Methyl and pentyl chloride in microhydrated environment and at the liquid water-vapor interface – a theoretical study

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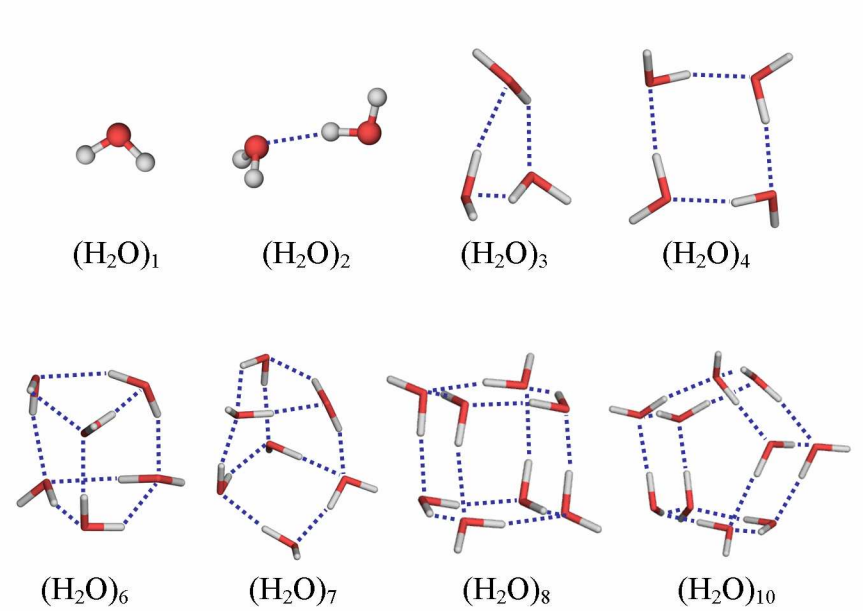

Figure S1. RI-MP2/TZVPP optimized water clusters $(H_2O)_n$, n = 1, 2, 3, 4, 6, 7, 8, 10.

Table S1. Cartesian coordinates (Å) and energies (a.u.) for the RI-MP2/TZVPP optimized water clusters $(H_2O)_n$, n = 1, 2, 3, 4, 6, 7, 8, 10.

n = 1

O	0.0000000	0.0000000	0.3942630
H	0.7544975	0.0000000	-0.1971315
H	-0.7544975	0.0000000	-0.1971315

Energy: -76.323499

n = 2

O	1.2573484	1.0538768	-0.2079741
O	-0.9508009	-0.8025949	0.1631202
H	-1.7361519	-0.2818670	0.3454823
H	-1.1293938	-1.2112950	-0.6867982
H	1.9742236	0.8509755	0.3935661
H	0.5847745	0.3909049	-0.0073965

Energy: -152.655558

n = 3

O	2.4727246	5.0660402	-1.6746035
O	0.3150329	4.4446511	-3.3244038
O	-0.0841782	4.8813630	-0.6066861
H	1.9776549	4.7859880	-2.4623477
H	3.2150428	4.4629581	-1.6159896
H	-0.0246945	3.6187172	-3.6717557
H	-0.1233728	4.5578789	-2.4640194
H	-0.4077944	5.6836210	-0.1939265
H	0.8777455	5.0034293	-0.6758848

Energy: -228.997959

n = 4

O	-1.0168725	-0.5553284	1.6575440
O	1.1036545	1.0772795	1.1253575
O	1.2121718	0.0941225	-1.4299467
O	-0.9081908	-1.5384628	-0.8977355
H	1.7682579	0.9430531	1.8025972
H	0.3324203	0.5528828	1.4235964
H	-1.8849930	-0.2098945	1.8702034
H	-1.1130665	-0.9698637	0.7763592
H	2.0803329	-0.2511312	-1.6427901
H	1.3084529	0.5087289	-0.5488145
H	-0.1369400	-1.0141376	-1.1961219
H	-1.5728359	-1.4044292	-1.5749781

Energy: -305.340052

n = 6

O	2.6371908	5.2210470	-2.0080764
O	0.2017848	4.6587605	-3.2425677
O	-0.0747422	5.2491253	-0.6619669
O	2.0133844	8.0143671	-2.3547393
O	-0.1419033	7.3986958	-4.0596885

O	-0.3211842	7.9652494	-1.0422329
H	1.9844577	4.8561257	-2.6287443
H	3.4618805	4.7742694	-2.2074072
H	-0.2556619	3.8743726	-3.5513634
H	-0.0709326	4.7851127	-2.3013834
H	-0.2503420	6.2098628	-0.6459900
H	0.8697621	5.1844326	-0.4844943
H	1.4805453	7.8895443	-3.1592460
H	2.4168088	7.1443559	-2.2178089
H	-0.1258731	6.4359459	-3.9515965
H	-0.6894852	7.6956056	-3.3249204
H	-0.4812205	8.6736114	-0.4165083
H	0.5906043	8.1071737	-1.3902982

Energy: -458.019630

n = 7

O	-0.6005305	-1.1593766	1.8672348
O	0.7869572	1.0224012	1.3040706
O	1.0467385	0.2940593	-1.3468921
O	-1.3304266	-1.2384626	-0.7088799
O	-1.2958578	2.7648453	0.3080407
O	-0.5412482	2.4636649	-2.3880723
O	-2.8658542	1.0680355	-1.0739213
H	1.4605352	1.2241632	1.9564341
H	0.2946243	0.2379111	1.6521715
H	-1.3638881	-1.1955591	2.4455954
H	-0.9539661	-1.2859954	0.9539073
H	1.9146916	-0.0129693	-1.6160966
H	1.1373276	0.5638769	-0.4123580
H	-0.5189806	-0.9052159	-1.1169018
H	-1.9775903	-0.5320567	-0.8798330
H	-0.8955768	2.9361437	-0.5622071
H	-0.5995911	2.2943130	0.7885393
H	0.0839280	1.7428372	-2.2240659
H	-1.3902231	2.0113597	-2.4521329
H	-3.8090720	1.2166976	-0.9902409
H	-2.4357239	1.6809921	-0.4351666

Energy: -534.361688

n = 8

O	-0.8905822	-0.6019064	1.6252036
O	1.1349304	0.9859672	1.1505757
O	1.3247688	0.1920926	-1.4635049
O	-0.8934046	-1.6021769	-0.9416734
O	-2.9807917	1.2330083	0.9282907
O	-0.7626064	3.0272764	0.4064774
O	-0.7654647	2.0269974	-2.1603916
O	-2.7909603	0.4391104	-1.6857889
H	1.7836642	0.9553203	1.8564610
H	0.4027407	0.3640943	1.4238919
H	-1.6891780	-0.0545804	1.5931885
H	-0.9249231	-1.1018387	0.7832444
H	2.2085058	0.0516147	-1.8082465
H	1.4410624	0.4742165	-0.5332885
H	-0.0951676	-1.1646409	-1.2702887
H	-1.6155367	-1.0833359	-1.3254689
H	-0.0404930	2.5084308	0.7902672
H	-1.5608598	2.5897497	0.7350985

H	−3.8645280	1.3734691	1.2730493
H	−3.0970914	0.9508804	−0.0019316
H	0.0331436	1.4796783	−2.1283815
H	−0.7311018	2.5269379	−1.3184618
H	−2.0587818	1.0609970	−1.9591082
H	−3.4396852	0.4697664	−2.3916730

Energy: −610.709811

n = 10

O	3.6292062	4.8421041	−2.0093372
O	3.6059720	6.5988750	−0.0344378
O	1.0105187	3.8372409	−2.4616555
O	−0.6029791	5.3298479	−0.8542119
O	0.8824450	7.0566482	0.4469488
O	3.4393936	6.7372114	−4.0863749
O	3.2926060	8.6294971	−2.0161053
O	0.9872866	5.9007538	−4.4993925
O	−0.7761553	7.3345263	−2.9661218
O	0.7686536	9.1576967	−1.4208779
H	3.7166822	5.3995132	−2.8007122
H	2.7772617	4.3925626	−2.1291237
H	4.3108248	6.4164453	0.5895971
H	3.6478392	5.8759335	−0.7124313
H	0.3883422	4.2640731	−1.8351881
H	0.7698011	2.9090623	−2.4784159
H	−1.2885993	5.0179232	−0.2602350
H	−0.0356276	5.9412406	−0.3085065
H	1.8362796	6.8683705	0.4167418
H	0.7892420	7.8887010	−0.0468649
H	3.9034061	6.8227352	−4.9212580
H	2.5076110	6.4712460	−4.3179420
H	3.5721746	8.0513339	−1.2895164
H	3.3947232	8.0760104	−2.8096520
H	0.3281908	6.4731372	−4.0522917
H	0.9339388	5.0720385	−4.0034590
H	−0.9463339	6.6896921	−2.2658561
H	−0.3278867	8.0614944	−2.5053499
H	1.7123389	9.0419416	−1.7030769
H	0.6408075	10.1019732	−1.3137078

Energy: −763.397114

Table S2. Cartesian coordinates (Å) and energies (a.u.) for the RI-MP2/TZVPP optimized microhydrated methyl chloride complexes.

1wM1

Cl	-0.7057276	0.1186107	1.7910388
C	0.0014710	0.0070340	0.1589033
O	1.3698882	0.0257036	-2.6506084
H	0.1423886	1.0065787	-0.2300894
H	-0.6772420	-0.5481400	-0.4755943
H	0.9515084	-0.5063470	0.2265970
H	1.0772161	-0.2903074	-3.5075408
H	2.3023733	0.2088462	-2.7804571

Energy: -575.838884

1wM2

Cl	0.9197389	-1.4951171	1.1005505
C	-0.0153633	-0.1045706	0.4832871
O	-0.2274336	0.0917747	3.7529021
H	-0.3013200	0.5070635	1.3300980
H	-0.8884368	-0.4884165	-0.0295202
H	0.6172463	0.4468967	-0.2010507
H	0.2641454	-0.6178864	3.3277256
H	0.2689300	0.2753622	4.5521939

Energy: -575.841970

2wM

Cl	1.7256312	-0.5296132	0.0361806
C	0.0098557	-0.0226248	-0.0419398
O	-0.8722350	-0.9326910	-3.1236758
O	1.9521133	-0.9501904	-3.2296901
H	-0.0175595	1.0588558	0.0057471
H	-0.4949658	-0.4541127	0.8133732
H	-0.4132606	-0.3842713	-0.9720778
H	0.0745426	-0.9731049	-3.3285363
H	-1.2404010	-1.7121039	-3.5417975
H	2.4419532	-0.2148294	-3.6031263
H	2.0785305	-0.8650472	-2.2761093

Energy: -652.178358

3wM

Cl	-0.5035264	8.2649270	-0.8629234
C	0.5193716	8.0001251	-2.3054514
O	2.4701320	5.2407213	-1.7901038
O	0.2532539	4.6989812	-3.3723464
O	-0.1185328	4.9644836	-0.6720013
H	1.9523059	4.9444294	-2.5570424
H	3.2722613	4.7162785	-1.8036683
H	-0.1304064	3.9398087	-3.8140240
H	-0.1299682	4.6997593	-2.4737251
H	-0.4290278	5.8449744	-0.4334194
H	0.8465286	5.0531127	-0.6835968
H	1.4684458	7.5925193	-1.9804234
H	0.6525282	8.9571602	-2.7942271

H	0.0150984	7.2982763	−2.9579080

Energy: −728.518981

4wM1

Cl	3.1624006	−1.4922853	1.2237049
C	1.6057476	−2.3556685	1.3923089
O	−1.0289819	−0.2265225	1.5467430
O	1.1893759	1.3085219	0.9137723
O	1.3255742	0.0393047	−1.5092492
O	−0.8414768	−1.4460846	−0.8976250
H	1.9018121	0.9193638	1.4284404
H	0.3847708	0.8691438	1.2474983
H	−1.8908051	0.1347218	1.7600860
H	−1.1383818	−0.6790319	0.6865685
H	2.1759450	−0.4058345	−1.5155353
H	1.3472662	0.5837041	−0.6930731
H	−0.0688166	−0.9447610	−1.2409624
H	−1.4660890	−1.4786407	−1.6238860
H	1.1542945	−2.4472725	0.4126340
H	0.9613946	−1.7803625	2.0450523
H	1.8139518	−3.3308034	1.8147650

Energy: −804.861298

4wM2

Cl	−2.1430863	0.2526918	−2.2838312
C	−0.4725002	0.6959352	−1.8124005
O	−0.0050594	−0.9007562	1.6188783
O	0.4554117	1.7362261	1.2888292
O	2.2091110	−0.0126098	0.0188772
O	−2.0316203	−2.0464975	0.0352371
H	0.4671036	2.2617591	2.0901283
H	0.1133455	0.8567012	1.5566920
H	−0.7102050	−1.3463003	1.1215541
H	0.7954832	−1.0327213	1.0940118
H	3.1591697	0.0303062	0.1372783
H	1.8617235	0.7922926	0.4379065
H	−2.2568323	−1.4339721	−0.6771135
H	−2.8747178	−2.3099466	0.4088256
H	0.0922005	−0.2125987	−1.6487763
H	−0.5174946	1.2868147	−0.9065730
H	−0.0454187	1.2667478	−2.6272894

Energy: −804.854755

6wM

Cl	1.6344443	4.3602026	−3.9085202
C	1.4125484	6.0358242	−4.5121904
O	2.8705015	5.6953276	−1.0229678
O	−1.2073619	4.7789483	−2.0681207
O	0.2742707	5.9641254	−0.0106543
O	2.7374671	8.1628537	−2.1649292
O	−1.5712680	7.1953223	−3.2684694
O	0.0865459	8.2483995	−1.2793072
H	2.7619865	5.0507142	−1.7293848
H	2.0202440	5.6728456	−0.5491868
H	−0.5376564	4.3095057	−2.5754253
H	−0.7424501	5.0518722	−1.2574049

H	0.1703285	6.8764475	-0.4019331
H	0.0217917	6.0362235	0.9120175
H	3.4459687	8.7522759	-1.9012856
H	2.9231900	7.3102343	-1.7181297
H	-1.5797952	6.2981385	-2.8734018
H	-2.4906634	7.4182651	-3.4230742
H	-0.4995477	8.0634354	-2.0335893
H	0.9716842	8.3937631	-1.6560952
H	1.6813267	6.0368589	-5.5611279
H	2.0611617	6.6900416	-3.9428541
H	0.3740407	6.3109169	-4.3753158

Energy: -957.545320

8wM1

Cl	-2.8854284	-1.0786802	-4.8533934
C	-1.5718569	0.0379041	-5.3308545
O	-1.0990931	0.1340231	2.0379214
O	0.8717611	1.7007677	1.3404699
O	1.8228456	-0.0914751	-0.4901223
O	-0.3480051	-1.8722976	0.3068724
O	-3.0203032	1.1133131	0.1559533
O	-0.8647243	2.8695184	-0.6383810
O	-0.0639906	0.9098643	-2.3770634
O	-2.0726349	-0.6798086	-1.6560952
H	1.2991007	2.0901549	2.1059271
H	0.1324473	1.1312857	1.6994253
H	-1.8899032	0.4651254	1.5861564
H	-0.8773960	-0.6818656	1.5424743
H	2.7731795	-0.2177149	-0.5157907
H	1.6587055	0.5726359	0.2109002
H	0.4794737	-1.4866113	-0.0126897
H	-0.9715304	-1.7128806	-0.4175720
H	-0.2508159	2.7010716	0.0917974
H	-1.6969451	2.4792034	-0.3332911
H	-3.9720984	1.2225493	0.1991387
H	-2.8574665	0.4367777	-0.5356718
H	0.7211573	0.5739522	-1.9176209
H	-0.3040483	1.7119571	-1.8645610
H	-1.3247219	-0.1158958	-1.9802829
H	-2.4971116	-0.9999211	-2.4607449
H	-0.9180182	-0.4943480	-6.0105024
H	-1.0358803	0.3483582	-4.4416787
H	-2.0246746	0.8882038	-5.8252659

Energy: -1110.230646

8wM2

Cl	-1.7691323	-0.9613701	-2.8775129
C	-0.3631243	0.1514939	-2.9683956
O	-1.0507049	-0.4117859	2.1349444
O	1.0600294	1.0508748	1.6602899
O	1.8032224	-0.6399228	-0.3954599
O	-0.5082435	-2.1566921	0.0600305
O	-3.0152995	1.4667521	1.3821673
O	-0.7449328	3.0838847	0.7626390
O	-1.4650111	3.1675047	-1.8192612
O	-3.5071923	1.4357245	-1.2420127
H	1.5559223	1.2012929	2.4679302
H	0.2750604	0.4909633	1.9264583

H	-1.8310756	0.1238736	1.9194376
H	-1.0057870	-1.1008741	1.4442687
H	2.7075059	-0.9515046	-0.3305191
H	1.6982399	0.0049349	0.3307431
H	0.3580486	-1.7689438	-0.1526758
H	-1.0083281	-2.0728024	-0.7575841
H	-0.0159831	2.5056848	1.0375728
H	-1.5311434	2.6636957	1.1442298
H	-3.8267640	1.6435575	1.8617261
H	-3.2756651	1.3962209	0.4320018
H	-1.5436145	4.0811922	-2.0983978
H	-1.1043000	3.2029673	-0.9024554
H	-2.8750313	2.1117895	-1.5574283
H	-3.2642398	0.6408752	-1.7281046
H	-0.7149847	1.1574625	-2.7740384
H	0.0460973	0.0669683	-3.9674849
H	0.3614871	-0.1572140	-2.2247697

Energy: -1110.225772

10wM1

Cl	1.6730274	1.3257160	0.0511560
C	3.4041467	1.7691371	-0.0030563
O	3.4007605	5.1563698	-1.0178868
O	3.1462278	7.4035109	0.3793310
O	0.9001368	4.1070196	-1.5627424
O	-0.9778034	5.9173594	-0.7592959
O	0.3736992	7.9333592	0.2664724
O	3.6629290	6.4062171	-3.5207223
O	3.2203736	8.7975765	-2.1144200
O	1.2869753	5.4518409	-4.0830439
O	-0.6681732	7.2251061	-3.3441023
O	0.6460566	9.4242751	-2.1062576
H	3.6859041	5.4829271	-1.8887403
H	2.5058559	4.8024945	-1.1860821
H	3.7284166	7.4170756	1.1411841
H	3.2775958	6.5214669	-0.0511070
H	0.1630756	4.6373076	-1.1968353
H	0.8311202	3.2297885	-1.1694849
H	-1.7703305	5.7703488	-0.2394465
H	-0.4863921	6.6499882	-0.3007991
H	1.3107726	7.7496702	0.4460502
H	0.3959937	8.5913550	-0.4485016
H	4.2515275	6.2855987	-4.2681830
H	2.7724628	6.0676656	-3.8166211
H	3.3600741	8.4479776	-1.2209927
H	3.4337738	8.0475497	-2.6961137
H	0.5798836	6.1149386	-3.9318972
H	1.1140525	4.7852659	-3.4035682
H	-0.9912435	6.7986908	-2.5381988
H	-0.2829482	8.0565102	-3.0251004
H	1.6189642	9.2527715	-2.1867024
H	0.5278698	10.3580069	-2.2898571
H	3.4871088	2.8199082	-0.2539724
H	3.8816953	1.1540601	-0.7556506
H	3.8261204	1.5705580	0.9742945

Energy: -1262.917378

10wM2

Cl	2.5569600	3.6954965	-0.9106293
C	2.1521356	5.4351260	-0.7461787
O	5.0358901	5.2318568	-2.6108085
O	5.1058228	7.1543110	-0.7029549
O	-0.1760472	3.9484301	-2.8305826
O	-1.7180425	5.8393105	-1.3437735
O	-0.3225448	7.3596624	0.4254422
O	3.3721404	6.6999076	-4.2766276
O	3.2671475	8.5958827	-2.1968353
O	0.8964253	5.9461478	-4.4728642
O	-0.7947028	7.7839518	-3.3031486
O	0.8516627	9.0788819	-1.3368977
H	4.4596691	5.6474273	-3.2798440
H	4.5379566	4.4682149	-2.3028130
H	5.9989412	7.4232963	-0.4819262
H	5.2053889	6.4230867	-1.3506402
H	-0.7157231	4.4943347	-2.2374411
H	0.4776766	3.5368746	-2.2568527
H	-2.6162091	5.6371747	-1.0744404
H	-1.3231886	6.3432717	-0.6032026
H	-0.5537420	7.7774542	1.2562515
H	0.1263334	8.0497768	-0.1047208
H	3.6674265	6.8899735	-5.1697372
H	2.4299994	6.3759443	-4.3744010
H	3.9415539	8.2097715	-1.6081838
H	3.3065332	8.0436883	-2.9966567
H	0.2948736	6.6510655	-4.1600650
H	0.5775530	5.1529231	-4.0059907
H	-1.2991137	7.1887921	-2.7317094
H	-0.2755490	8.3172631	-2.6820381
H	1.7858901	8.8838385	-1.6309193
H	0.8030725	10.0360101	-1.2879684
H	1.8832754	5.8081096	-1.7275852
H	3.0270842	5.9442727	-0.3622778
H	1.3186902	5.5228438	-0.0616142

Energy: -1262.908099

Table S3. Cartesian coordinates (Å) and energies (a.u.) for the RI-MP2/TZVPP optimized microhydrated pentyl chloride complexes.

1wP1

Cl	0.5734937	-1.7137182	0.5247254
C	0.0079569	-0.0592015	0.1054880
C	1.1314350	0.9445747	0.2228483
C	0.6489182	2.3460890	-0.1335015
C	1.7537622	3.3883688	-0.0185175
C	1.2659764	4.7890327	-0.3632752
O	-2.6355971	-1.8101393	-0.1978477
H	-0.8115436	0.1635270	0.7823493
H	-0.3831295	-0.1177604	-0.9059841
H	1.5212910	0.9328737	1.2416815
H	1.9483409	0.6521092	-0.4383868
H	-0.1796690	2.6256528	0.5224875
H	0.2540655	2.3494037	-1.1528554
H	2.1517536	3.3756764	0.9981769
H	2.5779119	3.1102663	-0.6785692
H	2.0646058	5.5235217	-0.2755298
H	0.4581546	5.0912446	0.3026299
H	0.8866479	4.8265931	-1.3840568
H	-1.7885522	-2.1901370	0.0561491
H	-3.2445616	-2.5495703	-0.1625738

Energy: -732.736198

1wP2

Cl	-0.4751070	-0.5714133	1.3925568
C	-0.3341035	0.7297182	0.1584013
C	0.8726546	1.6021140	0.4172903
C	0.9517337	2.7293658	-0.6054859
C	2.1555112	3.6346183	-0.3786541
C	2.2284818	4.7649636	-1.3963401
O	-1.5680607	2.2598377	2.6453324
H	-1.2546397	1.3028792	0.2162593
H	-0.2740449	0.2280387	-0.8034405
H	0.7975111	2.0223638	1.4198949
H	1.7771125	0.9932337	0.3769058
H	0.0380574	3.3269763	-0.5542932
H	1.0006880	2.3117439	-1.6151158
H	2.1035774	4.0477115	0.6305053
H	3.0677429	3.0361328	-0.4244377
H	3.0920438	5.4047595	-1.2229662
H	1.3351800	5.3869452	-1.3468378
H	2.3024036	4.3696682	-2.4092012
H	-1.3674872	1.3188295	2.6883793
H	-2.1065838	2.4219407	3.4219812

Energy: -732.737693

2wP1

Cl	1.7968178	-0.0076094	-0.0081336
C	-0.0114542	-0.0016674	0.0058694
C	-0.5487199	1.4096864	0.0096180
C	-2.0724599	1.3938410	0.0513219
C	-2.6644740	2.7971033	0.0535769

C	-4.1860684	2.7808498	0.1098040
O	0.7027071	0.6054841	3.0481869
O	0.6965180	0.6098631	-3.0577237
H	-0.2980907	-0.5448414	0.9011171
H	-0.3128331	-0.5468022	-0.8833925
H	-0.1627717	1.9380494	0.8812253
H	-0.2080159	1.9259664	-0.8878283
H	-2.4066938	0.8616986	0.9458047
H	-2.4568046	0.8429346	-0.8111825
H	-2.2686342	3.3487943	0.9085354
H	-2.3320384	3.3255579	-0.8420732
H	-4.5981318	3.7885470	0.1104886
H	-4.5332131	2.2763155	1.0111556
H	-4.5989417	2.2504900	-0.7479210
H	1.4101920	0.5041363	2.4036137
H	1.1505749	0.5778628	3.8956594
H	1.3970680	0.5042966	-2.4062616
H	1.1519361	0.5737419	-3.9008231

Energy: -809.067946

2wP2

Cl	0.8537046	-2.2163523	-0.3119672
C	0.4979250	-0.5661494	-0.9465864
C	0.9345017	0.5021265	0.0271382
C	0.6504146	1.8866656	-0.5429270
C	0.9592857	2.9931767	0.4564875
C	0.6832338	4.3781913	-0.1129319
O	-1.9147892	-2.0243961	1.4108046
O	-2.3247904	0.5967260	0.4326666
H	-0.5730876	-0.5235228	-1.1201470
H	1.0262999	-0.4958677	-1.8933482
H	0.3862586	0.3774533	0.9605539
H	1.9979770	0.3893850	0.2433587
H	-0.4025681	1.9420423	-0.8239633
H	1.2418684	2.0415937	-1.4497601
H	0.3550736	2.8345392	1.3518016
H	2.0041421	2.9218869	0.7667669
H	0.8942763	5.1605160	0.6143400
H	-0.3606767	4.4695635	-0.4116841
H	1.2978700	4.5647778	-0.9932968
H	-1.0489236	-2.2318609	1.0347192
H	-2.4832037	-2.7307647	1.0966982
H	-2.2958078	-0.2828166	0.8414793
H	-2.8924265	1.1089084	1.0103551

Energy: -809.074807

3wP

Cl	-1.5255714	8.4154946	-1.0642749
C	-0.0948479	9.1952037	-1.8304034
C	-0.1229617	9.0339736	-3.3329168
C	1.1309345	9.6273977	-3.9640848
C	1.1599473	9.4352968	-5.4742365
C	2.4319431	9.9916594	-6.0995451
O	2.7148888	7.1417129	-1.4487292
O	1.8593909	6.2022247	-3.9066786
O	0.2983355	5.7001264	-1.7090392
H	2.7409031	6.8560063	-2.3779136
H	3.6045756	7.0159597	-1.1147645

H	2.0855867	5.4446876	-4.4493268
H	1.1489988	5.8907888	-3.3131182
H	-0.4544380	6.2581711	-1.4820655
H	1.0431166	6.1094841	-1.2441594
H	0.7846812	8.7272301	-1.3973914
H	-0.1303436	10.2401682	-1.5346679
H	-0.1823458	7.9747479	-3.5814311
H	-1.0155518	9.5156130	-3.7353358
H	2.0107786	9.1508766	-3.5265019
H	1.1953306	10.6940733	-3.7306128
H	1.0777610	8.3690232	-5.6892913
H	0.2867537	9.9196440	-5.9168831
H	2.4430620	9.8514089	-7.1792893
H	3.3098045	9.4942557	-5.6877456
H	2.5298243	11.0586747	-5.8996732

Energy: -885.416084

4wP

Cl	0.0766413	-2.2792610	4.0998280
C	0.7041925	-2.8218878	2.5022646
C	1.9249280	-3.6980806	2.6568359
C	2.4176526	-4.1642075	1.2907927
C	3.6746707	-5.0185406	1.3852935
C	4.1437835	-5.5049476	0.0205365
O	-1.4127223	-2.5379087	-0.0553570
O	-1.8465767	-0.6109769	1.9069167
O	0.3081112	0.7468232	0.9643490
O	0.9600942	-1.2952568	-0.6853434
H	-1.6317456	-1.0510066	2.7363470
H	-1.8451014	-1.3287178	1.2466444
H	-1.9959593	-2.6651974	-0.8055290
H	-0.5866636	-2.1705232	-0.4271924
H	0.8242996	1.1013885	1.6900837
H	-0.4945821	0.3611492	1.3804409
H	0.8412781	-0.4894994	-0.1387074
H	1.2507465	-0.9775002	-1.5419410
H	0.9293869	-1.9209142	1.9404164
H	-0.1102998	-3.3468234	2.0123473
H	2.7107282	-3.1401770	3.1687426
H	1.6797904	-4.5585025	3.2812818
H	2.6089538	-3.2958739	0.6560967
H	1.6273956	-4.7365064	0.7976771
H	4.4670782	-4.4386867	1.8632604
H	3.4807695	-5.8743465	2.0354470
H	5.0467984	-6.1082079	0.0977311
H	4.3575091	-4.6623838	-0.6366405
H	3.3750131	-6.1115478	-0.4574802

Energy: -961.756920

6wP

Cl	2.3832969	5.4943911	-3.6680344
C	1.7802121	4.2408822	-2.5092365
C	1.1257799	3.0919578	-3.2366960
C	0.6669735	2.0385136	-2.2350999
C	-0.0921874	0.9022849	-2.9064238
C	-0.5406010	-0.1581633	-1.9100013
O	4.5210940	2.9851934	-3.4309836
O	-0.9368903	6.1728206	-4.3660904

O	-1.7289591	4.5544288	-2.2608944
O	1.0203613	7.7582127	-1.3809490
O	-0.5318396	8.6916230	-3.4099712
O	-0.6031896	5.9481150	-0.2340049
H	5.3955231	2.7903509	-3.7732944
H	4.2814389	3.8162635	-3.8520876
H	-0.0377379	5.8832597	-4.5469905
H	-1.2469696	5.5757102	-3.6579026
H	-1.3922219	5.0016577	-1.4572020
H	-2.6735061	4.4643882	-2.1207525
H	0.4617941	8.2065771	-2.0500739
H	1.7357309	7.3806020	-1.9006400
H	-0.7848265	7.8307517	-3.8044019
H	-1.3426158	9.1981087	-3.3491361
H	-0.2570044	5.7063803	0.6258067
H	0.0146312	6.6266258	-0.5910489
H	1.0852227	4.7545591	-1.8517370
H	2.6552157	3.9161225	-1.9542886
H	0.2649032	3.4546588	-3.7983487
H	1.8373472	2.6548386	-3.9369164
H	0.0196807	2.5073008	-1.4908010
H	1.5358296	1.6350599	-1.7085203
H	-0.9604906	1.3165259	-3.4224879
H	0.5417456	0.4479003	-3.6707383
H	-1.0862346	-0.9634101	-2.3991923
H	-1.1921594	0.2767060	-1.1523274
H	0.3166579	-0.5962535	-1.3993170

Energy: -1114.427848

7wP

Cl	-0.2885874	5.0138153	0.5526121
C	1.4362029	4.7685521	0.1014566
C	1.7413441	3.3290456	-0.2415826
C	3.2166440	3.1835439	-0.6057549
C	3.5940912	1.7474740	-0.9447361
C	5.0640234	1.6110347	-1.3175711
O	-1.3765848	0.0985995	1.9549186
O	1.3851335	0.4152152	1.7970505
O	1.1699543	-0.9687038	-0.6955470
O	-1.4737554	-1.3898426	-0.1923910
O	-2.0888545	2.2483527	0.3339420
O	0.5339358	0.8958239	-2.7485391
O	-2.1252230	0.8420269	-1.9179838
H	1.8633511	0.0007532	2.5177028
H	0.4439752	0.3044079	2.0235140
H	-1.9261651	-0.2446494	2.6621584
H	-1.4792774	-0.5367108	1.1890193
H	1.4093533	-0.4651484	0.0981366
H	1.1176857	-0.3113744	-1.4078760
H	-0.5165555	-1.3829931	-0.4179905
H	-1.8650902	-0.8260851	-0.8750087
H	-1.4821134	2.9918540	0.4287448
H	-1.8499597	1.6178253	1.0358689
H	0.6312373	0.6152076	-3.6604416
H	-0.4279677	0.9151333	-2.5926216
H	-2.9111806	1.0727894	-2.4169432
H	-2.1351054	1.4326072	-1.1244419
H	2.0160929	5.1083557	0.9552794
H	1.6188253	5.4306559	-0.7405198
H	1.5087374	2.6868022	0.6085664

H	1.1229078	3.0064641	-1.0803413
H	3.8345765	3.5317494	0.2272398
H	3.4494636	3.8283605	-1.4583820
H	3.3668792	1.1103889	-0.0891458
H	2.9662474	1.4019376	-1.7664322
H	5.3193747	0.5799212	-1.5563266
H	5.7058431	1.9333735	-0.4974457
H	5.3031981	2.2249791	-2.1860202

Energy: -1190.779438

8wP

Cl	4.5273989	-1.5396629	-0.6313431
C	4.6818328	0.1788334	-1.1507801
C	4.4954331	1.1239550	0.0137830
C	4.6233855	2.5750853	-0.4357174
C	4.4672840	3.5516482	0.7226435
C	4.4898466	5.0003151	0.2566451
O	-1.6504783	1.1010154	1.0317788
O	0.9056442	1.0570155	1.5874644
O	1.3473095	-0.8138955	-0.4005381
O	-1.4854226	-0.7947511	-0.9599201
O	-1.5763816	3.2185437	-0.9150263
O	1.2414311	3.1966502	-0.2838439
O	1.4580730	1.2776144	-2.2552539
O	-1.0982518	1.3624238	-2.8732926
H	1.0640563	0.9927355	2.5317675
H	-0.0872963	1.0759130	1.4775255
H	-1.8062708	1.8930165	0.4968953
H	-1.7263360	0.3694623	0.3842389
H	2.1740869	-1.3094072	-0.3490284
H	1.3071283	-0.2807021	0.4166066
H	-0.5659389	-1.0760121	-0.8529037
H	-1.4641147	-0.2218889	-1.7397452
H	1.2171369	2.6071240	0.4865050
H	0.3116804	3.4318793	-0.4226028
H	-2.2012619	3.9165595	-1.1202556
H	-1.5309453	2.6548742	-1.7139434
H	1.4830064	0.4921405	-1.6784777
H	1.4986550	2.0196296	-1.6167187
H	-0.1084783	1.3323083	-2.7643971
H	-1.2608574	1.3867340	-3.8183858
H	3.9331087	0.3401934	-1.9211431
H	5.6736113	0.2671086	-1.5854472
H	3.5103947	0.9661542	0.4554285
H	5.2362604	0.9007445	0.7834981
H	3.8632572	2.7902813	-1.1892232
H	5.5971076	2.7296077	-0.9091537
H	3.5230712	3.3511264	1.2306437
H	5.2641976	3.3782495	1.4494625
H	4.3954767	5.6906028	1.0933936
H	3.6643471	5.1864461	-0.4287001
H	5.4214046	5.2279448	-0.2617132

Energy: -1267.129594

10wP1

Cl	1.6740729	8.3277200	-7.6658793
C	0.5899995	9.3257580	-6.6290923
C	1.3734457	10.0700474	-5.5720200

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C    0.4463901   10.8947764   -4.6859929
C    1.2024910   11.6081521   -3.5724235
C    0.2693316   12.3661724   -2.6380273
O    1.8065500    4.3031962   -3.3057764
O    3.5104121    5.0020574   -1.4071637
O   -0.8340913    5.0538500   -2.5102479
O   -0.5396920    6.4991365   -0.2163185
O    2.0185556    6.5901803    0.3469743
O    2.1547073    6.6218108   -4.8540237
O    3.8780230    7.4508328   -2.8252572
O   -0.2525231    7.4180228   -4.0417225
O   -0.0900378    8.9158809   -1.7623516
O    2.6402101    8.9582494   -1.0570919
H    1.9590731    4.9542915   -4.0112751
H    0.8830321    4.4452906   -3.0453831
H    4.1057970    4.2774851   -1.2067681
H    2.8780922    4.6543810   -2.0879956
H   -0.8109694    5.4837221   -1.6292930
H   -1.5845397    4.4568745   -2.4922543
H   -1.0224078    6.3859803    0.6050317
H    0.4243195    6.4773033    0.0377697
H    2.5660749    5.9592869   -0.1524623
H    2.3176513    7.4607853    0.0365333
H    2.2444640    6.8709881   -5.7815742
H    1.2650209    6.9652581   -4.5887166
H    3.9733284    6.6012310   -2.3672000
H    3.3514317    7.2321041   -3.6160526
H   -0.1998655    8.0199624   -3.2676707
H   -0.6454038    6.6127852   -3.6740016
H   -0.3943300    8.2539484   -1.1244897
H    0.8389059    9.0632469   -1.5161843
H    3.1356378    8.4698528   -1.7678324
H    3.1844897    9.7144989   -0.8287063
H   -0.1241496    8.6420513   -6.1802199
H    0.0773187   10.0046031   -7.3050650
H    1.9199220    9.3522604   -4.9590940
H    2.1121964   10.7152926   -6.0502204
H   -0.3100019   10.2444275   -4.2421558
H   -0.0848992   11.6331805   -5.2930959
H    1.7699447   10.8685832   -3.0039448
H    1.9319741   12.2922241   -4.0122387
H    0.8215440   12.8848922   -1.8553592
H   -0.4273371   11.6774856   -2.1626196
H   -0.3073021   13.1106537   -3.1870941

Energy: -1419.817642
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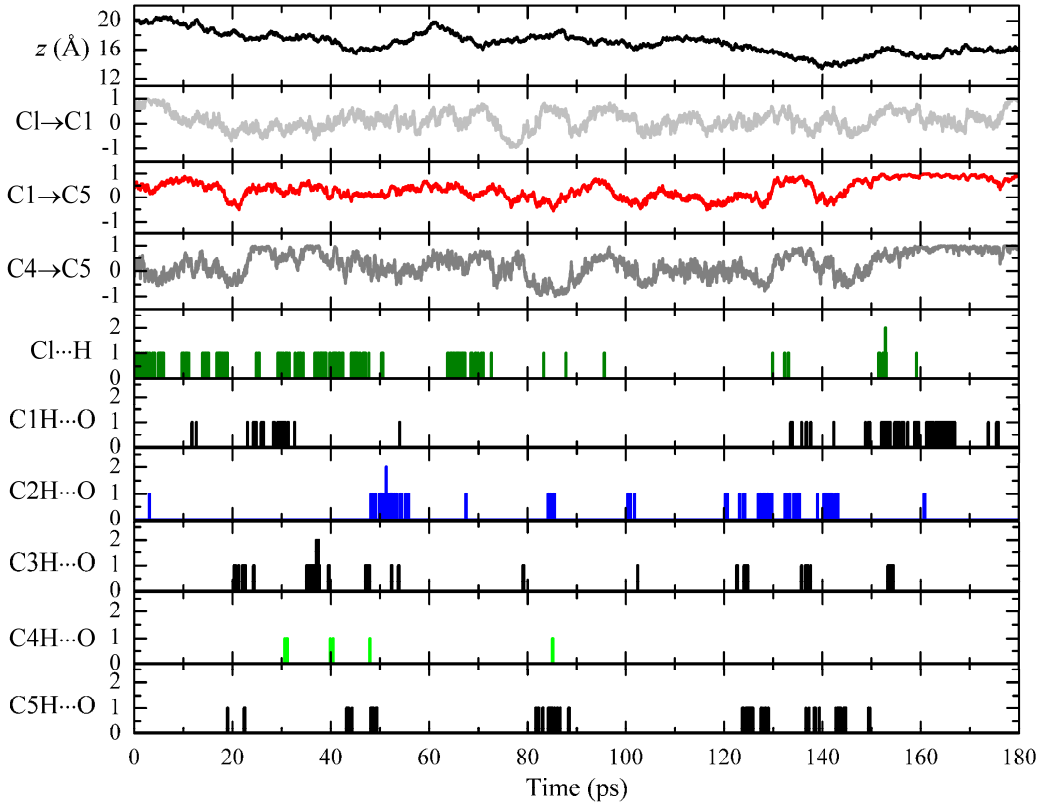

Figure S2. Evolution of the distance of the midpoint on the hydrocarbon chain along the *z*-axis, molecular orientations (cos θ of the Cl→C1, C1→C5, and C4→C5 vectors with the interface normal) and number of hydrogen bonds with simulation time for the pentyl chloride molecule at the liquid water-vapor interface.