CHEMPHYSCHEM

Supporting Information

Spectroscopic Evidence for Clusters of Like-Charged Ions in Ionic Liquids Stabilized by Cooperative Hydrogen Bonding

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Spectroscopic evidence for clusters of like-charged ions in ionic liquids stabilized by cooperative hydrogen bonding*

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Supplementary Information

Contents

SI0 Sample preparation

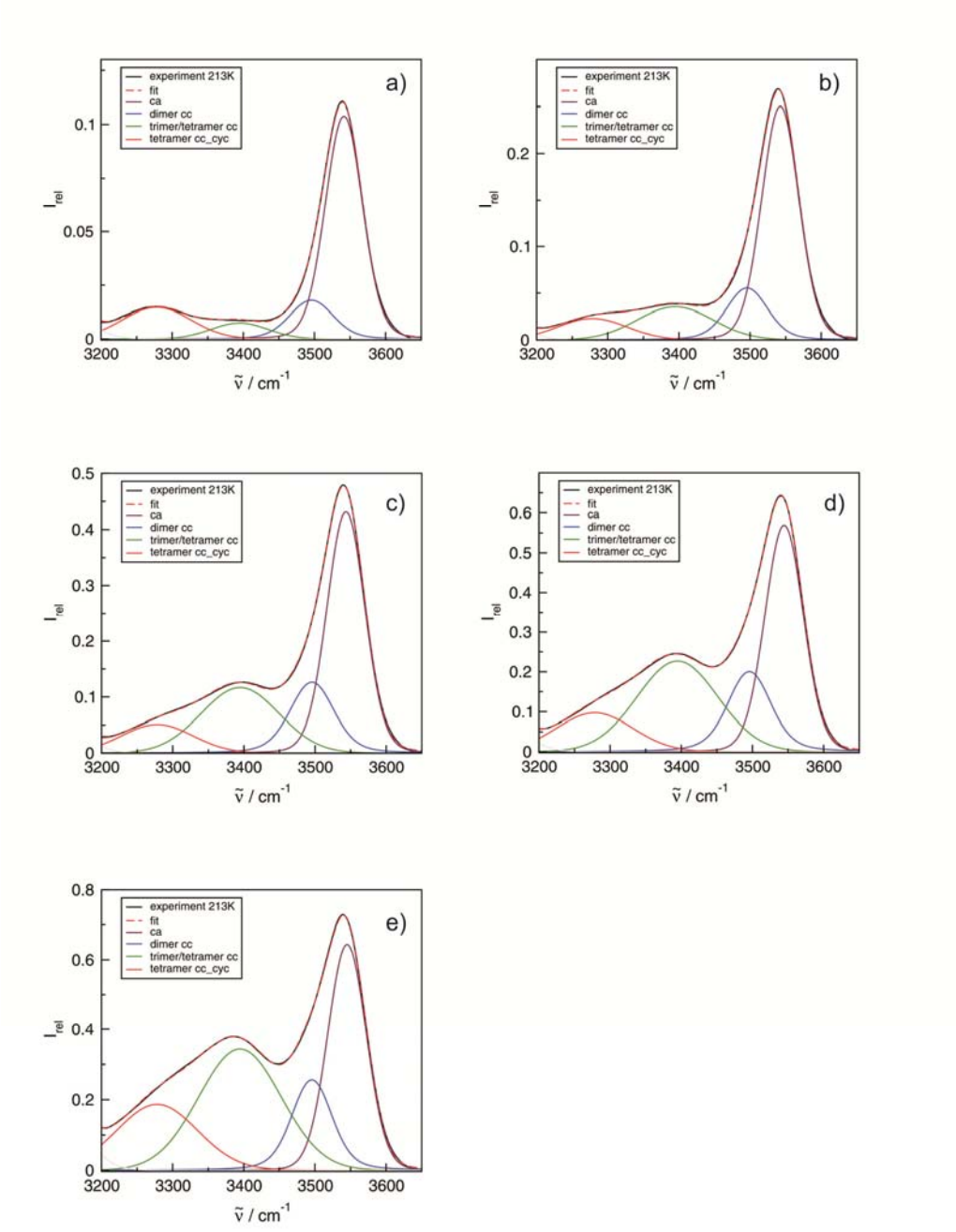
The sample of [HEMim][BF_4] and [PMIm][BF_4]were purchased from Iolitec (>99% mass fraction). The ionic liquids were dried under vacuum for around 48 hours in order to reduce the water content under 100 ppm and remove other volatile impurities as well. The water content was checked using a Karl Fischer titrator (Titroline KF Trace, Schott Instruments GmbH) resulting in 64 ppm and 85 ppm.

SI1 Experimental

Mid infrared (MIR) measurements were performed with a Bruker Vector 22 FTIR spectrometer. An L.O.T.-Oriel variable-temperature cell equipped with CaF_2 windows having a path length of 12 μm was used for the variable-temperature experiments between 213 and 353 K. Cooling of the cell is achieved by means of a cooling dewar with liquid ethanol/nitrogen mixture. For each spectrum 128 scans were recorded at a spectral resolution of 1 cm^{-1}.

The spectra were deconvoluted separately into a number of Voigt-profiles (convolution of Lorentzian and Gaussian functions) following the Levenberg-Marquardt procedure. The Voigt-profile has four parameters: the intensity, the frequency, the half-width of the Lorentzian, and the half-width of the Gaussian.

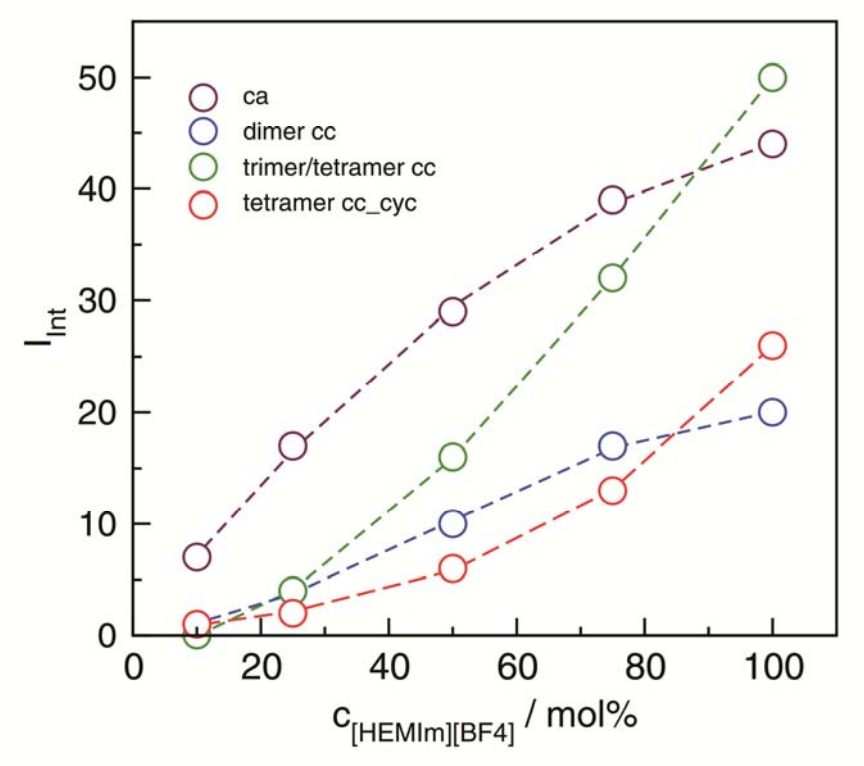
SI2 Deconvoluted mid infrared (MIR) spectra of [HEMIm][BF_4] in 10, 25, 50, 75 and 100 mol% mixtures with [PMIm][BF_4] at 213 K.



SI-FIG1 Deconvoluted mid infrared (MIR) spectra of [HEMIm][BF_4] in a) 10, b) 25, c) 50, d) 75 and e) 100 mol% mixtures with [PMIm][BF_4] at 213 K.

All spectra were deconvoluted separately into a number of Voigt profiles (convolution of Lorentzian and Gassian functions) following the Levenberg-Marquardt procedure. The Voigt profile has four parameters: the intensity, the frequency, the half-width of the Lorentzian, and the half-width of the Gaussian.

SI3 Intensities of the deconvoluted mid infrared (MIR) spectra of [HEMIm][BF_4] in 10, 25, 50, 75 and 100 mol% mixtures with [PMIm][BF_4] at 213 K.



SI-FIG2 Intensities of the deconvoluted mid infrared (MIR) spectra of [HEMIm][BF_4] in 10, 25, 50, 75 and 100 mol% mixtures with [PMIm][BF_4] at 213 K.

SI4 DFT-D3 optimized geometries of [HEMIm][BF_4] clusters ca and cc

The IL clusters have been calculated at the DFT level B3LYP, using the internal stored 6-31+G* basis set of the Gaussian 09 program.[24] Grimme's DFT-D3 method was applied for calculating dispersion forces.[SI1-3]

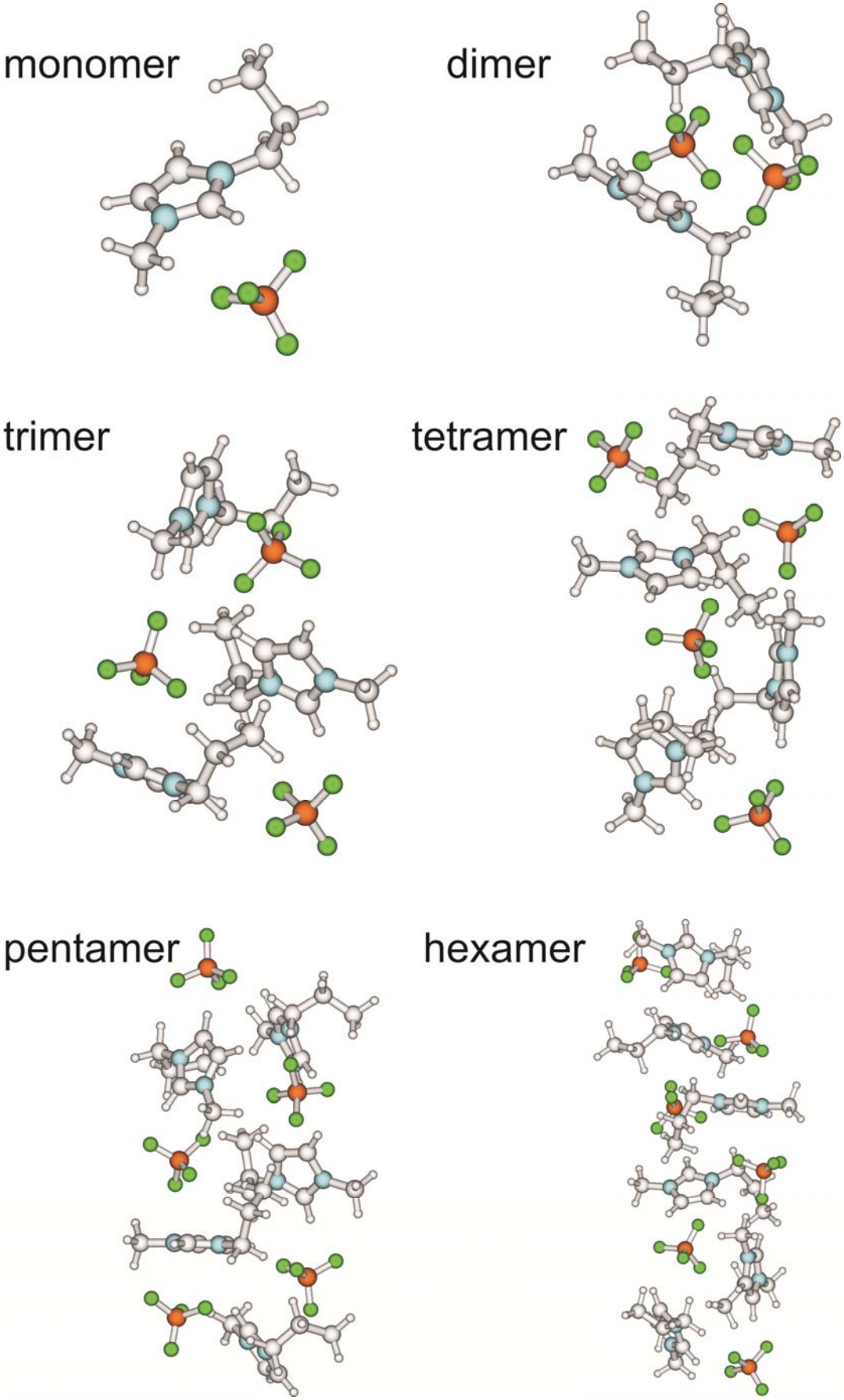
Literature

[SI1] Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

[SI2] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, 132, 154104.

[SI3] S. Ehrlich, J. Moellmann, W. Reckien, T. Bredow, S. Grimme**,** ChemPhysChem. **2011**, 12, 3414-3420.

[PMIm][BF_4]



Monomer

*** imCH3_BF4_b3lyp_6-31+Gp_D3.g09, E(RB3LYP) = -808.592825032, 9.11.2015

7	0	0.118402	1.788019	0.322548
6	0	0.412238	0.491213	0.449592
7	0	1.331459	0.165168	-0.464738
6	0	1.632197	1.293125	-1.206486
6	0	0.866757	2.310614	-0.715946
6	0	1.838245	-1.204812	-0.685360
6	0	2.681809	-1.705304	0.490237
6	0	3.928380	-0.855584	0.756445
6	0	-0.990318	2.463559	1.005189
9	0	-2.223529	-0.378719	1.277736
5	0	-2.300249	-0.827511	-0.082704
9	0	-1.226814	-1.752822	-0.278321
9	0	-2.059342	0.301493	-0.916965
9	0	-3.522328	-1.407948	-0.350650
1	0	-0.649859	3.436699	1.366178
1	0	-1.816757	2.564257	0.298958
1	0	-1.325269	1.836631	1.830182
1	0	0.962538	-1.836455	-0.853437
1	0	2.431698	-1.166391	-1.603519
1	0	-0.083258	-0.191182	1.122063
1	0	2.351163	1.270105	-2.010254
1	0	0.781123	3.343105	-1.016677
1	0	2.967239	-2.739712	0.261455
1	0	2.051499	-1.754457	1.387561
1	0	4.508059	-1.262681	1.591753
1	0	4.583842	-0.827539	-0.123685
1	0	3.662459	0.177965	1.010042

Dimer

*** imCH3_BF4_b3lyp_6-31+Gp_dimer_D3.g09, E(RB3LYP) = -1617.23646365, 9.11.2015

7	0	-0.731982	2.432604	1.569132
6	0	-1.060902	2.381093	0.274228
7	0	-1.859717	1.328394	0.073400
6	0	-2.051625	0.677864	1.280316
6	0	-1.343046	1.370675	2.217586
6	0	-2.410112	0.929013	-1.239507
6	0	-3.788987	1.540505	-1.508347
6	0	-4.869858	1.094035	-0.517032
6	0	0.263326	3.333193	2.151765
6	0	2.513319	-0.119699	2.959883
6	0	1.389938	-1.108844	2.635949
6	0	1.821467	-2.296470	1.770216
7	0	2.254414	-1.885317	0.421439
6	0	3.535156	-1.516689	0.045570
6	0	3.477915	-1.143548	-1.263849
7	0	2.164584	-1.292973	-1.665567
6	0	1.440575	-1.729468	-0.629860
6	0	1.636692	-1.007638	-3.002379
9	0	1.636240	3.340612	-0.678090
5	0	1.765482	1.984848	-1.051451
9	0	0.686674	1.646421	-1.919231
9	0	1.659116	1.179184	0.117651
9	0	2.981486	1.739390	-1.697032
9	0	-1.487387	-2.220506	-1.250721
5	0	-2.078595	-2.656652	-0.016658

9	0	-2.294089	-4.020981	-0.035425
9	0	-1.159983	-2.303495	1.022619
9	0	-3.275958	-1.930339	0.181751
1	0	0.987509	-2.987564	1.641066
1	0	2.663601	-2.834154	2.218345
1	0	1.863713	0.028233	-3.253937
1	0	2.087015	-1.696855	-3.721743
1	0	0.555538	-1.147549	-2.980498
1	0	0.376530	-1.925327	-0.648347
1	0	4.230995	-0.743878	-1.923093
1	0	4.357980	-1.534370	0.742125
1	0	-0.165124	3.835271	3.022784
1	0	1.142602	2.749941	2.434124
1	0	0.564819	4.058621	1.397379
1	0	-1.672979	1.242067	-1.982199
1	0	-2.453630	-0.160177	-1.238819
1	0	-0.676799	3.035505	-0.490898
1	0	-2.631197	-0.230395	1.340178
1	0	-1.203295	1.192473	3.272164
1	0	0.975544	-1.534279	3.559823
1	0	0.566532	-0.601187	2.124736
1	0	-4.068914	1.234408	-2.524836
1	0	-3.708008	2.636657	-1.522838
1	0	-5.850450	1.482915	-0.813718
1	0	-4.928524	0.001055	-0.468752
1	0	-4.663021	1.462540	0.495085
1	0	2.156472	0.653232	3.651832
1	0	3.362800	-0.620614	3.443926
1	0	2.866715	0.386775	2.056872

Trimer

*** imCH3_BF4_b3lyp_6-31+Gp_trimer_D3.g09, E(RB3LYP) = -2425.85790823, 9.11.2015

6	0	5.630807	-2.200121	-1.999415
6	0	4.418557	-1.346974	-2.382991
6	0	4.678192	0.164777	-2.361402
7	0	4.908756	0.704187	-1.010885
6	0	6.088611	0.654961	-0.287510
6	0	5.825844	1.188394	0.939188
7	0	4.495608	1.559839	0.943937
6	0	3.959380	1.243777	-0.236036
6	0	3.767518	2.144635	2.076334
9	0	4.120523	-1.638868	0.685149
5	0	3.471820	-1.385292	1.920689
9	0	2.899717	-2.569164	2.415429
9	0	4.394511	-0.841254	2.834603
9	0	2.436910	-0.433362	1.680498
6	0	0.274557	-1.116730	-0.221033
7	0	-0.806269	-1.287652	-1.074381
6	0	-1.373065	-2.473294	-0.818360
7	0	-0.683737	-3.068515	0.162652
6	0	0.358356	-2.239477	0.547830
6	0	-1.302076	-0.326742	-2.075548
6	0	-0.477651	-0.324932	-3.368448
6	0	0.972371	0.141546	-3.189195
6	0	-1.017813	-4.362185	0.761857
9	0	-0.535813	2.872915	-1.520488
5	0	-0.149834	2.724735	-0.162884
9	0	1.212373	2.329725	-0.120338
9	0	-0.335943	3.932839	0.526571
9	0	-0.941137	1.714501	0.427288

6	0	-2.401813	-0.701108	2.043957
6	0	-2.975557	0.437666	2.887818
6	0	-4.249161	1.050309	2.294441
7	0	-4.000956	1.782466	1.031758
6	0	-4.226743	1.304200	-0.246232
6	0	-3.851450	2.293674	-1.108191
7	0	-3.402013	3.356989	-0.346797
6	0	-3.487822	3.015506	0.942425
6	0	-2.932509	4.643118	-0.867213
9	0	-5.376154	-1.461152	0.588804
5	0	-4.924903	-2.405746	-0.371421
9	0	-4.220880	-1.673744	-1.392757
9	0	-5.981713	-3.103587	-0.926192
9	0	-3.993674	-3.285499	0.242584
1	0	-4.706407	1.764501	2.986767
1	0	-4.979736	0.274647	2.057340
1	0	-2.220375	4.451195	-1.669238
1	0	-3.787203	5.223499	-1.225808
1	0	-2.409438	5.173239	-0.072334
1	0	-3.159532	3.624177	1.769884
1	0	-3.851611	2.329933	-2.185908
1	0	-4.611655	0.309970	-0.417681
1	0	-0.375876	-5.143128	0.345015
1	0	-0.858819	-4.296584	1.839855
1	0	-2.068890	-4.576212	0.564720
1	0	-2.341046	-0.600664	-2.270101
1	0	-1.285848	0.655833	-1.605644
1	0	-2.284149	-2.839757	-1.262729
1	0	0.838168	-0.200656	-0.176610
1	0	1.051861	-2.500619	1.333782
1	0	-3.243416	0.071927	3.888103
1	0	-2.221699	1.223897	3.025193
1	0	-0.994510	0.351301	-4.061829
1	0	-0.506276	-1.324503	-3.822819
1	0	3.822402	0.709030	-2.770337
1	0	5.556460	0.422732	-2.963237
1	0	3.779885	1.425686	2.895649
1	0	4.252347	3.082289	2.360587
1	0	2.740156	2.328645	1.764151
1	0	2.926968	1.407993	-0.503866
1	0	6.447743	1.300441	1.812710
1	0	6.990075	0.230335	-0.698385
1	0	4.093692	-1.586912	-3.404684
1	0	3.586856	-1.573899	-1.708451
1	0	5.885151	-2.064238	-0.944905
1	0	6.504649	-1.958924	-2.620782
1	0	5.405696	-3.262851	-2.139200
1	0	1.543864	-0.565017	-2.577689
1	0	1.474667	0.217367	-4.161184
1	0	1.002378	1.124498	-2.704850
1	0	-1.494001	-1.096057	2.510967
1	0	-3.124696	-1.513079	1.920211
1	0	-2.122617	-0.335847	1.053410

Tetramer

*** imOH_BF4_b3lyp_6-31+Gp_tetramer_D3.g09, E(RB3LYP) = -3234.49318694, 9.11.2015

7	0	-5.932373	2.683775	-0.638086
6	0	-6.235432	1.603181	0.090480
7	0	-5.348829	1.496179	1.086624
6	0	-4.441383	2.537943	0.992300

6	0	-4.812573	3.286499	-0.085595
6	0	-5.341464	0.401775	2.079804
6	0	-5.945333	0.813857	3.426508
6	0	-5.156089	1.901074	4.165369
6	0	-6.633878	3.105544	-1.852842
6	0	-3.711208	0.525424	-2.050323
6	0	-2.462908	-0.284580	-2.403407
6	0	-2.623147	-1.795817	-2.187179
7	0	-2.674998	-2.165503	-0.759269
6	0	-3.814404	-2.330708	0.008697
6	0	-3.392876	-2.613086	1.275405
7	0	-2.009455	-2.616163	1.260938
6	0	-1.599514	-2.332674	0.021972
6	0	-1.135984	-2.842674	2.417752
9	0	-5.892899	-1.904880	-2.349023
5	0	-7.048416	-1.334545	-1.763385
9	0	-6.835820	-1.287034	-0.338718
9	0	-8.184005	-2.063365	-2.055255
9	0	-7.178034	0.014722	-2.209440
9	0	-2.338536	0.422607	0.814641
5	0	-1.561592	0.665895	1.976091
9	0	-1.395428	2.066199	2.117741
9	0	-2.245547	0.149521	3.100060
9	0	-0.314420	0.036448	1.836164
6	0	1.505124	0.703186	-0.469435
7	0	2.526828	0.932077	-1.380112
6	0	2.821224	2.237695	-1.377044
7	0	2.013695	2.852807	-0.504228
6	0	1.176232	1.910564	0.072127
6	0	3.240960	-0.075917	-2.187006
6	0	2.459306	-0.526820	-3.426078
6	0	1.159245	-1.277566	-3.114874
6	0	2.061903	4.277920	-0.172334
9	0	3.239642	-3.155907	-0.995343
5	0	2.763443	-2.833483	0.300580
9	0	1.348763	-2.745141	0.253364
9	0	3.171224	-3.809314	1.223237
9	0	3.287951	-1.575943	0.679014
6	0	4.186932	1.350738	1.741590
6	0	4.958608	0.528254	2.773756
6	0	6.349160	0.101545	2.289504
7	0	6.295543	-0.885738	1.187880
6	0	6.453274	-0.614719	-0.159368
6	0	6.316681	-1.802742	-0.817539
7	0	6.075084	-2.777125	0.133407
6	0	6.051369	-2.193633	1.335433
6	0	5.906958	-4.209188	-0.126925
9	0	6.894199	2.455459	0.096976
5	0	6.283960	3.059651	-1.034096
9	0	5.771234	1.999598	-1.862882
9	0	7.186961	3.828061	-1.744326
9	0	5.174428	3.838276	-0.603766
1	0	6.926979	-0.359505	3.096944
1	0	6.907224	0.957243	1.904167
1	0	5.285167	-4.327148	-1.013415
1	0	6.887534	-4.672286	-0.268259
1	0	5.378542	-4.657610	0.713599
1	0	5.831242	-2.694339	2.264862
1	0	6.355167	-2.036315	-1.869568
1	0	6.623140	0.389950	-0.516872
1	0	1.278438	4.815087	-0.714412
1	0	1.906012	4.389080	0.902508
1	0	3.048081	4.662425	-0.434131
1	0	4.192449	0.381855	-2.465294

1	0	3.443830	-0.919026	-1.528607
1	0	3.635376	2.695979	-1.914965
1	0	1.160326	-0.287240	-0.225340
1	0	0.452589	2.165784	0.830955
1	0	5.113577	1.114862	3.689126
1	0	4.381561	-0.361800	3.055879
1	0	3.133734	-1.185403	-3.988787
1	0	2.259405	0.341052	-4.069226
1	0	-1.779046	-2.340616	-2.620832
1	0	-3.547921	-2.159867	-2.639781
1	0	-1.307600	-2.047050	3.143888
1	0	-1.364499	-3.821821	2.846805
1	0	-0.100879	-2.813004	2.080002
1	0	-0.566522	-2.265392	-0.281417
1	0	-3.949313	-2.803133	2.179440
1	0	-4.803428	-2.223422	-0.410458
1	0	-7.242084	3.989844	-1.643426
1	0	-5.894376	3.336502	-2.622908
1	0	-7.256688	2.279909	-2.197655
1	0	-5.903344	-0.416580	1.625204
1	0	-4.302422	0.093542	2.192384
1	0	-7.010315	0.888229	-0.137260
1	0	-3.589468	2.617112	1.649754
1	0	-4.368845	4.168301	-0.520528
1	0	-2.207524	-0.145193	-3.462545
1	0	-1.609544	0.072688	-1.814171
1	0	-5.973452	-0.097622	4.038150
1	0	-6.989329	1.123122	3.280309
1	0	-5.569495	2.062635	5.167255
1	0	-4.102719	1.616247	4.267994
1	0	-5.199424	2.861094	3.637674
1	0	-3.945463	0.414882	-0.989768
1	0	-4.580615	0.202177	-2.629201
1	0	-3.531749	1.590788	-2.237800
1	0	0.425500	-0.620943	-2.636223
1	0	0.704296	-1.657946	-4.037001
1	0	1.353036	-2.125471	-2.448434
1	0	3.201267	1.618860	2.134977
1	0	4.728301	2.261537	1.469118
1	0	4.025726	0.763989	0.834777

Pentamer

*** imCH3_BF4_b3lyp_6-31+Gp_pentamer_D3.g09, E(RB3LYP) = -4043.13951749, 9.11.2015

6	0	-3.405671	2.495486	1.185223
7	0	-3.455498	1.164525	1.079323
6	0	-3.292135	0.822026	-0.251960
6	0	-3.146511	1.986967	-0.942643
7	0	-3.217366	3.015840	-0.027391
6	0	-3.635565	0.227120	2.199350
6	0	-2.314797	-0.090910	2.907973
6	0	-1.268720	-0.707203	1.976560
6	0	-3.169283	4.439984	-0.346362
9	0	-5.827625	4.022460	1.580019
5	0	-6.567652	2.959725	1.034811
9	0	-6.121260	2.728576	-0.306974
9	0	-7.934162	3.193059	1.050289
9	0	-6.275706	1.763440	1.783550
9	0	-0.375837	2.388869	0.667385
5	0	0.363687	2.783527	-0.471521
9	0	1.031421	3.995454	-0.199657

9	0	-0.490769	2.941435	-1.580005
9	0	1.320731	1.771287	-0.759232
6	0	-6.949158	-0.093837	-0.473813
7	0	-7.172426	-0.097645	-1.789974
6	0	-8.277417	-0.884782	-2.050350
6	0	-8.729543	-1.345475	-0.849020
7	0	-7.888360	-0.834148	0.122704
6	0	-6.320943	0.568634	-2.777516
6	0	-7.965834	-1.071087	1.577110
6	0	-7.047649	-2.213093	2.027635
6	0	-7.360975	-3.560349	1.370078
9	0	-5.863460	-2.747685	-1.718707
5	0	-4.517702	-2.598178	-1.389341
9	0	-3.809924	-3.808442	-1.537638
9	0	-4.386959	-2.136152	-0.052917
9	0	-3.914588	-1.617962	-2.247634
6	0	-1.038542	-2.506969	-1.495434
7	0	-0.362340	-1.353812	-1.573462
6	0	0.696382	-1.393255	-0.676772
6	0	0.645092	-2.609146	-0.058571
7	0	-0.446780	-3.283629	-0.579058
6	0	-0.717112	-0.242141	-2.476863
6	0	0.102365	-0.238466	-3.772723
6	0	1.603503	-0.010559	-3.564254
6	0	-0.918584	-4.605520	-0.156080
9	0	1.581297	-2.096246	3.228306
5	0	2.818126	-2.151760	2.576606
9	0	3.868820	-1.865603	3.466135
9	0	2.835072	-1.192304	1.518991
9	0	3.006630	-3.431069	1.985931
6	0	3.251390	2.724823	1.415096
7	0	4.501586	2.752219	0.940768
6	0	5.243181	1.770104	1.579475
6	0	4.401669	1.149503	2.459096
7	0	3.164123	1.759686	2.336698
6	0	4.948731	3.594229	-0.188611
6	0	4.342696	3.120883	-1.516297
6	0	4.684912	1.664453	-1.844787
6	0	1.943803	1.416182	3.074169
6	0	4.691917	-2.378350	-0.604194
7	0	5.893544	-1.913119	-0.098621
6	0	6.607315	-1.381980	-1.096614
7	0	5.901651	-1.485983	-2.229381
6	0	4.697256	-2.110847	-1.942258
6	0	6.332714	-0.984206	-3.536234
6	0	6.346915	-1.992884	1.307143
6	0	7.104764	-3.291383	1.604645
6	0	6.272594	-4.561483	1.396863
9	0	8.128165	1.048411	-1.785982
5	0	8.583025	1.540429	-0.517100
9	0	9.963021	1.561590	-0.474316
9	0	8.019333	2.807647	-0.286948
9	0	8.067689	0.636064	0.480920
1	0	-5.523784	-0.115156	-3.078306
1	0	-6.935777	0.846939	-3.635592
1	0	-5.908621	1.467117	-2.316423
1	0	-7.703333	-0.127412	2.061760
1	0	-9.013937	-1.295073	1.798491
1	0	-6.178506	0.461606	0.031989
1	0	-9.560486	-1.986055	-0.600636
1	0	-8.630125	-1.055878	-3.054941
1	0	-7.146123	-2.283436	3.119170
1	0	-6.009428	-1.939122	1.812834
1	0	-6.718580	-4.345744	1.782635

1	0	-8.404701	-3.857173	1.542888
1	0	-7.177431	-3.524507	0.291474
1	0	-4.374917	0.672404	2.868869
1	0	-4.065531	-0.679005	1.767994
1	0	-2.253357	4.640112	-0.906125
1	0	-4.058516	4.702045	-0.924165
1	0	-3.174380	5.007489	0.584070
1	0	-3.571283	3.060858	2.086817
1	0	-2.968814	2.176259	-1.987696
1	0	-3.321923	-0.202958	-0.578617
1	0	-0.254231	-5.378702	-0.551046
1	0	-0.916290	-4.643474	0.935336
1	0	-1.934258	-4.747138	-0.527386
1	0	-1.782680	-0.355137	-2.691453
1	0	-0.568582	0.683327	-1.922671
1	0	-1.934958	-2.754158	-2.042216
1	0	1.342945	-0.544478	-0.518193
1	0	1.257895	-3.034120	0.719998
1	0	-2.550629	-0.779762	3.729930
1	0	-1.917945	0.824183	3.368054
1	0	-0.307261	0.570575	-4.391094
1	0	-0.076695	-1.174871	-4.319061
1	0	4.652552	4.624087	0.032082
1	0	6.037382	3.534845	-0.206966
1	0	1.872970	0.332532	3.153740
1	0	1.977651	1.865476	4.070741
1	0	1.085259	1.793267	2.515032
1	0	2.441881	3.352682	1.072912
1	0	4.546642	0.306808	3.116851
1	0	6.281880	1.596085	1.333573
1	0	6.637395	-1.819949	-4.172240
1	0	5.502402	-0.446676	-3.998527
1	0	7.164854	-0.295765	-3.384277
1	0	6.981358	-1.120512	1.473848
1	0	5.456628	-1.909846	1.929314
1	0	7.557191	-0.882450	-0.994028
1	0	3.950138	-2.821227	0.041143
1	0	3.955710	-2.289973	-2.704280
1	0	4.739109	3.785051	-2.295198
1	0	3.256225	3.257575	-1.492256
1	0	7.425345	-3.223806	2.652027
1	0	8.020470	-3.323613	0.998693
1	0	6.835934	-5.446478	1.713229
1	0	5.340410	-4.520094	1.971176
1	0	6.009396	-4.700923	0.340947
1	0	4.243314	0.980574	-1.110106
1	0	5.768783	1.509859	-1.861647
1	0	4.275650	1.393905	-2.825115
1	0	2.060261	-0.837344	-3.008127
1	0	2.117980	0.067843	-4.529185
1	0	1.783475	0.905852	-2.994546
1	0	-0.388259	-1.044697	2.529033
1	0	-1.686966	-1.574020	1.447778
1	0	-0.934686	0.020846	1.231122

Hexamer

*** imCH3_BF4_b3lyp_6-31+Gp_hexamer_D3.g09, E(RB3LYP) = -4851.76568712, 9.11.2015

7	0	5.574445	0.438808	-2.388828
6	0	5.457110	0.328387	-1.063250
7	0	6.177404	1.295693	-0.486599

6	0	6.785528	2.049061	-1.477958
6	0	6.394221	1.517207	-2.670359
6	0	6.266568	1.512095	0.967742
6	0	5.401911	2.682340	1.455213
6	0	5.845594	4.054599	0.935023
6	0	4.898308	-0.418893	-3.360978
6	0	8.336864	-1.377043	-1.530653
6	0	9.768561	-1.814001	-1.220275
6	0	9.925591	-2.455142	0.163910
7	0	9.749248	-1.492501	1.273284
6	0	8.605693	-1.314333	2.030952
6	0	8.877609	-0.319765	2.925224
7	0	10.176293	0.096102	2.698592
6	0	10.673882	-0.616142	1.684356
6	0	10.890321	1.131080	3.451634
9	0	6.812712	-3.442012	0.571953
5	0	5.468441	-3.017210	0.594066
9	0	5.394589	-1.781723	1.320213
9	0	4.653509	-3.969728	1.215510
9	0	5.016279	-2.772791	-0.724776
9	0	9.331326	1.208615	-0.020569
5	0	9.851775	2.457925	0.427176
9	0	9.587157	3.441174	-0.529518
9	0	9.194066	2.788664	1.648731
9	0	11.232818	2.306550	0.666559
1	0	10.923209	-2.889949	0.283236
1	0	9.185011	-3.242403	0.320687
1	0	10.230277	1.990152	3.564646
1	0	11.194480	0.729332	4.422164
1	0	11.753985	1.450408	2.869940
1	0	11.644277	-0.465967	1.238760
1	0	8.262679	0.136682	3.684385
1	0	7.712671	-1.893289	1.852173
1	0	4.030189	0.107885	-3.763457
1	0	5.599166	-0.667011	-4.161395
1	0	4.591206	-1.333747	-2.851743
1	0	5.957337	0.571766	1.430484
1	0	7.316420	1.685465	1.200985
1	0	4.935992	-0.460846	-0.549014
1	0	7.478280	2.843383	-1.247006
1	0	6.610276	1.816325	-3.683161
1	0	10.104872	-2.563873	-1.949128
1	0	10.448204	-0.956596	-1.300468
1	0	5.463699	2.666211	2.552354
1	0	4.353265	2.505150	1.188599
1	0	5.287129	4.851846	1.438676
1	0	6.915214	4.216836	1.111791
1	0	5.652285	4.153435	-0.138299
1	0	8.009319	-0.622242	-0.813849
1	0	7.641590	-2.220866	-1.489945
1	0	8.288163	-0.921129	-2.525339
7	0	-9.685881	2.924498	-0.397064
6	0	-9.918656	2.025978	0.566641
7	0	-8.868760	2.005671	1.395493
6	0	-7.926454	2.916062	0.947426
6	0	-8.442785	3.496948	-0.173183
6	0	-8.750073	1.111050	2.565756
6	0	-9.068175	1.813972	3.889676
6	0	-8.093883	2.940020	4.255666
6	0	-10.569765	3.191182	-1.533892
6	0	-7.942414	0.362074	-1.771030
6	0	-6.897976	-0.652233	-2.240503
6	0	-7.118746	-2.066693	-1.687966
7	0	-6.867846	-2.159162	-0.236735

6	0	-7.812167	-2.064415	0.770882
6	0	-7.133552	-2.163405	1.950783
7	0	-5.792643	-2.316203	1.646299
6	0	-5.656574	-2.300157	0.317908
6	0	-4.697144	-2.452638	2.613099
9	0	-10.318914	-1.904371	-1.143370
5	0	-11.283426	-1.088757	-0.504980
9	0	-10.802779	-0.804899	0.823145
9	0	-12.518582	-1.702843	-0.449334
9	0	-11.364720	0.159314	-1.193715
9	0	-6.000262	0.631562	0.778741
5	0	-5.037270	0.982667	1.757548
9	0	-4.777757	2.374568	1.654565
9	0	-5.556247	0.688510	3.038737
9	0	-3.859813	0.252571	1.535577
6	0	-2.305601	0.483447	-0.984605
7	0	-1.381130	0.498964	-2.018271
6	0	-0.944965	1.752700	-2.189831
7	0	-1.566691	2.542042	-1.303984
6	0	-2.428200	1.767859	-0.542654
6	0	-0.905207	-0.658494	-2.798523
6	0	-1.880474	-1.093184	-3.897698
6	0	-3.218821	-1.631108	-3.377381
6	0	-1.314903	3.972829	-1.123155
9	0	-0.923870	-3.547178	-1.230847
5	0	-1.363576	-3.039837	0.018044
9	0	-2.762945	-2.772888	-0.074169
9	0	-1.106096	-3.956882	1.038213
9	0	-0.703518	-1.816832	0.278444
6	0	0.493321	1.214928	1.092775
6	0	1.483762	0.561105	2.058657
6	0	2.705927	-0.038140	1.356934
7	0	2.371702	-1.168338	0.474639
6	0	2.147308	-1.107310	-0.890539
6	0	1.887519	-2.380413	-1.300590
7	0	1.947788	-3.193070	-0.187568
6	0	2.240290	-2.438283	0.871362
6	0	1.806583	-4.649581	-0.171969
9	0	2.988696	2.001087	-1.208843
5	0	2.567384	2.336715	-2.521938
9	0	1.941749	1.170014	-3.087458
9	0	3.657113	2.699649	-3.306784
9	0	1.601057	3.362101	-2.461350
1	0	3.447459	-0.407812	2.069493
1	0	3.181283	0.710340	0.722373
1	0	1.136920	-4.932469	-0.983304
1	0	2.794734	-5.102443	-0.278658
1	0	1.344351	-4.946417	0.769713
1	0	2.394518	-2.803850	1.872687
1	0	1.638500	-2.776297	-2.271146
1	0	2.177880	-0.176069	-1.432337
1	0	-2.179696	4.547431	-1.465847
1	0	-1.142740	4.166662	-0.062026
1	0	-0.422985	4.246389	-1.687721
1	0	0.056454	-0.358704	-3.221860
1	0	-0.733744	-1.468222	-2.090966
1	0	-0.181359	2.063166	-2.885022
1	0	-2.731192	-0.430842	-0.605804
1	0	-3.024411	2.177389	0.258109
1	0	1.864744	1.302522	2.774264
1	0	0.980476	-0.218828	2.644555
1	0	-1.367609	-1.881712	-4.463844
1	0	-2.043395	-0.260309	-4.595524
1	0	-6.443301	-2.780595	-2.169379

1	0	-8.148051	-2.392867	-1.849767
1	0	-4.668439	-1.557884	3.235772
1	0	-4.868717	-3.346566	3.218561
1	0	-3.760830	-2.546071	2.064163
1	0	-4.716881	-2.399942	-0.203206
1	0	-7.480742	-2.128398	2.971143
1	0	-8.861401	-1.934376	0.552466
1	0	-11.030979	4.176352	-1.422754
1	0	-9.980640	3.156597	-2.453195
1	0	-11.329329	2.410273	-1.574012
1	0	-9.438300	0.284179	2.379817
1	0	-7.729860	0.728135	2.561564
1	0	-10.769645	1.365539	0.620523
1	0	-6.962308	3.021175	1.420274
1	0	-8.029749	4.237307	-0.840177
1	0	-6.918047	-0.737658	-3.335445
1	0	-5.892836	-0.311396	-1.962558
1	0	-9.034316	1.034655	4.662341
1	0	-10.101394	2.186729	3.868184
1	0	-8.302672	3.317004	5.263170
1	0	-7.057625	2.583736	4.228436
1	0	-8.180392	3.788547	3.566699
1	0	-7.892775	0.483147	-0.686692
1	0	-8.955763	0.050048	-2.038963
1	0	-7.741593	1.342703	-2.219288
1	0	-3.807179	-0.845175	-2.891242
1	0	-3.820948	-2.025140	-4.204364
1	0	-3.057507	-2.434880	-2.650598
1	0	-0.337732	1.668443	1.643397
1	0	0.986509	1.986611	0.490170
1	0	0.064200	0.466484	0.422697

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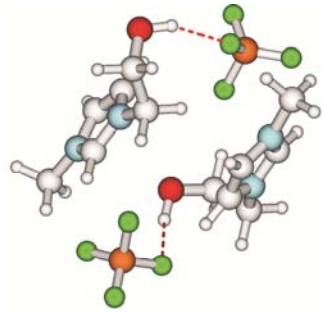

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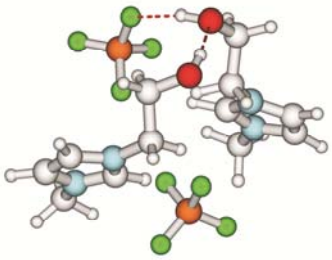

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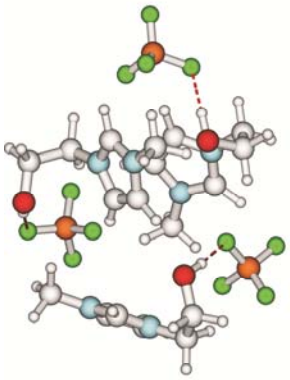

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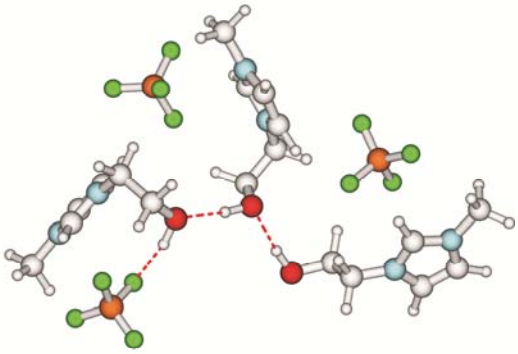
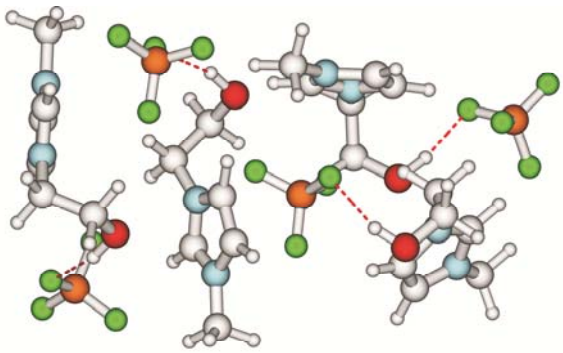
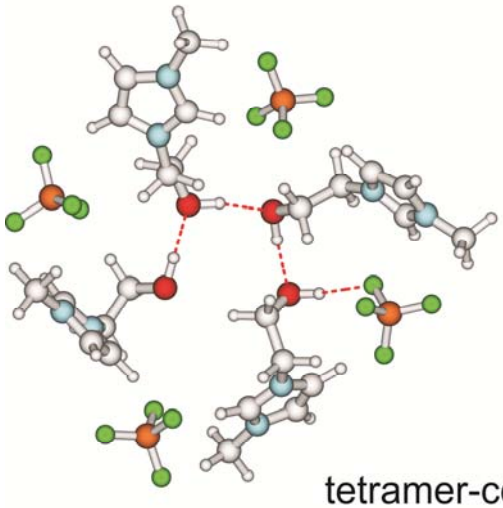


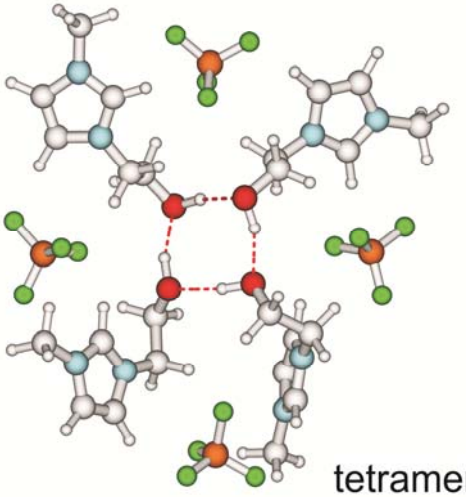
trimer-cc



tetramer-ca



tetramer-cc



tetramer-cc-cyc

dimer ca

*** imOH_BF4_b3lyp_6-31+Gp_dimer_D3.g09, -1689.04027659

7	0	-0.537230	2.319948	-0.849060
6	0	0.079166	2.495557	0.378231
6	0	-0.912544	2.535375	1.313038
7	0	-2.116215	2.375168	0.644149
6	0	-1.861669	2.239428	-0.660930
6	0	-3.445624	2.364704	1.264570
6	0	0.153948	2.190193	-2.143103
6	0	0.471964	0.736349	-2.516030
9	0	-3.396662	-0.575774	0.785971
5	0	-3.434495	-0.673529	-0.651724
9	0	-4.179467	0.420674	-1.145587
9	0	-2.091476	-0.547555	-1.110951
9	0	-3.962621	-1.893346	-1.025618
9	0	3.063705	1.887146	-0.557436
5	0	3.664061	1.276807	0.610635
9	0	4.605071	2.117429	1.155981
9	0	4.213600	0.036264	0.207973
9	0	2.601133	1.015687	1.527377
6	0	1.839458	-1.829425	0.462156
7	0	0.510647	-1.835911	0.598695
6	0	-0.031927	-2.712530	-0.323312
6	0	1.013750	-3.251248	-1.013232
7	0	2.173859	-2.687739	-0.505817
6	0	-0.233465	-0.942558	1.494133
6	0	-0.991614	-1.707895	2.581816
6	0	3.531223	-2.903695	-1.006543
1	0	-0.481997	2.643849	-2.909662
1	0	1.072707	2.777098	-2.063693
1	0	-3.462103	1.608232	2.049623
1	0	-3.658887	3.356107	1.672803
1	0	-4.180338	2.085988	0.510694
1	0	-2.604360	2.033660	-1.415881
1	0	-0.867805	2.654890	2.384243
1	0	1.152987	2.533363	0.473610
1	0	3.855583	-3.922107	-0.775778
1	0	3.538433	-2.745477	-2.087637
1	0	4.194778	-2.176246	-0.538432
1	0	0.492315	-0.249400	1.926880
1	0	-0.930319	-0.381831	0.871286
1	0	2.522700	-1.182102	0.989228
1	0	-1.096106	-2.855575	-0.405769
1	0	1.035111	-3.970288	-1.817122
1	0	0.954008	0.763122	-3.507669
8	0	1.278180	0.084090	-1.559758
1	0	-0.450823	0.156199	-2.590389
1	0	-1.442228	-0.963583	3.258327
8	0	-1.960196	-2.593838	2.056131
1	0	-0.296218	-2.317125	3.169473
1	0	2.051799	0.642068	-1.337432
1	0	-2.663904	-2.059752	1.637846

trimer ca

*** imOH_BF4_b3lyp_6-31+Gp_trimer_D3.g09, E(RB3LYP) = -2533.58418824

7	0	-4.064985	-0.332992	1.265784

6	0	-4.366573	0.087975	-0.017134
6	0	-4.046948	1.412308	-0.093849
7	0	-3.547021	1.777878	1.142664
6	0	-3.561927	0.705278	1.944411
6	0	-3.054134	3.110004	1.521251
6	0	-4.252609	-1.707117	1.766127
6	0	-3.214995	-2.093921	2.830115
9	0	-1.200337	-2.755119	0.086003
5	0	-2.248965	-3.423288	-0.648734
9	0	-2.988475	-4.198180	0.246152
9	0	-1.657500	-4.185156	-1.662266
9	0	-3.072199	-2.414932	-1.213638
1	0	-5.264795	-1.795689	2.177426
1	0	-4.169918	-2.362936	0.900640
1	0	-3.045794	3.738437	0.632533
1	0	-3.713438	3.541050	2.278875
1	0	-2.031650	3.035507	1.897062
1	0	-3.194620	0.679716	2.956888
1	0	-4.059579	2.100315	-0.925503
1	0	-4.720804	-0.604723	-0.763467
1	0	-3.308542	-3.177619	2.984089
8	0	-1.897777	-1.716386	2.485450
1	0	-3.433877	-1.602517	3.785725
1	0	-1.628022	-2.167531	1.654516
7	0	1.490873	-1.824402	-2.014285
6	0	1.902852	-0.500537	-2.015113
6	0	0.842193	0.241347	-2.449100
7	0	-0.200100	-0.640459	-2.689371
6	0	0.216195	-1.881712	-2.420506
6	0	-1.536874	-0.278767	-3.172868
6	0	2.282186	-2.980378	-1.567080
6	0	2.111410	-3.256104	-0.068341
9	0	-0.390233	3.189987	-2.661729
5	0	-1.471528	3.187293	-1.776210
9	0	-2.695580	3.045759	-2.439037
9	0	-1.315286	2.085618	-0.872322
9	0	-1.473989	4.378244	-0.996579
9	0	4.770713	-1.318589	-0.506558
5	0	5.291716	-0.053712	-0.051899
9	0	6.558584	0.154176	-0.542443
9	0	5.264380	-0.068410	1.368223
9	0	4.384710	0.953274	-0.501779
6	0	2.584576	1.050780	1.832497
7	0	1.602320	1.587662	1.099321
6	0	0.417752	0.934061	1.398354
6	0	0.711803	-0.014583	2.333115
7	0	2.067941	0.080371	2.592515
6	0	1.770575	2.721726	0.180761
6	0	1.443265	4.055000	0.862378
6	0	2.837700	-0.806854	3.466567
1	0	1.960241	-3.851188	-2.146188
1	0	3.325924	-2.763694	-1.804612
1	0	-1.905102	0.559873	-2.583587
1	0	-1.478991	0.008696	-4.225703
1	0	-2.196099	-1.136956	-3.040327
1	0	-0.383754	-2.778318	-2.481422
1	0	0.717762	1.301513	-2.606186
1	0	2.892411	-0.211067	-1.691986
1	0	2.580287	-0.608911	4.510622
1	0	2.605461	-1.837173	3.194305
1	0	3.899110	-0.627111	3.292318
1	0	2.803258	2.698717	-0.177433
1	0	1.101295	2.559812	-0.663768
1	0	3.631201	1.300292	1.766780

1	0	-0.496665	1.186975	0.889926
1	0	0.081046	-0.757215	2.797012
1	0	2.701921	-4.156385	0.166449
8	0	2.493878	-2.156891	0.736933
1	0	1.061096	-3.458498	0.155613
1	0	1.692191	4.863691	0.160144
8	0	0.091077	4.131250	1.284345
1	0	2.062804	4.179183	1.757502
1	0	3.401187	-1.885907	0.485405
1	0	-0.464044	4.286925	0.494585

tetramer ca

*** imOH_BF4_b3lyp_6-31+Gp_tetramer_D3.g09, E(RB3LYP) = -3378.11575625

7	0	5.957772	-0.794729	0.751501
6	0	6.212942	-0.176621	-0.460819
6	0	6.231346	-1.159585	-1.405661
7	0	5.980658	-2.359129	-0.758375
6	0	5.808439	-2.109700	0.543591
6	0	5.933334	-3.679231	-1.394365
6	0	5.806651	-0.104670	2.043320
6	0	4.393552	0.455038	2.256973
9	0	2.995800	-3.162769	-1.284385
5	0	2.731328	-3.254876	0.128969
9	0	3.629475	-4.168190	0.700410
9	0	2.934716	-1.973312	0.683700
9	0	1.399025	-3.652173	0.297071
9	0	6.011063	2.929302	0.357727
5	0	5.573146	3.560442	-0.870368
9	0	6.603844	4.285997	-1.421564
9	0	4.448088	4.361730	-0.569648
9	0	5.154025	2.509032	-1.741601
6	0	2.195904	2.375681	-0.765900
7	0	2.019899	1.053219	-0.858265
6	0	1.164873	0.643575	0.151059
6	0	0.807610	1.761046	0.844937
7	0	1.463270	2.829155	0.256791
6	0	2.764845	0.191708	-1.780486
6	0	1.861516	-0.504667	-2.798164
6	0	1.437300	4.216333	0.720727
1	0	6.058364	-0.816470	2.835329
1	0	6.546269	0.701064	2.054315
1	0	5.249396	-3.635409	-2.242138
1	0	6.938919	-3.960159	-1.718435
1	0	5.540366	-4.398710	-0.677586
1	0	5.531266	-2.844271	1.283108
1	0	6.397214	-1.110398	-2.470455
1	0	6.325500	0.893209	-0.543056
1	0	0.512065	4.703098	0.399334
1	0	1.494438	4.220243	1.811226
1	0	2.304819	4.737044	0.313310
1	0	3.503369	0.824042	-2.279433
1	0	3.295352	-0.545290	-1.176317
1	0	2.881401	2.963737	-1.355126
1	0	0.924277	-0.390555	0.319746
1	0	0.165661	1.875960	1.704652
1	0	4.388301	0.945372	3.244247
8	0	3.998569	1.333134	1.228389
1	0	3.662541	-0.357145	2.268188
1	0	2.500135	-0.950925	-3.574803
8	0	1.022136	-1.489318	-2.207510
1	0	1.201051	0.223079	-3.281994

1	0	4.676094	2.025410	1.081383
1	0	1.595602	-2.231450	-1.929223
7	0	-2.416142	-2.000209	-0.997043
6	0	-3.653124	-2.274386	-0.442454
6	0	-3.417455	-2.939246	0.725498
7	0	-2.045656	-3.056814	0.865758
6	0	-1.461204	-2.473673	-0.184641
6	0	-1.353946	-3.664740	2.007707
6	0	-2.174625	-1.245452	-2.235896
6	0	-2.185493	0.270841	-2.013007
9	0	-2.394627	-0.875434	3.353879
5	0	-1.441950	-0.140280	2.581980
9	0	-0.220073	-0.818342	2.556099
9	0	-1.936387	-0.011049	1.262727
9	0	-1.302800	1.147730	3.142437
9	0	-5.288562	-0.734299	-2.954985
5	0	-6.611486	-0.597688	-2.398083
9	0	-7.508266	-1.382181	-3.082883
9	0	-6.956096	0.777534	-2.441191
9	0	-6.520457	-0.983903	-1.023836
6	0	-5.603862	1.747310	0.082294
7	0	-4.908051	1.363722	1.156968
6	0	-3.918727	2.298848	1.408340
6	0	-4.048651	3.268021	0.458099
7	0	-5.108407	2.907236	-0.357491
6	0	-5.111632	0.089842	1.861187
6	0	-5.478102	0.280469	3.334501
6	0	-5.511978	3.576763	-1.593100
1	0	-1.198096	-1.550269	-2.616820
1	0	-2.952929	-1.535606	-2.946290
1	0	-1.580441	-3.082118	2.901518
1	0	-1.693666	-4.697896	2.117312
1	0	-0.282486	-3.642988	1.817360
1	0	-0.397913	-2.405934	-0.349992
1	0	-4.096841	-3.326942	1.468083
1	0	-4.573660	-1.959560	-0.911536
1	0	-5.841164	4.595361	-1.371366
1	0	-4.659671	3.593619	-2.276998
1	0	-6.320028	3.006151	-2.051458
1	0	-5.901779	-0.444846	1.326911
1	0	-4.184841	-0.475481	1.766190
1	0	-6.392366	1.184857	-0.392391
1	0	-3.221461	2.179068	2.220854
1	0	-3.481200	4.168758	0.284323
1	0	-1.837175	0.732334	-2.952944
8	0	-3.448593	0.782721	-1.629494
1	0	-1.485350	0.534871	-1.215303
1	0	-5.702633	-0.715209	3.749096
8	0	-4.471281	0.943035	4.076866
1	0	-6.381428	0.893415	3.424923
1	0	-4.137572	0.392802	-2.205997
1	0	-3.670905	0.384335	4.082781

dimer cc

*** imOH_BF4_cation_cation_b3lyp_6-31+Gp_dimer_D3.g09, E(RB3LYP) = -1689.03077609

6	0	0.661378	-3.831511	-0.936789
6	0	-0.205805	-3.091176	-1.682808
7	0	-0.599404	-2.021456	-0.898186
6	0	0.012666	-2.107397	0.286650
7	0	0.777986	-3.201704	0.290184

6	0	-1.402857	-0.871893	-1.318061
6	0	-2.899534	-1.169905	-1.497565
8	0	-3.611299	0.067730	-1.497458
6	0	1.737561	-3.544597	1.340480
9	0	-2.839695	0.841067	1.062326
5	0	-2.476290	-0.137043	2.077163
9	0	-2.730395	-1.414351	1.540804
9	0	-1.072920	-0.007463	2.281446
9	0	-3.179143	0.105535	3.234614
8	0	-2.410707	2.397951	-2.669753
6	0	-1.737183	2.837716	-1.503548
6	0	-0.242950	2.502440	-1.646063
7	0	0.515219	2.595114	-0.380891
6	0	0.038845	2.335858	0.894814
6	0	1.120946	2.281362	1.720145
7	0	2.241439	2.502569	0.942785
6	0	1.851693	2.672853	-0.323621
6	0	3.626221	2.401864	1.406396
9	0	3.749402	0.456090	-0.861953
5	0	2.726031	-0.475675	-0.599073
9	0	3.091450	-1.770955	-0.985665
9	0	1.550981	-0.075589	-1.300465
9	0	2.433450	-0.468357	0.795768
1	0	-0.556121	-3.215655	-2.695321
1	0	-0.088428	-1.394123	1.092866
1	0	-1.288622	-0.119819	-0.539434
1	0	-0.960461	-0.483636	-2.237975
1	0	-3.099882	-1.648712	-2.461188
1	0	-3.249670	-1.819912	-0.690694
1	0	-3.646381	0.369847	-0.566104
1	0	-2.895647	1.575752	-2.442917
1	0	-1.874158	3.921271	-1.401404
1	0	-2.157982	2.361633	-0.613152
1	0	-0.123323	1.481773	-2.008420
1	0	0.229215	3.173466	-2.368465
1	0	2.513030	2.761981	-1.170144
1	0	-1.001574	2.165066	1.113224
1	0	1.184359	2.067026	2.774891
1	0	3.823594	1.361792	1.670007
1	0	4.293579	2.690788	0.595248
1	0	3.765482	3.063539	2.264576
1	0	1.714978	-4.623485	1.508921
1	0	2.728472	-3.214482	1.022107
1	0	1.454899	-3.022963	2.255356
1	0	1.221250	-4.722133	-1.174027

trimer cc

*** imOH_BF4_cation_cation_b3lyp_6-31+Gp_trimer_D3.g09, E(RB3LYP) = -2533.55624132

6	0	-5.585765	0.961949	-0.302834
7	0	-4.689276	-0.028361	-0.194928
6	0	-4.573977	-0.383411	1.137490
6	0	-5.436725	0.411900	1.831719
7	0	-6.061912	1.239849	0.914199
6	0	-3.868026	-0.582323	-1.284923
6	0	-2.772240	0.398536	-1.729217
8	0	-2.046564	0.902319	-0.613377
6	0	-7.008587	2.307810	1.242909
9	0	-2.195610	-2.565982	1.384621
5	0	-2.805441	-3.640369	0.661759
9	0	-2.498236	-3.462043	-0.716573

9	0	-4.184654	-3.599599	0.854284
9	0	-2.238370	-4.854902	1.102979
8	0	0.477507	0.471150	0.193863
6	0	0.240388	-0.360835	1.330083
6	0	1.242686	-1.511106	1.338681
7	0	1.053149	-2.411625	0.193557
6	0	0.388980	-3.572932	0.223134
7	0	0.377482	-4.089881	-1.008130
6	0	1.050446	-3.223150	-1.854391
6	0	1.476132	-2.169621	-1.100493
6	0	-0.296665	-5.326588	-1.406957
8	0	1.738428	2.696851	1.178978
6	0	3.104073	2.368695	1.240799
6	0	3.818050	2.926679	-0.006416
7	0	5.272088	2.691574	0.063499
6	0	6.129367	3.224898	1.010529
6	0	7.341583	2.623624	0.837814
7	0	7.206643	1.735300	-0.214178
6	0	5.946207	1.791189	-0.657086
6	0	8.206761	0.753336	-0.644293
9	0	4.217561	-2.241659	0.253760
5	0	4.798364	-1.015419	-0.057326
9	0	3.840524	-0.194998	-0.751187
9	0	5.926049	-1.163886	-0.897095
9	0	5.183127	-0.322749	1.115214
9	0	-3.474434	4.967013	-1.197835
5	0	-4.239479	3.857378	-0.908904
9	0	-3.541608	3.011624	0.047853
9	0	-5.483761	4.187443	-0.340433
9	0	-4.465063	3.063787	-2.070301
1	0	-2.480930	1.735025	-0.315988
1	0	-4.524660	-0.827649	-2.125952
1	0	-3.435912	-1.508746	-0.911060
1	0	-2.073794	-0.151719	-2.369467
1	0	-3.198399	1.229382	-2.298449
1	0	-0.399830	0.687367	-0.208450
1	0	-0.781461	-0.749966	1.311912
1	0	0.382770	0.216767	2.255174
1	0	2.270379	-1.147780	1.291335
1	0	1.124268	-2.104925	2.248905
1	0	1.254884	1.962465	0.730988
1	0	3.287225	1.289903	1.299182
1	0	3.523615	2.834394	2.142444
1	0	3.641503	4.001937	-0.095788
1	0	3.446499	2.424796	-0.900991
1	0	-0.113788	-3.995302	1.078811
1	0	1.175862	-3.439979	-2.903560
1	0	2.066414	-1.299672	-1.336397
1	0	5.805492	3.978420	1.711049
1	0	8.276254	2.747123	1.362333
1	0	5.523026	1.161731	-1.422613
1	0	-3.912380	-1.175904	1.453498
1	0	-5.665067	0.458245	2.884890
1	0	-5.816903	1.505565	-1.206082
1	0	7.985128	0.443745	-1.665009
1	0	9.195136	1.214893	-0.598128
1	0	8.147227	-0.121914	0.005231
1	0	-7.451180	2.685659	0.322764
1	0	-7.781934	1.902967	1.900181
1	0	-6.471665	3.128057	1.721498
1	0	-1.037351	-5.091462	-2.172951
1	0	0.443557	-6.036670	-1.785369
1	0	-0.819230	-5.733602	-0.542335

tetramer cc

*** imOH_BF4_cation_cation_b3lyp_6-31+Gp_tetramer_l_D3.g09, E(RB3LYP) = -3378.10686835

6	0	3.375127	4.822319	-0.243667
7	0	3.238869	3.479826	0.071855
6	0	4.434876	2.991169	0.420134
7	0	5.337828	3.975509	0.342540
6	0	4.692573	5.131395	-0.069533
6	0	2.021850	2.664146	-0.086616
6	0	1.744314	2.365880	-1.571063
8	0	0.722161	1.384699	-1.671094
6	0	6.763847	3.840066	0.647752
8	0	1.463272	-1.225182	-1.576939
6	0	2.237157	-1.797734	-0.531249
6	0	3.174882	-2.865097	-1.119108
7	0	3.772144	-3.672863	-0.039755
6	0	4.665224	-3.229202	0.922698
6	0	4.843997	-4.262017	1.795925
7	0	4.056401	-5.314878	1.357730
6	0	3.418752	-4.930807	0.246307
6	0	3.924803	-6.624071	2.002301
8	0	-1.862225	1.235709	-0.757099
6	0	-2.562653	2.150290	-1.586661
6	0	-3.844648	2.573603	-0.877912
7	0	-3.556742	3.169312	0.439494
6	0	-2.989819	4.365089	0.640958
7	0	-2.806160	4.533094	1.956153
6	0	-3.264271	3.400903	2.611122
6	0	-3.732687	2.543995	1.658496
6	0	-2.197713	5.702780	2.596300
9	0	-5.243987	-0.208981	1.341537
5	0	-6.365466	0.184626	0.517210
9	0	-7.426001	-0.696671	0.761430
9	0	-5.943862	0.036349	-0.835728
9	0	-6.680369	1.511262	0.786897
8	0	-0.834182	-2.629955	-1.115252
6	0	-1.379374	-2.026639	0.059726
6	0	-2.389172	-2.928202	0.772669
7	0	-3.482600	-3.342075	-0.118642
6	0	-4.639212	-2.682293	-0.258486
7	0	-5.367651	-3.297165	-1.195954
6	0	-4.646004	-4.380147	-1.675072
6	0	-3.460938	-4.409245	-0.999536
6	0	-6.694308	-2.869433	-1.658404
9	0	4.403878	0.489103	-1.422278
5	0	5.482836	0.035874	-0.637864
9	0	5.903417	-1.232860	-1.056004
9	0	5.004788	-0.064141	0.722927
9	0	6.532393	0.967222	-0.662982
9	0	-1.167287	-5.933750	0.507735
5	0	0.188337	-5.592213	0.482390
9	0	0.475221	-4.614106	1.454756
9	0	0.484238	-4.998333	-0.805161
9	0	1.013089	-6.714251	0.646754
9	0	-0.463124	4.694162	-1.223192
5	0	-0.111110	5.817368	-0.436924
9	0	-1.242087	6.651500	-0.286217
9	0	0.301645	5.348161	0.841915
9	0	0.945434	6.516307	-1.042148
1	0	-0.910925	1.299939	-1.000090

1	0	-4.392572	3.308622	-1.475089
1	0	-4.499263	1.721103	-0.706536
1	0	-2.854120	1.684955	-2.541689
1	0	-1.941040	3.026444	-1.804636
1	0	-0.411277	-3.490507	-0.908208
1	0	-1.842628	-1.091166	-0.266385
1	0	-0.590207	-1.786258	0.786824
1	0	-1.914681	-3.834915	1.150156
1	0	-2.832788	-2.386020	1.612722
1	0	0.597330	-1.699246	-1.611037
1	0	1.595177	-2.261828	0.228679
1	0	2.825694	-1.003567	-0.065668
1	0	3.978651	-2.403294	-1.693467
1	0	2.604075	-3.546672	-1.752976
1	0	1.112663	0.477814	-1.652841
1	0	1.382899	3.270282	-2.066639
1	0	2.663178	2.016776	-2.054665
1	0	2.191760	1.728514	0.451899
1	0	1.188132	3.205010	0.364544
1	0	-4.920883	-1.799607	0.299402
1	0	-5.041295	-5.031401	-2.438955
1	0	-2.626615	-5.092318	-1.034070
1	0	5.081915	-2.234454	0.891213
1	0	5.455599	-4.340756	2.681232
1	0	2.708001	-5.525151	-0.304284
1	0	4.639189	1.967957	0.697472
1	0	5.221557	6.062475	-0.201070
1	0	2.535320	5.432455	-0.547631
1	0	-4.193605	1.570170	1.729979
1	0	-3.227288	3.313952	3.685724
1	0	-2.689044	5.069624	-0.119531
1	0	3.033480	-7.115286	1.612117
1	0	4.816168	-7.225893	1.805042
1	0	3.807365	-6.474784	3.077793
1	0	7.336937	4.376861	-0.111233
1	0	6.974201	4.258225	1.636166
1	0	7.028201	2.783295	0.607787
1	0	-2.014027	6.462403	1.838544
1	0	-2.877297	6.079247	3.365173
1	0	-1.240068	5.414933	3.034399
1	0	-6.591922	-2.328296	-2.601864
1	0	-7.316658	-3.756604	-1.794650
1	0	-7.135195	-2.208026	-0.913261

tetramer cc_cyc

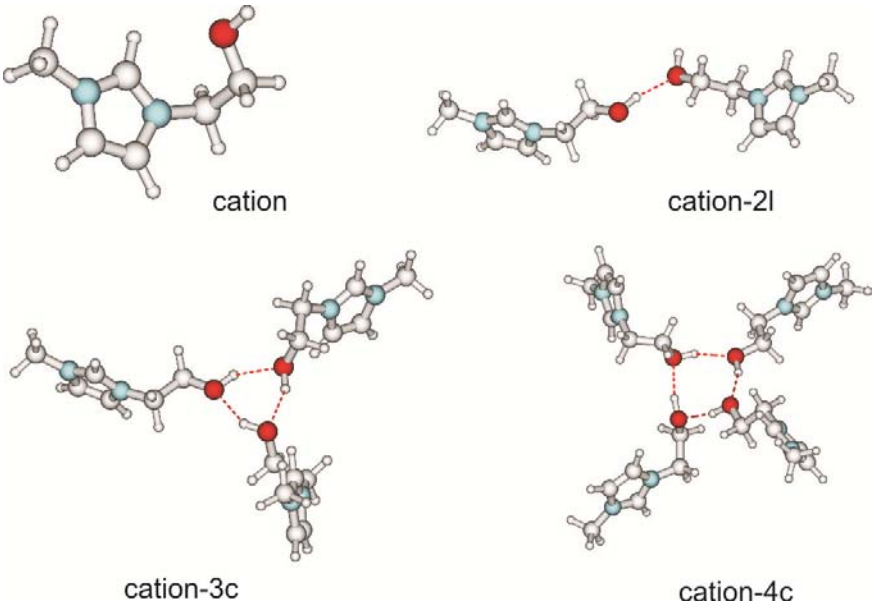
*** imOH_BF4_cation_cation_b3lyp_6-31+Gp_tetramer_D3.g09, E(RB3LYP) = -3378.11423979

6	0	-3.142778	3.321540	0.143202
7	0	-3.977421	2.392172	-0.341968
6	0	-5.279505	2.758963	-0.042073
6	0	-5.210077	3.942325	0.629066
7	0	-3.869314	4.276034	0.734239
6	0	-3.605389	1.158480	-1.064034
6	0	-2.164001	1.160890	-1.535842
8	0	-1.318939	1.095798	-0.387532
6	0	-3.335193	5.506473	1.324291
9	0	-5.101429	-0.397462	1.344496
5	0	-6.420761	-0.381544	0.798506
9	0	-6.296830	-0.196792	-0.612844
9	0	-7.162840	0.658950	1.345480
9	0	-7.021599	-1.639275	1.042938

8	0	-1.028569	-1.290581	0.812209
6	0	-1.966099	-1.594068	1.842243
6	0	-2.497342	-3.010062	1.629732
7	0	-3.205342	-3.122665	0.345247
6	0	-4.531608	-3.034450	0.184676
7	0	-4.808850	-3.091411	-1.121603
6	0	-3.615291	-3.216597	-1.818219
6	0	-2.607970	-3.236545	-0.898544
6	0	-6.146903	-3.018139	-1.714851
8	0	1.607958	-0.777006	1.139046
6	0	2.577351	-1.821023	1.087844
6	0	2.925462	-2.120166	-0.380475
7	0	3.810732	-3.293920	-0.465338
6	0	5.154845	-3.340761	-0.129711
6	0	5.528301	-4.652067	-0.204073
7	0	4.406910	-5.379869	-0.575500
6	0	3.384071	-4.532418	-0.730652
6	0	4.318724	-6.830309	-0.758043
8	0	1.284684	0.929757	-0.931183
6	0	2.237139	1.985644	-0.962994
6	0	2.202346	2.763020	0.362723
7	0	3.256739	3.791375	0.366544
6	0	4.511694	3.569074	0.772294
7	0	5.251537	4.644239	0.479934
6	0	4.436369	5.587071	-0.129659
6	0	3.183490	5.050205	-0.208949
6	0	6.685802	4.766210	0.750664
9	0	4.693476	0.630545	1.185499
5	0	5.791053	0.363612	0.308287
9	0	6.515066	-0.738914	0.793708
9	0	6.608365	1.515204	0.258445
9	0	5.271491	0.072713	-0.969931
9	0	-1.109344	-5.620537	0.321529
5	0	0.222769	-5.212707	0.227745
9	0	0.372742	-4.339720	-0.909777
9	0	1.091681	-6.311013	0.043207
9	0	0.598549	-4.485010	1.377325
9	0	0.517250	5.918122	-1.522721
5	0	-0.469118	5.034518	-1.058857
9	0	-0.310467	4.859878	0.357701
9	0	-1.759475	5.520516	-1.310232
9	0	-0.304506	3.760543	-1.657534
1	0	-0.370128	1.216430	-0.664071
1	0	-4.285052	1.071688	-1.914837
1	0	-3.802647	0.319457	-0.394580
1	0	-2.019531	0.277901	-2.175171
1	0	-1.930423	2.059131	-2.120014
1	0	-1.233897	-0.410395	0.404377
1	0	-2.793020	-0.875120	1.840811
1	0	-1.471374	-1.559929	2.822535
1	0	-1.682924	-3.735169	1.619023
1	0	-3.201747	-3.276078	2.422637
1	0	0.692755	-1.151703	1.102988
1	0	2.191904	-2.727599	1.566415
1	0	3.463903	-1.463803	1.617671
1	0	3.438419	-1.275960	-0.843898
1	0	2.016076	-2.359697	-0.935756
1	0	1.522374	0.297935	-0.203655
1	0	1.954299	2.641908	-1.789135
1	0	3.244585	1.584989	-1.134224
1	0	2.398261	2.086341	1.198043
1	0	1.242426	3.259992	0.503358
1	0	-5.261205	-2.883717	0.965012
1	0	-3.592933	-3.300971	-2.893516

```
1           0       -1.541271   -3.355422   -1.004650
1           0        5.710189   -2.448862    0.131894
1           0        6.481241   -5.125598   -0.025656
1           0        2.373280   -4.799164   -0.995750
1           0        4.865836    2.649314    1.212841
1           0        4.815798    6.544033   -0.452746
1           0        2.260910    5.437868   -0.622587
1           0       -6.116780    2.126358   -0.290173
1           0       -5.986633    4.561870    1.049414
1           0       -2.068813    3.304079    0.072595
1           0        3.266326   -7.117611   -0.723378
1           0        4.762515   -7.115189   -1.716013
1           0        4.852554   -7.322133    0.058063
1           0        7.165292    5.246855   -0.104705
1           0        6.848340    5.364989    1.651174
1           0        7.097712    3.763542    0.875594
1           0       -2.250704    5.426908    1.381136
1           0       -3.589545    6.352081    0.681567
1           0       -3.765828    5.636677    2.320166
1           0       -6.197294   -2.149393   -2.373125
1           0       -6.344126   -3.938874   -2.270167
1           0       -6.874655   -2.882261   -0.916381
```

SI7 B3LYP/6-31+G*-D3 optimized geometries of $HEMim^+$ clusters n=1-4



Cation monomer

```
*** imOH_BF4_b3lyp_6-31+Gp_D3.g09

N      4.527308     5.018642     4.717323
 C     3.724581     3.934916     4.370811
 C     2.502564     4.424990     4.118242
 N     2.572824     5.807388     4.293706
 C     3.807773     6.129964     4.647460
 C     1.464429     6.764243     4.094263
 C     5.945566     4.894271     5.161989
 C     6.838381     5.988055     4.565875
 H     5.950111     4.936052     6.242145
 H     6.259730     3.919028     4.833379
 H     0.793766     6.356808     3.353148
 H     0.934955     6.908165     5.024722
 H     1.887452     7.685969     3.737891
 H     4.174162     7.119661     4.795428
 H     1.607966     3.941551     3.812895
 H     4.140721     2.963850     4.282409
 H     7.830313     5.892439     4.991823
 O     6.935496     5.820137     3.179379
 H     6.471430     6.983322     4.767773
 H     6.426707     5.065982     2.916335
```

Cation dimer

```
***  imOH_b3lyp_6-31+Gp_dimer_D3.g09, E(RB3LYP) =  -839.515427871, 5.8.2015

                6           0       -5.598022    0.304464   -0.890386
                7           0       -4.694602    0.533524    0.073499
                6           0       -5.320507    0.389607    1.300154
                6           0       -6.623977    0.070291    1.052107
                7           0       -6.776344    0.021921   -0.322188
                6           0       -3.272571    0.858803   -0.136975
                6           0       -2.362684   -0.349519    0.115163
                8           0       -1.052737    0.121085   -0.123970
```

6	0	-8.033660	-0.266510	-1.032218
8	0	1.260208	-1.539015	0.165861
6	0	2.424710	-0.850799	-0.280790
6	0	3.528927	-0.956291	0.788449
7	0	4.721662	-0.172572	0.420415
6	0	4.837221	1.206236	0.494277
6	0	6.084570	1.529186	0.045108
7	0	6.713377	0.345597	-0.298280
6	0	5.871797	-0.667099	-0.063905
6	0	8.087672	0.228030	-0.817259
1	0	4.037874	1.828808	0.867177
1	0	6.087910	-1.713076	-0.225661
1	0	3.842344	-1.994469	0.928179
1	0	3.159917	-0.584214	1.747434
1	0	2.128270	0.193125	-0.419313
1	0	2.778889	-1.235268	-1.246095
1	0	1.332187	-2.490017	-0.014897
1	0	-0.396303	-0.589035	0.017063
1	0	-2.641140	-1.169255	-0.565995
1	0	-2.491678	-0.706308	1.149105
1	0	-3.010259	1.679026	0.535778
1	0	-3.152633	1.211646	-1.163811
1	0	-5.407550	0.350718	-1.952554
1	0	-4.793700	0.535106	2.231071
1	0	-7.447656	-0.117083	1.724833
1	0	-8.768820	0.503918	-0.790200
1	0	-7.843622	-0.266338	-2.106168
1	0	-8.401793	-1.247771	-0.726104
1	0	8.167533	0.789555	-1.750216
1	0	8.785762	0.624486	-0.077111
1	0	8.308982	-0.823687	-1.002495
1	0	6.576221	2.485880	-0.051611

Cation trimer

*** imOH_b3lyp_6-31+Gp_trimer_D3.g09, E(RB3LYP) = -1259.20900225, 5.8.2015

6	0	-1.656817	4.575160	0.553046
7	0	-1.801425	4.445635	-0.776382
6	0	-1.762286	5.709035	-1.345742
6	0	-1.590841	6.602709	-0.329343
7	0	-1.528394	5.874583	0.845508
6	0	-1.999593	3.180212	-1.508697
6	0	-0.778186	2.269133	-1.489650
8	0	-0.649972	1.694853	-0.179711
6	0	-1.367897	6.450331	2.192363
8	0	-1.411323	-1.051968	0.239550
6	0	-2.119886	-1.395686	1.438172
6	0	-2.301724	-2.908903	1.495288
7	0	-3.321860	-3.419026	0.559620
6	0	-4.393064	-4.152069	0.907087
7	0	-5.067236	-4.483468	-0.198265
6	0	-4.408609	-3.949351	-1.291746
6	0	-3.313691	-3.284240	-0.820117
6	0	-6.299554	-5.293020	-0.252587
8	0	1.357499	-0.340421	0.079737
6	0	2.541216	-1.123446	-0.067146
6	0	3.721721	-0.145738	-0.022021
7	0	5.010102	-0.833609	-0.208315
6	0	5.920581	-1.075986	0.750449
7	0	6.963830	-1.709209	0.205733
6	0	6.719993	-1.880560	-1.145415
6	0	5.498058	-1.333025	-1.406530

6	0	8.186481	-2.138173	0.912344
1	0	0.244805	1.306883	-0.087599
1	0	-2.245612	3.447877	-2.538673
1	0	-2.864826	2.666463	-1.079154
1	0	-0.926573	1.482607	-2.241655
1	0	0.122470	2.837119	-1.753668
1	0	-1.434331	-0.077818	0.113725
1	0	-3.096996	-0.896495	1.468716
1	0	-1.546609	-1.092752	2.324781
1	0	-1.355951	-3.411902	1.270701
1	0	-2.611730	-3.201884	2.501491
1	0	0.568542	-0.918395	0.149346
1	0	2.535844	-1.666930	-1.022200
1	0	2.634111	-1.854010	0.748062
1	0	3.749356	0.372267	0.939580
1	0	3.625701	0.605595	-0.810833
1	0	-4.662155	-4.437050	1.914047
1	0	-4.771506	-4.091832	-2.299014
1	0	-2.541281	-2.725857	-1.323974
1	0	5.830313	-0.794304	1.789462
1	0	7.432580	-2.364119	-1.797663
1	0	4.949002	-1.245764	-2.331906
1	0	-1.870641	5.864418	-2.408926
1	0	-1.517438	7.680374	-0.339872
1	0	-1.637299	3.758868	1.258213
1	0	8.301286	-3.218433	0.803762
1	0	9.047205	-1.621901	0.482321
1	0	8.095168	-1.882582	1.968565
1	0	-1.364552	5.643445	2.926011
1	0	-0.423767	6.996779	2.240355
1	0	-2.202130	7.125281	2.394836
1	0	-7.094482	-4.705174	-0.715704
1	0	-6.108659	-6.196129	-0.835826
1	0	-6.590003	-5.566991	0.762258

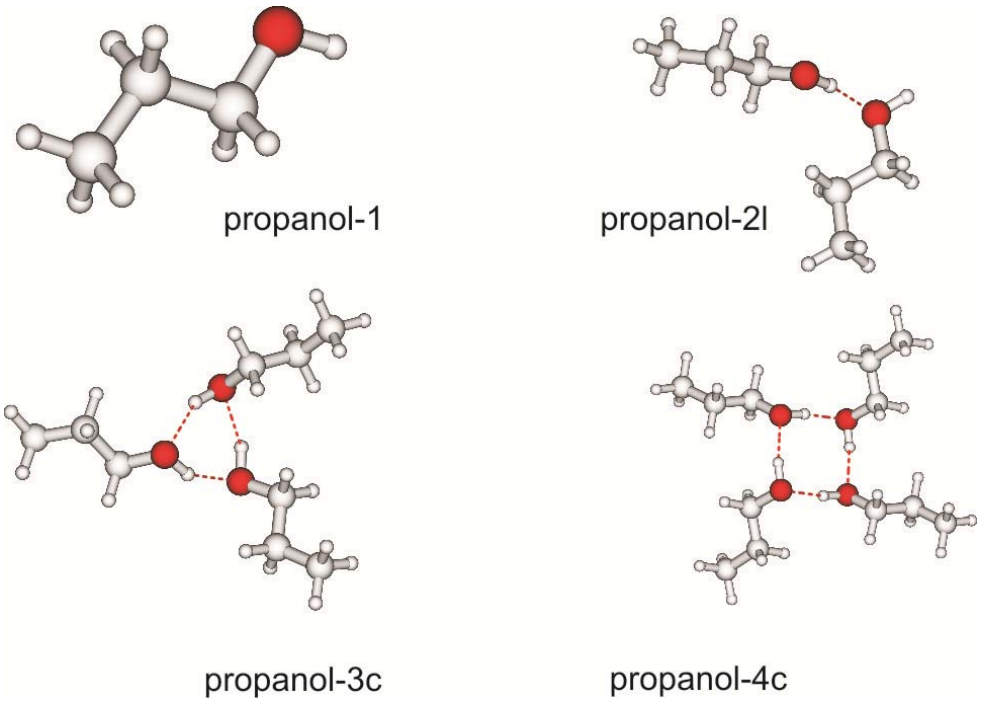
Cation tetramer

*** imOH_b3lyp_6-31+Gp_tetramer_D3.g09, E(RB3LYP) = -1678.85144940, 5.8.2015

6	0	2.388994	4.864478	-1.506478
7	0	1.997684	4.033072	-2.486465
6	0	2.930224	4.100274	-3.511414
6	0	3.889381	4.989794	-3.124718
7	0	3.531956	5.455263	-1.871483
6	0	0.761294	3.229561	-2.514822
6	0	0.930899	1.789058	-2.034479
8	0	0.949733	1.756997	-0.600041
6	0	4.270676	6.475622	-1.102605
8	0	-1.606862	1.287079	0.569826
6	0	-1.628196	1.669850	1.954393
6	0	-3.044603	1.534104	2.506888
7	0	-3.960454	2.614373	2.095273
6	0	-4.681053	3.378927	2.935261
7	0	-5.450318	4.202977	2.218430
6	0	-5.221608	3.961461	0.875361
6	0	-4.291358	2.965151	0.795147
6	0	-6.398804	5.197454	2.761268
8	0	-1.187919	-1.432579	-0.166158
6	0	-2.310252	-2.309383	-0.286802
6	0	-1.832325	-3.556368	-1.042863
7	0	-2.893955	-4.568254	-1.172023
6	0	-3.381871	-5.370858	-0.150348
6	0	-4.328738	-6.186464	-0.697459

7	0	-4.407711	-5.875790	-2.043354
6	0	-3.534872	-4.899851	-2.307980
6	0	-5.294417	-6.540649	-3.020815
8	0	1.606970	-0.906215	0.218241
6	0	2.543077	-1.940110	0.534037
6	0	3.851836	-1.254929	0.947927
7	0	4.919796	-2.229001	1.227901
6	0	5.414392	-2.533427	2.441947
7	0	6.387906	-3.436814	2.298445
6	0	6.528877	-3.724862	0.952544
6	0	5.612403	-2.970047	0.280690
6	0	7.203209	-4.019632	3.384375
1	0	1.364448	0.916064	-0.306020
1	0	0.408406	3.235070	-3.549664
1	0	0.012309	3.743482	-1.906333
1	0	0.081961	1.204774	-2.415174
1	0	1.852423	1.356486	-2.442883
1	0	-0.745184	1.565652	0.175745
1	0	-1.271911	2.700536	2.074256
1	0	-0.976318	1.008246	2.540606
1	0	-3.482283	0.581102	2.192553
1	0	-3.008549	1.544262	3.599209
1	0	-1.486348	-0.539964	0.125896
1	0	-3.122734	-1.826743	-0.846033
1	0	-2.691294	-2.593022	0.704287
1	0	-0.991134	-4.019145	-0.518394
1	0	-1.498561	-3.285499	-2.047313
1	0	0.714211	-1.294042	0.087693
1	0	2.715551	-2.586330	-0.337642
1	0	2.172959	-2.561244	1.360564
1	0	3.698188	-0.652406	1.846360
1	0	4.202514	-0.593057	0.150684
1	0	-4.651859	3.330135	4.014565
1	0	-5.740395	4.510985	0.103382
1	0	-3.832866	2.478611	-0.050746
1	0	-3.010436	-5.305893	0.861100
1	0	-4.940077	-6.958528	-0.252673
1	0	-3.362459	-4.460181	-3.279662
1	0	5.088463	-2.107328	3.379701
1	0	7.266675	-4.427723	0.592968
1	0	5.408147	-2.889109	-0.776219
1	0	2.820796	3.537587	-4.426789
1	0	4.774516	5.341975	-3.634718
1	0	1.860694	5.035577	-0.580937
1	0	-5.159481	-6.075053	-3.997631
1	0	-5.031749	-7.599002	-3.077602
1	0	-6.330773	-6.425715	-2.697493
1	0	7.082534	-5.104642	3.377786
1	0	8.250436	-3.755239	3.224163
1	0	6.864052	-3.616803	4.339286
1	0	3.782151	6.617600	-0.138014
1	0	5.296860	6.136030	-0.950010
1	0	4.265470	7.415418	-1.658970
1	0	-6.114288	6.191619	2.411314
1	0	-7.406825	4.950874	2.421775
1	0	-6.360952	5.166618	3.850684

SI8 B3LYP/6-31+G*-D3 optimized geometries of propanol clusters n=1-4



Propanol Monomer

```
*** propanol_1, B3LYP 6-31+G* opt, E(RB3LYP) =  -194.365963872, 15.09.2015

0 1
                6           0       -0.523007   -0.527116   -0.000073
                6           0        0.613310    0.486049    0.000073
                8           0        1.850182   -0.234972    0.000015
                1           0        2.586962    0.394498    0.000132
                6           0       -1.901364    0.143924   -0.000032
                1           0       -0.412648   -1.172868    0.880646
                1           0       -0.412602   -1.172666   -0.880934
                1           0        0.540928    1.131812   -0.890596
                1           0        0.540888    1.131601    0.890891
                1           0       -2.038104    0.777217   -0.886220
                1           0       -2.038145    0.777026    0.886286
                1           0       -2.702374   -0.603987   -0.000131
```

Propanol Dimer

```
*** propanol_2, B3LYP 6-31+G* opt,  E(RB3LYP) =  -388.745266754, 15.09.2015

0 1
                6           0       -2.065920    0.736552   -0.262501
                6           0       -2.587834   -0.664204    0.024373
                8           0       -1.620781   -1.612934   -0.469220
                1           0       -1.933426   -2.514316   -0.296789
                6           0       -3.044776    1.819577    0.205837
                1           0       -1.884590    0.826212   -1.341447
                1           0       -1.098310    0.857262    0.239380
                1           0       -2.731441   -0.802910    1.106191
```

```
1           0       -3.553301   -0.825630   -0.477612
1           0       -3.220908    1.756767    1.287206
1           0       -4.015659    1.728823   -0.298144
1           0       -2.651323    2.819439   -0.008024
1           0        0.046801   -1.274123    0.318186
8           0        0.856542   -0.956962    0.764923
6           0        1.719628   -0.380207   -0.209079
6           0        2.937795    0.199560    0.499304
1           0        1.200112    0.417805   -0.767899
1           0        2.040994   -1.137414   -0.944833
1           0        3.425889   -0.604881    1.064998
1           0        2.591951    0.936531    1.236269
6           0        3.930105    0.844990   -0.474608
1           0        3.462481    1.664981   -1.035478
1           0        4.305055    0.115494   -1.204415
1           0        4.795603    1.257513    0.056831
```

Propanol Trimer

```
% *** propanol_3, B3LYP 6-31+G* opt, E(RB3LYP) =  -583.134480305, 15.09.2015

0 1
      6           0        1.661484   -2.993956   -0.014440
      6           0        1.803387   -1.524433   -0.387241
      8           0        0.623845   -1.109977   -1.082614
      1           0        0.645447   -0.131584   -1.193883
      6           0        2.900503   -3.533601    0.708798
      1           0        1.473837   -3.567356   -0.931505
      1           0        0.772033   -3.109897    0.619568
      1           0        1.944660   -0.915953    0.521110
      1           0        2.687166   -1.379072   -1.028149
      1           0        3.090909   -2.983639    1.639576
      1           0        3.796871   -3.447354    0.081239
      1           0        2.776527   -4.591188    0.967545
      1           0       -0.896042   -0.901974   -0.042739
      8           0       -1.559473   -0.335507    0.414616
      6           0       -2.870204   -0.625692   -0.082423
      6           0       -3.846643    0.387188    0.500517
      1           0       -3.163332   -1.646316    0.208939
      1           0       -2.880462   -0.574249   -1.182639
      1           0       -3.522230    1.394921    0.207285
      1           0       -3.783541    0.340493    1.595570
      6           0       -5.287041    0.140572    0.037743
      1           0       -5.638315   -0.854075    0.341253
      1           0       -5.371412    0.204735   -1.054734
      1           0       -5.971529    0.880320    0.468049
      1           0       -0.673884    1.161763   -0.216550
      8           0        0.088691    1.578473   -0.680094
      6           0        0.936100    2.208041    0.285559
      6           0        2.263291    2.552405   -0.377735
      1           0        1.102991    1.535336    1.142235
      1           0        0.455395    3.121749    0.668418
      1           0        2.060626    3.180833   -1.254565
      1           0        2.720002    1.626118   -0.753102
      6           0        3.226191    3.263930    0.579305
      1           0        3.457771    2.638167    1.451029
      1           0        2.797176    4.203987    0.949082
      1           0        4.172430    3.503583    0.081209
```

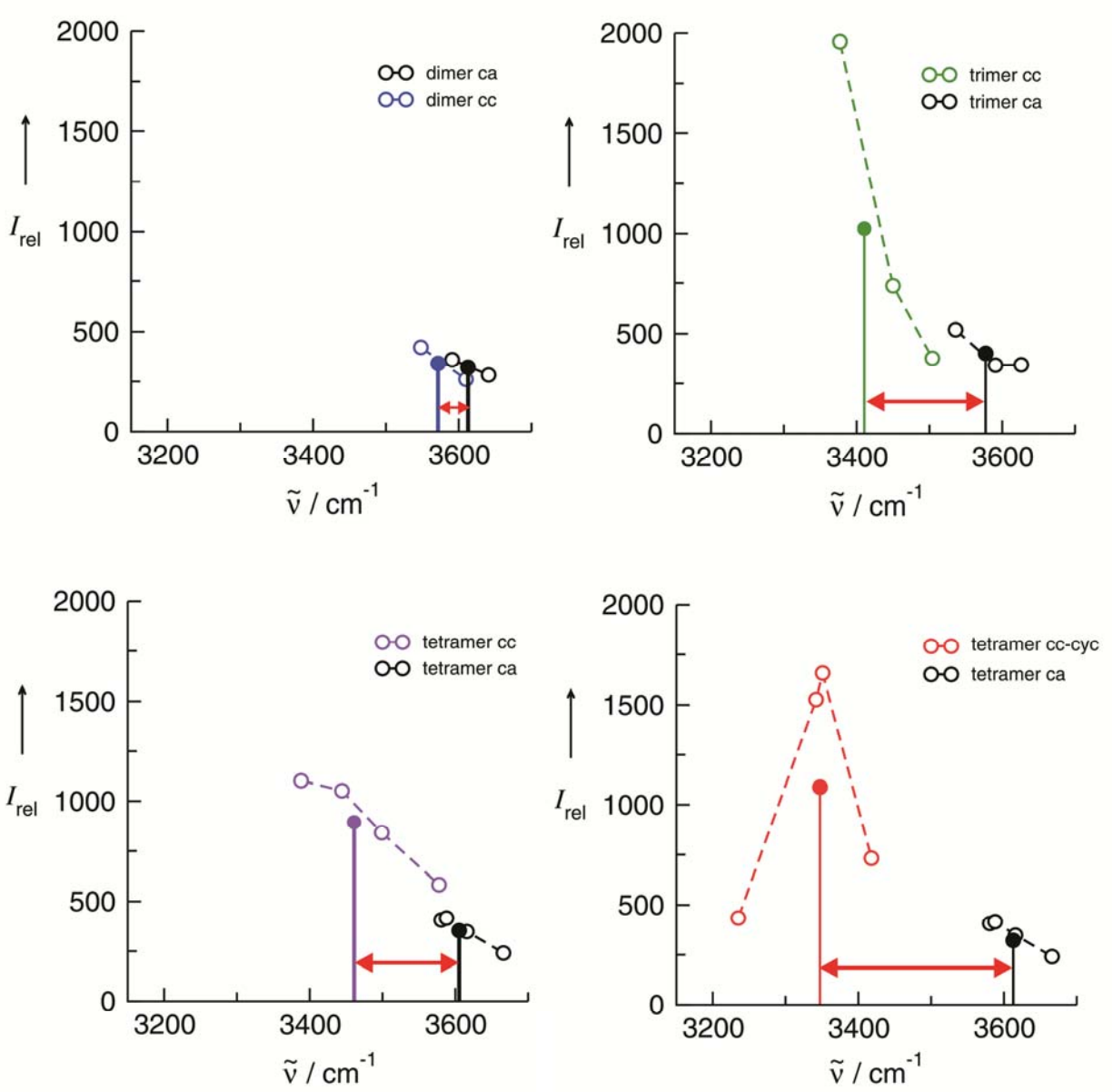
Propanol Tetramer

*** propanol_4, B3LYP 6-31+G* opt, E(RB3LYP) = -777.527236311, 25.09.2015

0 1

6	0	-2.308927	-3.174669	0.174170
6	0	-2.424392	-1.658628	0.269355
8	0	-1.256381	-1.143945	0.915308
1	0	-1.271817	-0.153355	0.872294
6	0	-3.537396	-3.809944	-0.486840
1	0	-2.168814	-3.575702	1.186519
1	0	-1.402980	-3.422177	-0.395097
1	0	-2.525463	-1.223034	-0.737916
1	0	-3.320823	-1.382279	0.846091
1	0	-3.679401	-3.432919	-1.507845
1	0	-4.452055	-3.592423	0.079680
1	0	-3.434309	-4.899314	-0.546302
1	0	0.205498	-1.494517	0.053964
8	0	1.048265	-1.537950	-0.468026
6	0	2.061281	-2.165546	0.322469
6	0	3.363288	-2.184072	-0.468166
1	0	1.755255	-3.193072	0.572288
1	0	2.198569	-1.619955	1.270096
1	0	3.637255	-1.150747	-0.720706
1	0	3.185107	-2.703226	-1.418733
6	0	4.504100	-2.856269	0.303803
1	0	4.260963	-3.899053	0.544860
1	0	4.707955	-2.335280	1.248276
1	0	5.430283	-2.857627	-0.282001
1	0	1.271726	0.153443	-0.872440
8	0	1.256501	1.144056	-0.915488
6	0	2.424311	1.658535	-0.269011
6	0	2.308999	3.174583	-0.173735
1	0	3.320946	1.382133	-0.845405
1	0	2.524924	1.222840	0.738263
1	0	1.402854	3.422150	0.395190
1	0	2.169343	3.575722	-1.186105
6	0	3.537282	3.809646	0.487825
1	0	4.452143	3.592050	-0.078340
1	0	3.678821	3.432520	1.508857
1	0	3.434314	4.899025	0.547332
1	0	-0.205487	1.494593	-0.054289
8	0	-1.048268	1.538075	0.467685
6	0	-2.061266	2.165590	-0.322878
6	0	-3.363275	2.184223	0.467758
1	0	-2.198580	1.619879	-1.270435
1	0	-1.755235	3.193081	-0.572841
1	0	-3.185081	2.703470	1.418272
1	0	-3.637255	1.150923	0.720403
6	0	-4.504081	2.856353	-0.304276
1	0	-4.707919	2.335290	-1.248713
1	0	-4.260946	3.899119	-0.545409
1	0	-5.430273	2.857749	0.281515

SI9 DFT-D3 calculated frequencies of the [HEMIm][BF_4] clusters ca and cc



SI-FIG3 DFT-D3 calculated frequencies and intensities of the OH stretches in the dimer cc (blue), the trimer cc (green), the tetramer cc (purple) and the tetramer cc-cyc (red) compared to the corresponding values of the ca clusters n=2-4 (black). The average values for each cluster ca and cc are given by the filled symbols.

SI10 B3LYP/6-31+G*-D3 calculated total energies and binding energies of [PMIm][BF_4] and [HEMIm][BF_4] clusters n=1-6.

SI Table 1. Total energies (in Hartrees) and binding energies (in $kJmol^{-1}$) for [PMIm][BF_4] and [HEMIm][BF_4] clusters.

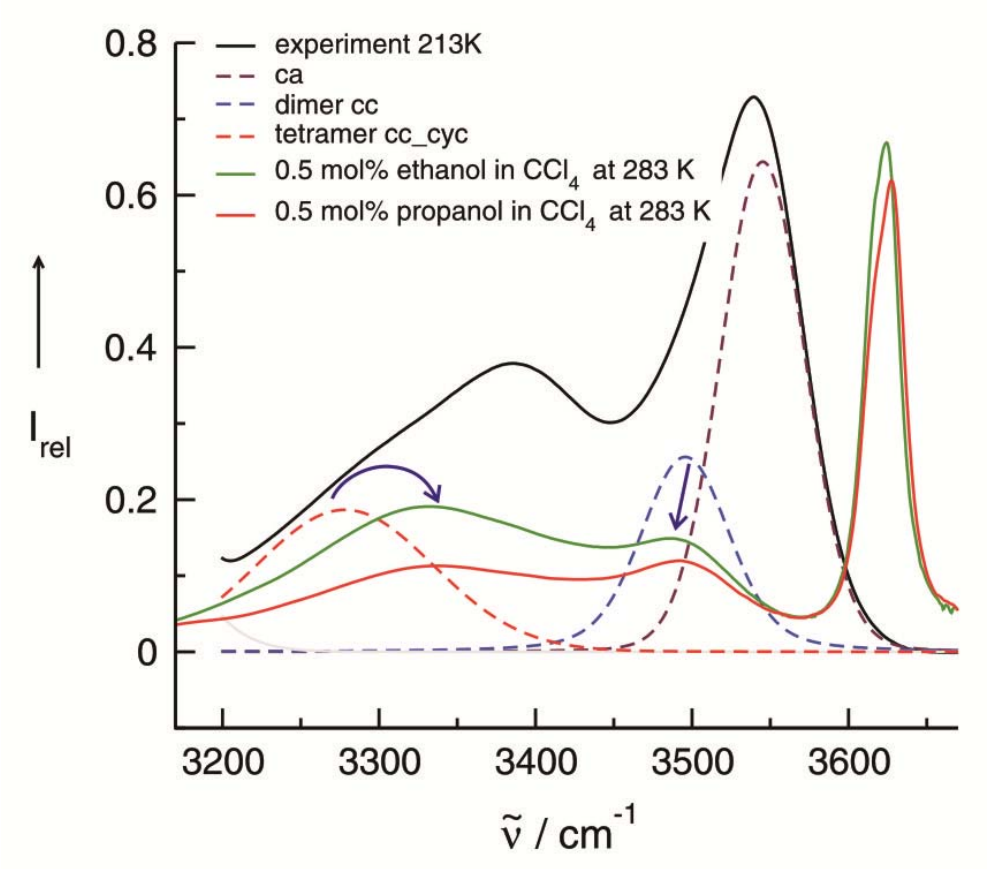
		total energy/ Hartree	**binding energy/ $kJmol^{-1}$**
[PMIm][BF_4]	**1**	-808.592825	-364.3506
	2	-1617.236463	-431.0562
	3	-2425.857908	-433.8685
	4	-3234.493186	-444.3543
	5	-4043.139364	-456.3695
	6	-4851.765687	-455.6913
[HEMIm][BF_4]	**1**	-844.496692	-375.9992
	2	-1689.040276	-437.5556
	3	-2533.584188	-458.3619
	4	-3378.115756	-460.6627
	5	-4222.669943	-473.9204
	6	-5067.193783	-469.4790

SI11 B3LYP/6-31+G*-D3 calculated geometries and frequencies of [HEMIm][BF_4], [HEMIm]$^+$ and propanol clusters n=1-4.

SI Table 2. Intramolecular bond lengths, r_{OH}, and intermolecular bond lengths, $r_{OH...O}$ and $r_{O...O}$, and average, intensity weighted OH vibrational frequencies, ν_{OH}, in [HEMIm][BF_4] clusters, cationic [HEMIm]$^+$ clusters and propanol clusters.

		rOH/Å	**rOH…O/Å**	**rO…O/Å**	**ν_{OH}/cm^{-1}**
[HEMIm][BF_4]	**2**	0.9805	1.9184	2.8715	3571.6
	3l	0.9880	1.7374	2.7130	3410.5
	4l	0.9863	1.7747	2.7536	3461.0
	4c	0.9923	1.7194	2.6900	3347.3
[HEMIm]+	**1**	0.9701	-	-	3765.8
	2	0.9740	1.9154	2.8618	3638.9
	3c	0.9809	1.9806	2.8716	3638.0
	4c	0.9836	1.8984	2.8579	3506.5
propanol	**1**	0.9701	-	-	3765.8
	2	0.9736	1.8750	2.8444	3615.2
	3c	0.9849	1.8581	2.7606	3504.0
	4c	0.9920	1.7439	2.7219	3360.0

SI12 Mid infrared spectra of [HEMim][BF_4] at 213 K, 0.5 mol% ethanol and propanol in CCl_4 at 283 K



SI-FIG4 Although the mid infrared spectra of pure [HEMIm][BF_4] at 213 K, 0.5 mol% ethanol and propanol in CCl_4 at 283 K show different systems at different concentrations and temperatures, it is shown that the deconvoluted bands of the H-bonded dimers and cyclic tetramers in the IL (dotted lines) and the alcohols indicate comparable red shifts.