819	1.003
6.388	1.129	0.869	1.058	1.793	0.847	1.013
6.431	1.178	0.911	1.061	1.687	0.882	1.018
6.474	1.202	0.938	1.057	2.231	0.937	1.014
6.517	1.201	0.906	1.036	2.113	0.935	1.009
6.559	1.195	0.942	1.046	1.915	0.959	1.000
6.602	1.184	1.011	1.051	2.291	0.989	1.007
6.645	1.179	1.021	1.065	2.294	1.011	1.009
6.688	1.162	1.037	1.063	2.615	1.007	1.008
6.731	1.186	0.988	1.069	2.325	1.018	1.017
6.774	1.143	0.983	1.048	2.409	1.011	1.013
6.817	1.141	0.944	1.038	2.373	0.997	1.010
6.860	1.137	0.889	1.046	2.377	1.028	1.020
6.902	1.072	0.926	1.019	2.153	1.039	0.992
6.945	1.030	0.883	1.015	1.848	1.033	0.980
6.988	1.071	0.909	1.021	1.856	1.014	0.987

system 7:25 DC1:D2O, RDF

r [Å]	g(O,O)	g(O,Cl)	g(O,D)	g(Cl,Cl)	g(Cl,D)	g(D,D)
0.043	0.000	0.000	0.000	0.000	0.000	0.000
0.087	0.000	0.000	0.000	0.000	0.000	0.000
0.130	0.000	0.000	0.000	0.000	0.000	0.000
0.174	0.000	0.000	0.000	0.000	0.000	0.000
0.217	0.000	0.000	0.000	0.000	0.000	0.000
0.261	0.000	0.000	0.000	0.000	0.000	0.000
0.304	0.000	0.000	0.000	0.000	0.000	0.000
0.348	0.000	0.000	0.000	0.000	0.000	0.000
0.391	0.000	0.000	0.000	0.000	0.000	0.000
0.435	0.000	0.000	0.000	0.000	0.000	0.000
0.478	0.000	0.000	0.000	0.000	0.000	0.000
0.521	0.000	0.000	0.000	0.000	0.000	0.000
0.565	0.000	0.000	0.000	0.000	0.000	0.000
0.608	0.000	0.000	0.000	0.000	0.000	0.000
0.652	0.000	0.000	0.000	0.000	0.000	0.000
0.695	0.000	0.000	0.000	0.000	0.000	0.000
0.739	0.000	0.000	0.000	0.000	0.000	0.000
0.782	0.000	0.000	0.000	0.000	0.000	0.000
0.826	0.000	0.000	0.000	0.000	0.000	0.000
0.869	0.000	0.000	0.000	0.000	0.000	0.000
0.912	0.000	0.000	0.031	0.000	0.000	0.000

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Electronic supplementary information for *PCCP*

0.956	0.000	0.000	4.123	0.000	0.000	0.000
0.999	0.000	0.000	28.527	0.000	0.000	0.000
1.043	0.000	0.000	25.674	0.000	0.000	0.000
1.086	0.000	0.000	7.739	0.000	0.000	0.000
1.130	0.000	0.000	2.451	0.000	0.000	0.000
1.173	0.000	0.000	1.178	0.000	0.000	0.000
1.217	0.000	0.000	0.768	0.000	0.003	0.000
1.260	0.000	0.000	0.638	0.000	0.142	0.000
1.303	0.000	0.000	0.645	0.000	1.101	0.000
1.347	0.000	0.000	0.728	0.000	1.953	0.001
1.390	0.000	0.000	0.843	0.000	1.214	0.005
1.434	0.000	0.000	0.917	0.000	0.448	0.035
1.477	0.000	0.000	0.982	0.000	0.189	0.178
1.521	0.000	0.000	1.016	0.000	0.092	0.679
1.564	0.000	0.000	1.044	0.000	0.054	1.672
1.608	0.000	0.000	1.040	0.000	0.051	2.581
1.651	0.000	0.000	1.025	0.000	0.071	2.606
1.694	0.000	0.000	0.934	0.000	0.107	2.075
1.738	0.000	0.000	0.865	0.000	0.163	1.569
1.781	0.000	0.000	0.745	0.000	0.257	1.220
1.825	0.000	0.000	0.641	0.000	0.391	1.024
1.868	0.000	0.000	0.550	0.000	0.620	0.923
1.912	0.000	0.000	0.462	0.000	0.895	0.863
1.955	0.000	0.000	0.391	0.000	1.217	0.860
1.999	0.000	0.000	0.328	0.000	1.522	0.904
2.042	0.000	0.000	0.268	0.000	1.803	0.987
2.085	0.000	0.000	0.201	0.000	1.914	1.061
2.129	0.000	0.000	0.172	0.000	1.876	1.121
2.172	0.000	0.000	0.143	0.000	1.861	1.145
2.216	0.000	0.000	0.115	0.000	1.742	1.146
2.259	0.001	0.000	0.103	0.000	1.522	1.105
2.303	0.008	0.000	0.091	0.000	1.346	1.030
2.346	0.108	0.000	0.094	0.000	1.153	0.957
2.390	0.546	0.000	0.089	0.000	0.922	0.885
2.433	1.260	0.000	0.086	0.000	0.790	0.834
2.476	2.042	0.000	0.082	0.000	0.680	0.767
2.520	2.325	0.000	0.097	0.000	0.577	0.701
2.563	2.424	0.000	0.113	0.000	0.512	0.651
2.607	2.354	0.000	0.129	0.000	0.430	0.609
2.650	2.242	0.000	0.167	0.000	0.385	0.577
2.694	2.116	0.003	0.214	0.000	0.363	0.553
2.737	1.884	0.033	0.286	0.000	0.353	0.533
2.781	1.689	0.078	0.376	0.000	0.343	0.534
2.824	1.412	0.214	0.498	0.000	0.349	0.541
2.867	1.308	0.420	0.666	0.000	0.367	0.553
2.911	1.147	0.915	0.851	0.000	0.380	0.570
2.954	0.960	1.290	1.048	0.000	0.412	0.603
2.998	0.887	1.759	1.252	0.000	0.448	0.634
3.041	0.779	2.179	1.445	0.058	0.505	0.663
3.085	0.690	2.300	1.594	0.189	0.569	0.702
3.128	0.666	2.420	1.649	0.430	0.656	0.746
3.172	0.695	2.368	1.688	0.620	0.727	0.778
3.215	0.665	2.326	1.648	0.774	0.843	0.823
3.258	0.736	2.215	1.589	1.071	0.965	0.873
3.302	0.751	1.976	1.528	1.283	1.091	0.934

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Electronic supplementary information for *PCCP*

3.345	0.772	1.737	1.451	1.732	1.209	0.998
3.389	0.772	1.617	1.393	1.681	1.320	1.046
3.432	0.816	1.612	1.340	1.654	1.438	1.100
3.476	0.795	1.575	1.283	1.606	1.469	1.150
3.519	0.781	1.393	1.242	1.167	1.505	1.197
3.563	0.817	1.308	1.214	1.251	1.530	1.240
3.606	0.858	1.246	1.203	1.318	1.555	1.285
3.649	0.877	1.316	1.171	1.086	1.550	1.318
3.693	0.902	1.301	1.147	1.077	1.508	1.332
3.736	0.924	1.276	1.144	1.075	1.497	1.358
3.780	0.998	1.203	1.118	1.161	1.440	1.375
3.823	1.054	1.157	1.108	1.039	1.433	1.361
3.867	1.061	1.209	1.120	1.153	1.372	1.329
3.910	1.140	1.211	1.103	1.118	1.311	1.308
3.954	1.210	1.263	1.096	1.385	1.287	1.271
3.997	1.210	1.227	1.088	1.299	1.283	1.237
4.040	1.264	1.200	1.069	1.199	1.271	1.215
4.084	1.296	1.202	1.063	1.297	1.203	1.196
4.127	1.337	1.211	1.068	1.010	1.206	1.173
4.171	1.406	1.172	1.064	0.992	1.175	1.146
4.214	1.346	1.160	1.048	1.148	1.148	1.140
4.258	1.357	1.134	1.047	1.060	1.150	1.126
4.301	1.347	1.229	1.046	1.026	1.123	1.104
4.345	1.370	1.229	1.047	1.012	1.100	1.088
4.388	1.338	1.201	1.033	0.963	1.092	1.072
4.431	1.338	1.204	1.025	0.917	1.107	1.064
4.475	1.266	1.188	1.010	0.947	1.115	1.045
4.518	1.225	1.142	1.002	1.005	1.110	1.014
4.562	1.221	1.235	1.013	0.981	1.068	1.012
4.605	1.176	1.225	1.013	0.898	1.021	1.003
4.649	1.155	1.215	1.007	1.055	1.028	0.985
4.692	1.091	1.159	1.008	1.256	1.004	0.983
4.736	1.098	1.125	1.023	1.061	1.003	0.985
4.779	1.068	1.097	1.015	0.901	1.000	0.983
4.822	1.007	1.112	1.009	0.899	1.003	0.969
4.866	0.950	1.081	1.027	0.965	1.017	0.965
4.909	0.906	1.073	1.024	0.868	1.002	0.958
4.953	0.898	1.075	1.020	0.822	0.990	0.959
4.996	0.847	1.016	1.029	0.819	0.965	0.956
5.040	0.813	1.014	1.011	0.888	0.976	0.937
5.083	0.773	0.942	0.983	0.799	0.980	0.925
5.127	0.759	0.936	0.969	0.769	0.972	0.920
5.170	0.723	0.904	0.952	0.854	0.939	0.928
5.213	0.730	0.877	0.933	0.726	0.951	0.923
5.257	0.708	0.882	0.922	0.678	0.973	0.915
5.300	0.692	0.873	0.909	0.654	0.982	0.911
5.344	0.688	0.917	0.891	0.675	0.992	0.913
5.387	0.695	0.902	0.875	0.678	0.977	0.911
5.431	0.703	0.895	0.861	0.761	0.970	0.911
5.474	0.710	0.895	0.851	0.730	0.945	0.922
5.518	0.693	0.874	0.839	0.563	0.945	0.919
5.561	0.712	0.889	0.841	0.626	0.929	0.912
5.604	0.717	0.898	0.831	0.628	0.935	0.916
5.648	0.755	0.861	0.847	0.623	0.946	0.922
5.691	0.759	0.856	0.846	0.653	0.960	0.919

Electronic supplementary information for *PCCP*

5.735	0.755	0.890	0.854	0.599	0.961	0.911
5.778	0.799	0.963	0.856	0.579	0.938	0.907
5.822	0.849	1.000	0.858	0.539	0.946	0.911
5.865	0.886	0.958	0.869	0.539	0.956	0.930
5.909	0.962	0.959	0.886	0.522	0.958	0.934
5.952	0.937	0.934	0.894	0.560	0.950	0.931
5.995	0.941	0.941	0.906	0.657	0.950	0.942
6.039	0.943	0.964	0.903	0.651	0.956	0.949
6.082	1.042	0.949	0.913	0.763	0.945	0.953
6.126	1.041	0.957	0.923	0.807	0.941	0.966
6.169	1.009	0.992	0.940	0.842	0.948	0.967
6.213	1.043	1.002	0.950	0.873	0.929	0.965
6.256	1.062	1.031	0.966	0.854	0.939	0.974
6.300	1.082	1.032	0.971	0.888	0.938	0.985
6.343	1.072	0.994	0.973	1.139	0.932	1.002
6.386	1.115	0.995	0.995	1.244	0.944	0.996
6.430	1.130	1.048	1.007	1.051	0.917	1.006
6.473	1.133	1.042	1.025	1.009	0.965	1.015
6.517	1.109	1.003	1.042	0.976	0.934	1.009
6.560	1.109	1.016	1.051	1.166	0.924	1.009
6.604	1.136	0.971	1.065	1.386	0.935	1.009
6.647	1.129	1.005	1.072	1.329	0.935	1.023
6.691	1.165	0.948	1.080	1.296	0.952	1.038
6.734	1.183	1.027	1.099	1.337	0.963	1.034
6.777	1.169	1.019	1.107	1.514	0.959	1.031
6.821	1.150	0.948	1.098	1.391	0.986	1.025
6.864	1.134	0.898	1.101	1.589	0.976	1.033
6.908	1.140	0.871	1.124	1.770	0.955	1.013
6.951	1.082	0.862	1.127	1.449	0.945	1.022
6.995	1.048	0.896	1.133	1.436	0.963	1.034

system 10:22 DCl:D2O, 330K, RDF

r [Å]	g(O,O)	g(O,Cl)	g(O,D)	g(Cl,Cl)	g(Cl,D)	g(D,D)
0.044	0.000	0.000	0.000	0.000	0.000	0.000
0.087	0.000	0.000	0.000	0.000	0.000	0.000
0.131	0.000	0.000	0.000	0.000	0.000	0.000
0.174	0.000	0.000	0.000	0.000	0.000	0.000
0.218	0.000	0.000	0.000	0.000	0.000	0.000
0.261	0.000	0.000	0.000	0.000	0.000	0.000
0.305	0.000	0.000	0.000	0.000	0.000	0.000
0.349	0.000	0.000	0.000	0.000	0.000	0.000
0.392	0.000	0.000	0.000	0.000	0.000	0.000
0.436	0.000	0.000	0.000	0.000	0.000	0.000
0.479	0.000	0.000	0.000	0.000	0.000	0.000
0.523	0.000	0.000	0.000	0.000	0.000	0.000
0.566	0.000	0.000	0.000	0.000	0.000	0.000
0.610	0.000	0.000	0.000	0.000	0.000	0.000
0.653	0.000	0.000	0.000	0.000	0.000	0.000
0.697	0.000	0.000	0.000	0.000	0.000	0.000
0.741	0.000	0.000	0.000	0.000	0.000	0.000
0.784	0.000	0.000	0.000	0.000	0.000	0.000
0.828	0.000	0.000	0.000	0.000	0.000	0.000
0.871	0.000	0.000	0.000	0.000	0.000	0.000
0.915	0.000	0.000	0.025	0.000	0.000	0.000
0.958	0.000	0.000	4.805	0.000	0.000	0.000



Electronic supplementary information for *PCCP*

1.002	0.000	0.000	30.444	0.000	0.000	0.000
1.045	0.000	0.000	26.934	0.000	0.000	0.000
1.089	0.000	0.000	9.542	0.000	0.000	0.000
1.133	0.000	0.000	3.543	0.000	0.000	0.000
1.176	0.000	0.000	1.656	0.000	0.000	0.000
1.220	0.000	0.000	1.056	0.000	0.000	0.000
1.263	0.000	0.000	0.862	0.000	0.214	0.000
1.307	0.000	0.000	0.825	0.000	1.921	0.000
1.350	0.000	0.000	0.905	0.000	1.987	0.000
1.394	0.000	0.000	0.967	0.000	1.038	0.001
1.438	0.000	0.000	0.998	0.000	0.394	0.022
1.481	0.000	0.000	1.005	0.000	0.175	0.151
1.525	0.000	0.000	0.966	0.000	0.107	0.601
1.568	0.000	0.000	0.928	0.000	0.096	1.459
1.612	0.000	0.000	0.866	0.000	0.141	2.458
1.655	0.000	0.000	0.815	0.000	0.214	2.795
1.699	0.000	0.000	0.740	0.000	0.331	2.519
1.742	0.000	0.000	0.647	0.000	0.540	2.069
1.786	0.000	0.000	0.528	0.000	0.810	1.746
1.830	0.000	0.000	0.442	0.000	1.082	1.445
1.873	0.000	0.000	0.376	0.000	1.260	1.189
1.917	0.000	0.000	0.315	0.000	1.401	1.024
1.960	0.000	0.000	0.261	0.000	1.536	0.948
2.004	0.000	0.000	0.242	0.000	1.632	0.931
2.047	0.000	0.000	0.193	0.000	1.696	0.943
2.091	0.000	0.000	0.143	0.000	1.719	0.940
2.134	0.000	0.000	0.119	0.000	1.626	0.927
2.178	0.000	0.000	0.099	0.000	1.549	0.910
2.222	0.000	0.000	0.094	0.000	1.362	0.879
2.265	0.003	0.000	0.089	0.000	1.211	0.837
2.309	0.027	0.000	0.072	0.000	1.024	0.785
2.352	0.185	0.000	0.066	0.000	0.852	0.727
2.396	0.816	0.000	0.071	0.000	0.720	0.661
2.439	1.788	0.000	0.077	0.000	0.636	0.604
2.483	2.602	0.000	0.075	0.000	0.543	0.567
2.527	2.659	0.000	0.080	0.000	0.435	0.553
2.570	2.471	0.000	0.094	0.000	0.406	0.526
2.614	2.284	0.000	0.119	0.000	0.364	0.526
2.657	1.959	0.001	0.172	0.000	0.339	0.514
2.701	1.899	0.046	0.244	0.000	0.329	0.521
2.744	1.507	0.171	0.321	0.000	0.310	0.517
2.788	1.284	0.423	0.451	0.000	0.298	0.544
2.831	1.169	0.887	0.591	0.000	0.297	0.561
2.875	0.987	1.383	0.757	0.000	0.321	0.567
2.919	0.927	1.705	0.946	0.000	0.339	0.604
2.962	0.906	1.908	1.187	0.011	0.370	0.644
3.006	0.795	2.172	1.380	0.053	0.429	0.698
3.049	0.733	2.305	1.520	0.081	0.477	0.743
3.093	0.740	2.321	1.615	0.222	0.566	0.796
3.136	0.761	2.317	1.654	0.341	0.649	0.848
3.180	0.769	2.256	1.670	0.581	0.756	0.895
3.223	0.753	2.017	1.623	0.883	0.862	0.945
3.267	0.728	1.848	1.569	0.974	0.989	1.002
3.311	0.799	1.630	1.509	1.121	1.106	1.043
3.354	0.819	1.556	1.426	1.100	1.231	1.110

Electronic supplementary information for *PCCP*

3.398	0.833	1.415	1.384	1.312	1.404	1.172
3.441	0.873	1.421	1.337	1.333	1.495	1.201
3.485	0.880	1.265	1.307	1.146	1.606	1.247
3.528	0.913	1.267	1.257	1.230	1.609	1.286
3.572	1.017	1.254	1.248	1.095	1.592	1.319
3.615	1.049	1.240	1.234	1.197	1.600	1.340
3.659	1.165	1.318	1.201	1.321	1.585	1.369
3.703	1.172	1.315	1.199	1.428	1.563	1.393
3.746	1.183	1.214	1.181	1.603	1.512	1.387
3.790	1.210	1.240	1.173	1.547	1.496	1.366
3.833	1.198	1.237	1.156	1.580	1.442	1.343
3.877	1.233	1.222	1.146	1.566	1.401	1.320
3.920	1.276	1.207	1.154	1.610	1.351	1.295
3.964	1.255	1.152	1.151	1.578	1.334	1.265
4.008	1.268	1.176	1.148	1.586	1.270	1.220
4.051	1.259	1.189	1.107	1.709	1.241	1.189
4.095	1.307	1.208	1.114	1.586	1.203	1.169
4.138	1.356	1.233	1.116	1.519	1.187	1.154
4.182	1.339	1.218	1.094	1.402	1.166	1.128
4.225	1.345	1.261	1.103	1.439	1.164	1.111
4.269	1.369	1.239	1.100	1.376	1.150	1.088
4.312	1.308	1.258	1.090	1.337	1.130	1.078
4.356	1.286	1.192	1.066	1.463	1.114	1.062
4.400	1.278	1.228	1.071	1.333	1.093	1.043
4.443	1.275	1.208	1.048	1.219	1.083	1.040
4.487	1.198	1.178	1.035	1.282	1.066	1.021
4.530	1.173	1.167	1.019	1.172	1.052	1.018
4.574	1.093	1.231	1.019	1.118	1.031	1.024
4.617	1.053	1.205	1.035	1.179	1.001	1.021
4.661	1.043	1.100	1.022	1.077	0.974	1.005
4.704	1.006	1.050	1.006	1.032	0.977	0.999
4.748	1.010	1.007	1.005	0.943	0.953	0.994
4.792	0.971	1.020	0.984	0.951	0.959	0.988
4.835	0.959	1.003	0.978	1.014	0.961	0.994
4.879	0.845	0.951	0.976	0.876	0.942	0.984
4.922	0.825	0.900	0.962	0.990	0.962	0.968
4.966	0.799	0.872	0.966	0.941	0.955	0.968
5.009	0.789	0.852	0.958	0.975	0.954	0.964
5.053	0.804	0.821	0.939	0.869	0.930	0.941
5.097	0.760	0.788	0.922	0.888	0.917	0.940
5.140	0.802	0.791	0.911	0.864	0.930	0.927
5.184	0.828	0.761	0.917	0.862	0.921	0.917
5.227	0.786	0.706	0.897	0.811	0.926	0.911
5.271	0.786	0.673	0.881	0.742	0.903	0.887
5.314	0.792	0.685	0.883	0.793	0.914	0.888
5.358	0.829	0.698	0.878	0.812	0.926	0.883
5.401	0.840	0.677	0.874	0.786	0.923	0.892
5.445	0.802	0.721	0.864	0.807	0.916	0.896
5.489	0.773	0.720	0.857	0.819	0.916	0.900
5.532	0.805	0.774	0.867	0.907	0.891	0.906
5.576	0.769	0.757	0.878	0.852	0.881	0.910
5.619	0.800	0.747	0.873	0.795	0.877	0.919
5.663	0.813	0.788	0.863	0.841	0.856	0.913
5.706	0.838	0.799	0.859	0.871	0.852	0.930
5.750	0.852	0.864	0.869	0.812	0.860	0.935

Electronic supplementary information for *PCCP*

5.793	0.795	0.922	0.869	0.686	0.871	0.934
5.837	0.847	0.950	0.895	0.843	0.864	0.944
5.881	0.849	1.005	0.874	0.781	0.871	0.943
5.924	0.885	0.997	0.876	0.799	0.881	0.948
5.968	0.904	1.070	0.892	0.834	0.903	0.941
6.011	0.878	1.062	0.894	0.843	0.892	0.959
6.055	0.891	1.086	0.897	0.845	0.912	0.944
6.098	0.937	1.158	0.902	0.731	0.935	0.941
6.142	0.930	1.175	0.918	0.705	0.948	0.934
6.186	0.947	1.143	0.935	0.754	0.973	0.939
6.229	0.949	1.111	0.946	0.783	1.000	0.929
6.273	0.951	1.107	0.974	0.784	1.032	0.925
6.316	1.042	1.101	0.972	0.779	1.077	0.932
6.360	0.959	1.135	0.994	0.811	1.088	0.938
6.403	0.952	1.163	0.995	0.859	1.083	0.947
6.447	1.037	1.232	1.017	0.891	1.084	0.963
6.490	0.974	1.241	1.026	0.813	1.097	0.963
6.534	0.971	1.206	1.029	0.662	1.119	0.967
6.578	1.019	1.249	1.047	0.802	1.141	0.979
6.621	0.970	1.340	1.025	0.864	1.118	0.993
6.665	0.986	1.298	1.041	0.997	1.196	1.000
6.708	0.958	1.354	1.044	1.132	1.234	0.991
6.752	0.981	1.310	1.049	1.059	1.234	1.018
6.795	1.028	1.336	1.030	1.002	1.228	1.027
6.839	1.079	1.371	1.006	1.079	1.235	1.025
6.882	1.104	1.334	1.008	1.138	1.238	1.046
6.926	1.082	1.250	0.991	1.195	1.227	1.049
6.970	1.039	1.135	0.998	0.991	1.250	1.051

system 10:22 DCl:D2O, 470K, RDF

r [Å]	g(O,O)	g(O,Cl)	g(O,D)	g(Cl,Cl)	g(Cl,D)	g(D,D)
0.044	0.000	0.000	0.000	0.000	0.000	0.000
0.087	0.000	0.000	0.000	0.000	0.000	0.000
0.131	0.000	0.000	0.000	0.000	0.000	0.000
0.174	0.000	0.000	0.000	0.000	0.000	0.000
0.218	0.000	0.000	0.000	0.000	0.000	0.000
0.261	0.000	0.000	0.000	0.000	0.000	0.000
0.305	0.000	0.000	0.000	0.000	0.000	0.000
0.349	0.000	0.000	0.000	0.000	0.000	0.000
0.392	0.000	0.000	0.000	0.000	0.000	0.000
0.436	0.000	0.000	0.000	0.000	0.000	0.000
0.479	0.000	0.000	0.000	0.000	0.000	0.000
0.523	0.000	0.000	0.000	0.000	0.000	0.000
0.566	0.000	0.000	0.000	0.000	0.000	0.000
0.610	0.000	0.000	0.000	0.000	0.000	0.000
0.653	0.000	0.000	0.000	0.000	0.000	0.000
0.697	0.000	0.000	0.000	0.000	0.000	0.000
0.741	0.000	0.000	0.000	0.000	0.000	0.000
0.784	0.000	0.000	0.000	0.000	0.000	0.000
0.828	0.000	0.000	0.000	0.000	0.000	0.000
0.871	0.000	0.000	0.000	0.000	0.000	0.000
0.915	0.000	0.000	0.205	0.000	0.000	0.000
0.958	0.000	0.000	9.132	0.000	0.000	0.000
1.002	0.000	0.000	29.732	0.000	0.000	0.000
1.045	0.000	0.000	23.091	0.000	0.000	0.000

Electronic supplementary information for *PCCP*

1.089	0.000	0.000	8.267	0.000	0.000	0.000
1.133	0.000	0.000	2.949	0.000	0.000	0.000
1.176	0.000	0.000	1.529	0.000	0.001	0.000
1.220	0.000	0.000	1.039	0.000	0.137	0.000
1.263	0.000	0.000	0.854	0.000	0.898	0.000
1.307	0.000	0.000	0.811	0.000	2.339	0.000
1.350	0.000	0.000	0.799	0.000	2.531	0.003
1.394	0.000	0.000	0.761	0.000	1.613	0.027
1.438	0.000	0.000	0.765	0.000	0.857	0.163
1.481	0.000	0.000	0.770	0.000	0.446	0.499
1.525	0.000	0.000	0.784	0.000	0.323	1.161
1.568	0.000	0.000	0.779	0.000	0.259	1.899
1.612	0.000	0.000	0.754	0.000	0.293	2.338
1.655	0.000	0.000	0.758	0.000	0.324	2.335
1.699	0.000	0.000	0.702	0.000	0.375	2.004
1.742	0.000	0.000	0.632	0.000	0.460	1.641
1.786	0.000	0.000	0.589	0.000	0.547	1.361
1.830	0.000	0.000	0.557	0.000	0.668	1.168
1.873	0.000	0.000	0.497	0.000	0.779	1.011
1.917	0.000	0.000	0.448	0.000	0.872	0.937
1.960	0.000	0.000	0.387	0.000	0.940	0.901
2.004	0.000	0.000	0.340	0.000	0.976	0.887
2.047	0.000	0.000	0.290	0.000	1.046	0.899
2.091	0.000	0.000	0.261	0.000	1.029	0.873
2.134	0.000	0.000	0.243	0.000	0.986	0.887
2.178	0.000	0.000	0.229	0.000	0.941	0.893
2.222	0.000	0.000	0.216	0.000	0.945	0.870
2.265	0.011	0.000	0.208	0.000	0.883	0.856
2.309	0.087	0.000	0.199	0.000	0.818	0.844
2.352	0.338	0.000	0.198	0.000	0.798	0.818
2.396	0.861	0.000	0.197	0.000	0.727	0.799
2.439	1.659	0.000	0.203	0.000	0.698	0.748
2.483	1.986	0.000	0.231	0.000	0.668	0.740
2.527	2.074	0.002	0.254	0.000	0.617	0.736
2.570	2.055	0.002	0.299	0.000	0.586	0.731
2.614	1.910	0.023	0.343	0.000	0.559	0.731
2.657	2.010	0.054	0.397	0.000	0.547	0.706
2.701	1.799	0.123	0.498	0.000	0.574	0.703
2.744	1.706	0.296	0.599	0.000	0.570	0.692
2.788	1.552	0.535	0.693	0.000	0.580	0.712
2.831	1.416	0.811	0.820	0.016	0.609	0.742
2.875	1.316	1.133	0.956	0.013	0.661	0.769
2.919	1.205	1.372	1.071	0.015	0.689	0.781
2.962	1.217	1.456	1.197	0.024	0.727	0.794
3.006	1.199	1.670	1.292	0.080	0.753	0.823
3.049	1.124	1.795	1.361	0.301	0.838	0.848
3.093	1.043	1.881	1.411	0.537	0.915	0.888
3.136	1.053	1.851	1.479	0.811	0.966	0.915
3.180	1.025	1.993	1.487	1.023	1.038	0.930
3.223	0.981	1.995	1.484	0.992	1.108	0.969
3.267	0.919	1.865	1.443	1.265	1.215	1.004
3.311	0.957	1.791	1.428	1.340	1.273	1.024
3.354	0.942	1.908	1.412	1.468	1.341	1.048
3.398	0.913	1.750	1.341	1.537	1.370	1.068
3.441	0.939	1.759	1.293	1.386	1.389	1.087

Electronic supplementary information for *PCCP*

3.485	0.939	1.749	1.245	1.465	1.485	1.123
3.528	0.950	1.687	1.215	1.711	1.486	1.147
3.572	0.968	1.665	1.200	1.622	1.466	1.166
3.615	0.974	1.670	1.183	1.653	1.441	1.186
3.659	1.029	1.632	1.140	1.515	1.427	1.191
3.703	0.963	1.530	1.111	1.393	1.443	1.210
3.746	0.966	1.560	1.116	1.330	1.394	1.211
3.790	1.020	1.464	1.114	1.298	1.374	1.214
3.833	1.053	1.372	1.079	1.399	1.330	1.204
3.877	1.078	1.347	1.047	1.228	1.320	1.193
3.920	1.076	1.387	1.031	1.280	1.330	1.189
3.964	1.019	1.455	1.031	1.197	1.292	1.168
4.008	1.011	1.400	1.045	1.324	1.244	1.155
4.051	1.034	1.377	1.024	1.208	1.235	1.137
4.095	1.036	1.361	1.009	1.201	1.216	1.117
4.138	1.057	1.396	1.021	1.159	1.207	1.095
4.182	1.077	1.353	0.992	1.345	1.195	1.077
4.225	1.110	1.227	0.997	1.213	1.193	1.047
4.269	1.079	1.226	0.992	1.098	1.185	1.039
4.312	1.032	1.193	0.976	1.055	1.157	1.040
4.356	1.045	1.165	0.966	0.946	1.114	1.039
4.400	1.005	1.104	0.954	1.054	1.089	1.027
4.443	0.992	1.101	0.948	1.070	1.074	1.010
4.487	0.929	1.017	0.963	1.035	1.040	1.003
4.530	0.937	1.036	0.958	1.066	1.048	1.008
4.574	0.942	1.009	0.950	0.942	1.061	1.000
4.617	0.964	0.925	0.938	0.950	1.037	0.989
4.661	0.901	0.940	0.942	0.992	1.044	0.992
4.704	0.907	0.955	0.950	0.971	1.008	0.982
4.748	0.872	0.948	0.955	0.865	0.981	0.981
4.792	0.892	0.906	0.961	0.790	0.962	0.970
4.835	0.900	0.894	0.962	0.799	0.953	0.970
4.879	0.911	0.865	0.970	0.707	0.944	0.977
4.922	0.907	0.874	0.975	0.824	0.950	0.962
4.966	0.876	0.857	0.979	0.916	0.940	0.967
5.009	0.886	0.881	0.979	0.768	0.959	0.970
5.053	0.878	0.851	0.969	0.780	0.925	0.962
5.097	0.844	0.859	0.955	0.872	0.911	0.948
5.140	0.858	0.824	0.959	0.782	0.913	0.957
5.184	0.873	0.839	0.951	0.884	0.910	0.946
5.227	0.872	0.876	0.955	0.887	0.898	0.953
5.271	0.865	0.841	0.950	0.858	0.905	0.947
5.314	0.852	0.834	0.962	0.883	0.898	0.958
5.358	0.898	0.854	0.956	0.789	0.905	0.953
5.401	0.954	0.847	0.956	0.800	0.882	0.949
5.445	0.968	0.903	0.955	0.823	0.893	0.955
5.489	0.980	0.854	0.960	0.824	0.888	0.958
5.532	0.970	0.858	0.966	0.808	0.879	0.969
5.576	0.978	0.848	0.976	0.765	0.895	0.962
5.619	0.985	0.782	0.970	0.803	0.905	0.964
5.663	1.013	0.786	0.970	0.853	0.894	0.966
5.706	1.064	0.823	0.973	0.826	0.900	0.968
5.750	1.046	0.854	0.974	0.869	0.908	0.978
5.793	1.067	0.866	0.980	0.877	0.923	0.982
5.837	1.058	0.888	0.987	0.857	0.911	0.989

Electronic supplementary information for *PCCP*

5.881	1.063	0.939	0.992	0.948	0.914	0.996
5.924	1.068	0.930	0.993	1.115	0.898	0.997
5.968	1.048	0.955	0.974	1.065	0.925	1.000
6.011	1.042	0.933	0.990	0.978	0.928	0.987
6.055	1.066	0.978	0.991	1.001	0.951	0.994
6.098	1.068	0.960	0.996	1.059	0.960	0.995
6.142	1.114	0.997	0.993	1.115	0.950	0.984
6.186	1.098	1.009	1.014	1.139	0.968	0.980
6.229	1.099	0.993	1.019	1.044	0.939	0.978
6.273	1.023	1.065	1.017	1.063	0.942	0.988
6.316	1.027	1.014	1.031	1.122	0.961	0.976
6.360	1.064	0.975	1.024	1.126	0.975	0.982
6.403	1.045	0.976	1.011	1.179	0.971	0.974
6.447	1.065	0.995	0.994	1.283	0.983	0.987
6.490	1.069	0.948	1.015	1.307	1.004	0.976
6.534	0.997	0.996	0.990	1.348	1.005	0.968
6.578	0.955	1.028	0.994	1.329	0.998	0.967
6.621	0.963	0.981	0.979	1.266	1.004	0.971
6.665	0.973	0.959	0.976	1.206	1.023	0.979
6.708	0.999	1.020	0.958	1.156	1.059	0.982
6.752	0.941	1.086	0.988	1.315	1.076	0.994
6.795	0.947	1.049	0.964	1.457	1.082	1.000
6.839	0.931	1.035	0.919	1.225	1.071	0.983
6.882	0.862	1.055	0.954	1.307	1.077	0.988
6.926	0.866	1.015	0.959	1.129	1.067	0.960
6.970	0.867	0.996	0.959	1.064	1.072	0.958

system 10:22 DCl:D2O, 909K, RDF

r [Å]	g(O,O)	g(O,Cl)	g(O,D)	g(Cl,Cl)	g(Cl,D)	g(D,D)
0.044	0.000	0.000	0.000	0.000	0.000	0.000
0.087	0.000	0.000	0.000	0.000	0.000	0.000
0.131	0.000	0.000	0.000	0.000	0.000	0.000
0.174	0.000	0.000	0.000	0.000	0.000	0.000
0.218	0.000	0.000	0.000	0.000	0.000	0.000
0.261	0.000	0.000	0.000	0.000	0.000	0.000
0.305	0.000	0.000	0.000	0.000	0.000	0.000
0.349	0.000	0.000	0.000	0.000	0.000	0.000
0.392	0.000	0.000	0.000	0.000	0.000	0.000
0.436	0.000	0.000	0.000	0.000	0.000	0.000
0.479	0.000	0.000	0.000	0.000	0.000	0.000
0.523	0.000	0.000	0.000	0.000	0.000	0.000
0.566	0.000	0.000	0.000	0.000	0.000	0.000
0.610	0.000	0.000	0.000	0.000	0.000	0.000
0.653	0.000	0.000	0.000	0.000	0.000	0.000
0.697	0.000	0.000	0.000	0.000	0.000	0.000
0.741	0.000	0.000	0.000	0.000	0.000	0.000
0.784	0.000	0.000	0.000	0.000	0.000	0.000
0.828	0.000	0.000	0.000	0.000	0.000	0.000
0.871	0.000	0.000	0.081	0.000	0.000	0.000
0.915	0.000	0.000	2.431	0.000	0.000	0.000
0.958	0.000	0.000	13.631	0.000	0.000	0.000
1.002	0.000	0.000	25.834	0.000	0.000	0.000
1.045	0.000	0.000	18.691	0.000	0.000	0.000
1.089	0.000	0.000	7.553	0.000	0.000	0.000
1.133	0.000	0.000	3.026	0.000	0.000	0.000

Electronic supplementary information for *PCCP*

1.176	0.000	0.000	1.311	0.000	0.098	0.000
1.220	0.000	0.000	0.815	0.000	0.647	0.000
1.263	0.000	0.000	0.606	0.000	1.897	0.005
1.307	0.000	0.000	0.459	0.000	2.898	0.032
1.350	0.000	0.000	0.430	0.000	2.970	0.122
1.394	0.000	0.000	0.451	0.000	2.064	0.312
1.438	0.000	0.000	0.449	0.000	1.308	0.605
1.481	0.000	0.000	0.444	0.000	0.784	1.056
1.525	0.000	0.000	0.475	0.000	0.658	1.501
1.568	0.000	0.000	0.459	0.000	0.469	1.852
1.612	0.000	0.000	0.443	0.000	0.390	1.999
1.655	0.000	0.000	0.459	0.000	0.357	1.852
1.699	0.000	0.000	0.444	0.000	0.340	1.574
1.742	0.000	0.000	0.444	0.000	0.352	1.301
1.786	0.000	0.000	0.487	0.000	0.394	1.009
1.830	0.000	0.000	0.497	0.000	0.404	0.892
1.873	0.000	0.000	0.492	0.000	0.415	0.805
1.917	0.000	0.000	0.493	0.000	0.478	0.754
1.960	0.000	0.000	0.474	0.000	0.493	0.730
2.004	0.000	0.000	0.479	0.000	0.493	0.745
2.047	0.000	0.000	0.454	0.000	0.521	0.747
2.091	0.000	0.000	0.436	0.000	0.547	0.762
2.134	0.000	0.000	0.436	0.000	0.573	0.772
2.178	0.000	0.000	0.438	0.000	0.624	0.841
2.222	0.000	0.000	0.446	0.000	0.691	0.835
2.265	0.059	0.000	0.453	0.000	0.700	0.859
2.309	0.256	0.000	0.469	0.000	0.699	0.872
2.352	0.382	0.000	0.506	0.000	0.712	0.869
2.396	0.575	0.000	0.534	0.000	0.733	0.870
2.439	0.916	0.000	0.550	0.000	0.721	0.871
2.483	1.108	0.008	0.571	0.000	0.720	0.864
2.527	1.300	0.033	0.612	0.000	0.740	0.887
2.570	1.422	0.041	0.671	0.000	0.726	0.889
2.614	1.406	0.130	0.715	0.000	0.721	0.912
2.657	1.492	0.263	0.785	0.000	0.737	0.915
2.701	1.663	0.441	0.815	0.000	0.759	0.920
2.744	1.727	0.638	0.885	0.000	0.827	0.915
2.788	1.783	0.867	0.933	0.000	0.773	0.902
2.831	1.737	0.984	1.012	0.000	0.845	0.939
2.875	1.751	1.005	1.054	0.016	0.875	0.925
2.919	1.673	1.238	1.090	0.089	0.885	0.946
2.962	1.747	1.332	1.158	0.480	0.962	0.963
3.006	1.680	1.501	1.203	0.730	1.020	0.962
3.049	1.551	1.631	1.245	0.824	1.061	0.976
3.093	1.495	1.714	1.259	1.135	1.083	0.991
3.136	1.542	1.807	1.271	1.050	1.075	0.992
3.180	1.395	1.832	1.278	1.468	1.134	1.014
3.223	1.372	1.997	1.290	1.841	1.146	1.033
3.267	1.363	1.903	1.289	1.891	1.162	1.050
3.311	1.353	1.826	1.283	1.644	1.221	1.075
3.354	1.244	1.834	1.278	1.750	1.233	1.098
3.398	1.307	1.786	1.287	1.535	1.237	1.098
3.441	1.227	1.728	1.264	1.654	1.225	1.098
3.485	1.202	1.573	1.233	1.717	1.282	1.114
3.528	1.102	1.604	1.225	1.687	1.253	1.126

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3.572	1.129	1.608	1.200	1.700	1.264	1.106
3.615	1.070	1.470	1.206	1.727	1.254	1.097
3.659	1.078	1.436	1.184	1.786	1.208	1.121
3.703	1.015	1.542	1.178	1.716	1.237	1.114
3.746	1.013	1.507	1.134	1.606	1.249	1.116
3.790	1.017	1.453	1.103	1.454	1.265	1.100
3.833	1.006	1.342	1.083	1.295	1.242	1.109
3.877	1.025	1.315	1.083	1.269	1.237	1.090
3.920	0.926	1.219	1.071	1.359	1.202	1.098
3.964	0.919	1.163	1.058	1.209	1.195	1.092
4.008	0.955	1.161	1.064	1.395	1.197	1.068
4.051	0.931	1.064	1.043	1.304	1.205	1.077
4.095	0.937	1.097	1.044	1.351	1.197	1.064
4.138	0.890	1.067	1.006	1.181	1.152	1.057
4.182	0.942	1.096	1.002	1.196	1.122	1.046
4.225	0.934	1.043	0.993	1.122	1.120	1.026
4.269	0.865	1.110	0.978	1.061	1.126	1.028
4.312	0.834	1.090	0.964	0.926	1.079	1.034
4.356	0.858	0.989	0.944	0.924	1.077	1.028
4.400	0.810	0.978	0.951	1.032	1.038	1.016
4.443	0.814	0.992	0.948	0.944	1.063	1.005
4.487	0.825	0.903	0.950	0.891	1.047	1.009
4.530	0.814	0.909	0.943	0.818	1.054	0.987
4.574	0.800	0.863	0.939	0.801	1.030	0.993
4.617	0.857	0.915	0.933	0.790	1.010	0.988
4.661	0.833	0.866	0.934	0.744	1.013	0.984
4.704	0.875	0.883	0.928	0.832	0.981	0.986
4.748	0.861	0.905	0.924	0.825	1.004	0.989
4.792	0.864	0.841	0.915	0.982	0.966	0.981
4.835	0.859	0.882	0.905	0.890	0.955	0.970
4.879	0.875	0.899	0.901	0.911	0.958	0.966
4.922	0.813	0.865	0.897	0.797	0.951	0.979
4.966	0.810	0.909	0.895	0.729	0.940	0.976
5.009	0.822	0.882	0.901	0.860	0.928	0.973
5.053	0.915	0.859	0.906	0.765	0.916	0.954
5.097	0.883	0.821	0.914	0.795	0.921	0.956
5.140	0.872	0.824	0.929	0.766	0.925	0.957
5.184	0.840	0.812	0.934	0.788	0.915	0.935
5.227	0.906	0.892	0.946	0.802	0.913	0.934
5.271	0.889	0.895	0.956	0.771	0.948	0.941
5.314	0.919	0.938	0.954	0.790	0.935	0.944
5.358	1.012	0.904	0.953	0.756	0.922	0.954
5.401	1.018	0.933	0.971	0.836	0.939	0.954
5.445	1.006	0.964	0.966	0.794	0.953	0.948
5.489	1.029	0.970	0.958	0.758	0.968	0.947
5.532	1.017	1.038	0.969	0.716	0.954	0.960
5.576	1.036	1.044	0.970	0.679	0.959	0.966
5.619	1.048	1.110	0.991	0.534	0.952	0.971
5.663	1.034	1.058	0.992	0.649	0.965	0.962
5.706	1.035	1.027	0.997	0.773	0.977	0.959
5.750	1.050	1.052	1.004	0.832	0.990	0.961
5.793	1.048	1.063	0.993	0.987	0.966	0.968
5.837	1.037	1.123	1.013	0.782	0.984	0.974
5.881	1.096	1.026	1.017	0.908	1.000	0.972
5.924	1.143	1.055	1.011	1.103	1.004	0.988



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5.968	1.133	1.080	1.023	1.122	1.015	0.992
6.011	1.143	1.145	1.010	1.191	1.044	0.990
6.055	1.064	1.140	1.019	1.072	1.056	0.999
6.098	1.056	1.078	1.025	1.133	1.055	0.987
6.142	1.063	1.078	1.010	1.105	1.043	0.989
6.186	1.095	1.046	0.994	1.105	1.042	1.019
6.229	1.023	1.086	1.008	1.284	1.009	1.011
6.273	1.039	1.078	1.010	1.054	0.999	0.999
6.316	0.987	1.128	0.999	1.035	1.024	0.990
6.360	0.914	1.218	1.000	1.083	1.039	0.999
6.403	0.980	1.185	0.997	1.049	1.033	0.997
6.447	1.018	1.160	0.995	1.026	1.016	1.013
6.490	0.923	1.074	0.977	0.925	1.036	0.998
6.534	0.958	1.052	0.976	1.236	0.999	1.004
6.578	0.989	1.011	0.986	1.207	0.998	1.002
6.621	0.947	1.019	0.989	1.213	1.005	0.996
6.665	0.975	0.987	0.969	1.252	1.009	0.977
6.708	0.934	0.942	0.968	1.029	0.984	0.985
6.752	1.018	0.993	0.972	0.923	0.954	0.988
6.795	1.004	0.979	0.945	0.816	0.949	0.992
6.839	0.958	0.955	0.939	0.854	0.976	0.995
6.882	0.913	0.928	0.961	0.866	0.986	0.962
6.926	0.913	0.855	0.950	0.676	0.986	0.959
6.970	0.867	0.920	0.932	0.882	0.976	0.958