

The potential role of hydrogen bonding in aprotic and protic ionic liquids

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TABLE I: Energies (E_{B3LYP}), counter poise corrected energies (E_{B3LYP}^{CP}) and average binding energies per ion (E_{bin}) for the clusters ($[dMeAm][NO_3]_x$) calculated at the B3LYP/6-31+G* level of theory.

cluster x	E_{B3LYP} Hartree	E_{B3LYP}^{CP} Hartree	E_{bin} kJmol ⁻¹
2	-832.232492673	-832.228651808	-259.895
3	-1248.366122910	-1248.360392568	-267.515
4	-1664.490923390	-1664.482325255	-268.106
6	-2496.729818317	-2496.743919700	-269.491
dMeAm ⁺	-135.535594841		
NO ₃ ⁻	-280.380753561		

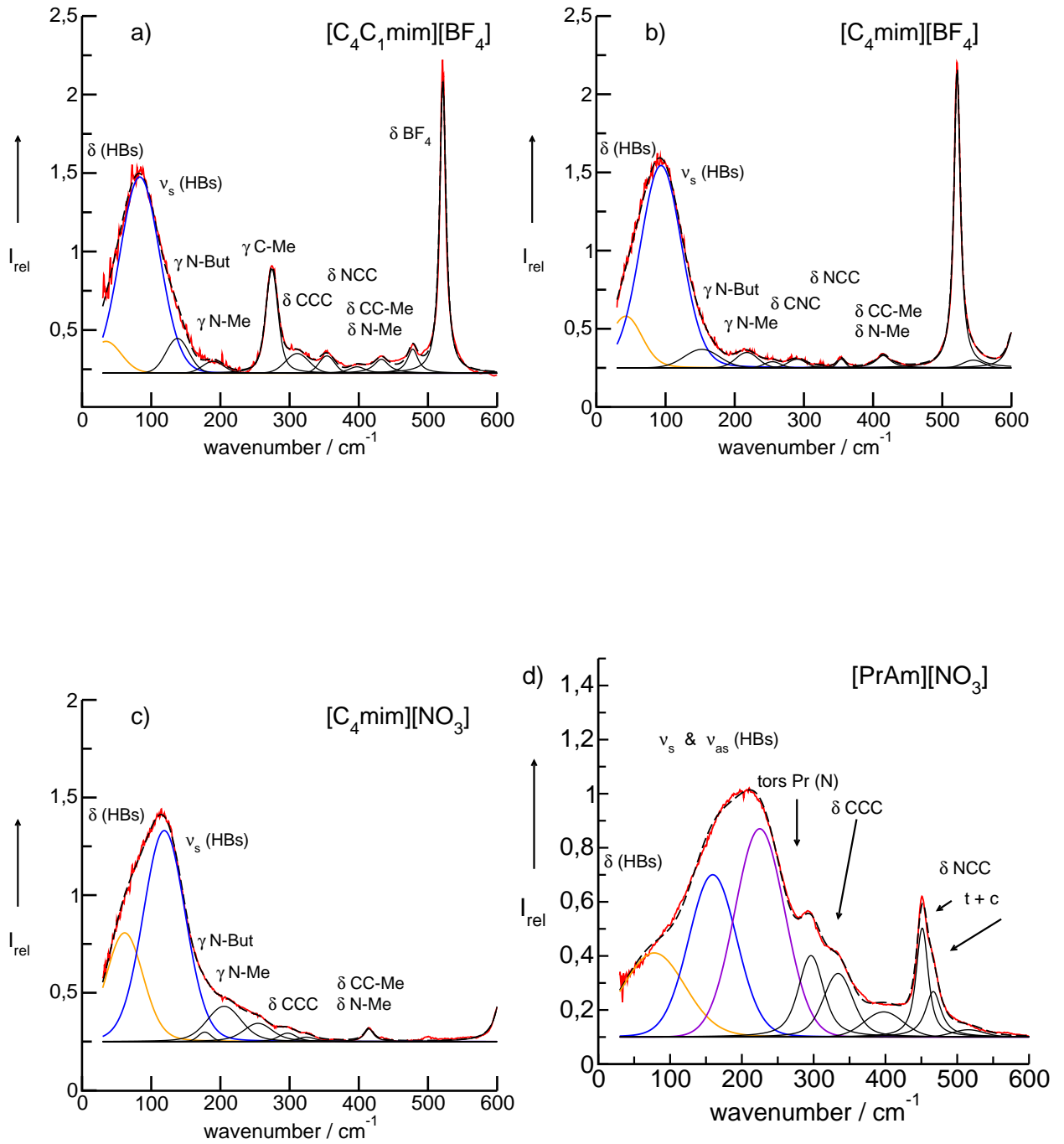


FIG. 1: Measured low-frequency vibrational FTIR spectra of the imidazolium-based ionic liquids $[\text{C}_4\text{C}_1\text{mim}][\text{BF}_4]$ (a), $[\text{C}_4\text{mim}][\text{BF}_4]$ (b), $[\text{C}_4\text{mim}][\text{NO}_3]$ (c) and the protic ionic liquid $[\text{PrAm}][\text{NO}_3]$ (d) deconvoluted into distinct vibrational bands, which can all be referred to DFT calculated frequencies. For all spectra, the detailed assignment to intramolecular bending modes as well as intermolecular stretching and bending modes is shown.

[C₄mim][BF₄]

Monomer

7 2.156205 -1.360348 0.099287
6 1.026110 -0.814649 0.563144
7 0.020244 -1.673664 0.365865
6 0.522831 -2.809034 -0.246263
6 1.863245 -2.614512 -0.409598
6 -1.399678 -1.370748 0.645561
6 -2.194682 -1.111903 -0.639847
6 -3.676046 -0.798186 -0.362910
6 3.469290 -0.701689 0.114047
9 0.059066 1.872758 1.159659
5 0.557745 2.299562 -0.122075
9 0.249862 3.621734 -0.357536
9 -0.014020 1.439769 -1.098218
9 1.966441 2.078154 -0.109095
1 4.054831 -1.056138 0.966812
1 3.988162 -0.937842 -0.817090
1 3.305312 0.375909 0.172495
1 -1.809082 -2.214713 1.212241
1 -1.396864 -0.488599 1.288069
1 0.913708 0.175355 0.992036
1 -0.106646 -3.643215 -0.514232
1 2.622815 -3.247707 -0.841490
1 -1.725390 -0.275852 -1.170653
1 -2.128549 -1.996825 -1.288462
1 -4.188195 -0.747855 -1.332350
1 -4.137673 -1.636769 0.180603
6 -3.915046 0.513745 0.397925
1 -4.988149 0.725046 0.472023
1 -3.519636 0.481610 1.420146
1 -3.436792 1.358000 -0.111483

Dimer

7 0.072872 -0.325178 -2.319849
6 -0.484225 -1.591336 -2.382033
6 0.536343 -2.481226 -2.215217
7 1.698551 -1.745740 -2.051616
6 1.394191 -0.442194 -2.117609
6 3.049661 -2.285136 -1.853515
6 -0.672612 0.938362 -2.546309
6 -0.303289 2.054742 -1.567287
9 3.237244 -0.067844 0.320872
5 3.633574 1.313493 0.196953
9 3.107849 1.775362 -1.050709
9 3.034776 2.033154 1.249931
9 5.010408 1.414515 0.213995
9 -3.400543 -0.734653 -1.881862
5 -3.794792 -1.188985 -0.595789
9 -4.851112 -2.072525 -0.675524
9 -4.123011 -0.062069 0.212522
9 -2.653173 -1.819352 0.009094
6 -1.651216 0.270153 1.913978
7 -0.323372 0.094288 1.910426
6 0.285601 1.254542 2.357417
6 -0.715423 2.138908 2.639312
7 -1.915651 1.507491 2.352615
6 0.360350 -1.147503 1.490270
6 0.410071 -2.194206 2.610966
6 -3.260140 2.081912 2.476463
1 -0.474076 1.248065 -3.578718
1 -1.729058 0.674585 -2.462089
1 2.973449 -3.215625 -1.288232
1 3.518498 -2.480152 -2.821744

1 3.628392 -1.562123 -1.277644
1 2.100267 0.367652 -1.965048
1 0.531901 -3.559527 -2.175437
1 -1.552216 -1.726573 -2.476352
1 -3.576871 2.065554 3.522943
1 -3.238132 3.112092 2.114608
1 -3.942829 1.494995 1.860305
1 -0.200394 -1.539557 0.637533
1 1.357090 -0.849068 1.160541
1 -2.380302 -0.438734 1.545257
1 1.361228 1.378305 2.350847

Trimer

7 -5.100244 -1.908450 0.937713
6 -4.257322 -0.994942 1.435814
7 -3.059917 -1.565624 1.610070
6 -3.133081 -2.889817 1.213276
6 -4.414587 -3.104719 0.794306
6 -1.876225 -0.891337 2.165028
6 -6.514484 -1.641077 0.599418
6 -6.878259 -2.028637 -0.838287
9 -5.390773 1.782177 1.210808
5 -4.354238 2.262371 0.367264
9 -3.103404 1.952665 0.989080
9 -4.408118 1.542936 -0.860637
9 -4.455931 3.624389 0.142488
9 -0.289062 -4.048823 0.750500
5 0.949322 -3.436936 0.491205
9 0.883609 -2.061231 0.833375
9 1.967047 -4.052040 1.267791
9 1.281825 -3.549922 -0.876529
6 4.391102 -2.422617 0.607886

7 4.793337 -3.018472 -0.522019
6 5.635450 -2.152432 -1.199297
6 5.731643 -1.015883 -0.451423
7 4.953704 -1.208193 0.675575
6 4.400133 -4.361459 -0.962031
6 4.763138 -0.234312 1.775657
6 3.352834 0.363071 1.796936
9 5.490087 2.033310 -0.387869
5 4.559261 2.355204 -1.407849
9 5.078539 3.284111 -2.290241
9 3.362815 2.847315 -0.800092
9 4.214522 1.147401 -2.091963
6 0.773659 1.546418 -1.694084
7 0.558923 0.323006 -2.194503
6 -0.803354 0.086737 -2.215280
6 -1.415947 1.199413 -1.716829
7 -0.413919 2.097596 -1.395210
6 1.594788 -0.623085 -2.627735
6 -0.618084 3.452185 -0.829449
6 0.080937 3.635245 0.521928
1 5.001842 -0.756565 2.706708
1 5.503362 0.551213 1.614465
1 3.947070 -4.296722 -1.953203
1 5.282980 -5.005851 -0.990962
1 3.660255 -4.753537 -0.265568
1 3.687734 -2.853273 1.307584
1 6.071007 -2.407795 -2.152729
1 6.219933 -0.071551 -0.638610
1 -7.134471 -2.189207 1.317419
1 -6.664579 -0.570411 0.760812
1 -1.815055 -1.094730 3.238036
1 -0.984819 -1.274913 1.666730

1 -1.983508 0.179447 1.988109
1 -4.510145 0.041031 1.625404
1 -2.261258 -3.530527 1.225487
1 -4.882334 -3.992058 0.398184
1 -1.697559 3.578143 -0.737359
1 -0.243803 4.175376 -1.562265
1 2.569662 -0.155107 -2.486874
1 1.513595 -1.536253 -2.032970
1 1.445302 -0.850406 -3.687091
1 1.746105 2.003967 -1.538499
1 -1.209744 -0.849427 -2.565156
1 -2.460977 1.414632 -1.538146
6 3.175829 1.393016 2.926112
1 3.181208 0.857229 0.835762
1 2.608460 -0.437426 1.896898
6 -0.082908 5.060209 1.081161
1 -0.334627 2.907377 1.230856
1 1.150023 3.421198 0.406407
1 -7.950049 -1.813234 -0.948499
6 -6.087569 -1.285505 -1.923208
1 -6.777175 -3.115661 -0.971332
1 2.197107 1.869510 2.787672
6 3.252049 0.814514 4.346436
1 3.918654 2.192978 2.804744
6 -6.571887 -1.631994 -3.335979
1 -6.159929 -0.204334 -1.755468
1 -5.020673 -1.530877 -1.834011
1 0.570758 5.147330 1.958980
1 0.305287 5.782155 0.347822
6 -1.516306 5.435994 1.480437
1 3.025035 1.585033 5.092477

1 2.530819 -0.002192 4.481626
1 4.248374 0.421728 4.585158
1 -5.990930 -1.092270 -4.092238
1 -6.474746 -2.705831 -3.543599
1 -7.626313 -1.360395 -3.472806
1 -1.539856 6.437593 1.926316
1 -2.205886 5.438538 0.629317
1 -1.920729 4.729326 2.214765

Tetramer

7 2.408321 0.740015 -3.248278
6 3.309881 0.982083 -2.288254
7 3.872952 -0.175292 -1.923134
6 3.307450 -1.191574 -2.676642
6 2.387966 -0.618859 -3.507614
6 4.882887 -0.337063 -0.852894
6 6.209803 -0.902848 -1.369695
6 6.959754 -0.022246 -2.383323
6 1.579388 1.755703 -3.912221
9 4.818719 -2.357570 2.033954
5 3.523152 -2.152577 2.510201
9 2.855985 -1.221954 1.645180
9 2.780867 -3.351903 2.510028
9 3.543104 -1.600472 3.814827
6 -0.666933 -2.693857 3.958700
6 -0.539905 -1.883626 5.255710
6 -0.978855 -0.422428 5.144023
7 -0.111923 0.416988 4.282288
6 1.223454 0.355298 4.163790
7 1.627031 1.360904 3.377372
6 0.522202 2.088421 2.976385
6 -0.568446 1.496686 3.543274

6 3.012542 1.640897 2.982787
9 0.853225 3.945478 -1.409707
5 1.732729 3.502247 -0.401696
9 1.509639 2.119338 -0.155508
9 1.523455 4.219593 0.789823
9 3.073129 3.655543 -0.843349
6 -1.900654 5.620424 1.758605
6 -1.983171 4.509320 0.698072
6 -3.359167 4.433194 0.029593
7 -3.436738 3.346835 -0.966666
6 -2.768636 3.302197 -2.179916
6 -3.083677 2.114107 -2.771688
7 -3.933461 1.449179 -1.904782
6 -4.130641 2.211802 -0.822535
6 -4.536077 0.128505 -2.124511
9 -5.147069 0.346454 1.440737
5 -3.835134 0.291444 1.963631
9 -3.374416 1.629851 2.151004
9 -3.789673 -0.391765 3.183837
9 -2.997500 -0.348253 1.014432
9 -2.151780 0.076017 -5.089220
5 -1.414708 -0.888682 -4.388229
9 -0.348181 -1.381157 -5.151888
9 -2.267074 -1.950711 -3.980338
9 -0.889175 -0.286030 -3.200322
6 -3.884361 -4.649977 -1.027613
6 -2.778290 -5.574696 -1.553527
6 -1.614590 -4.846904 -2.238893
7 -0.847809 -3.989801 -1.314736
6 -0.923042 -2.652955 -1.260662
7 -0.096502 -2.210640 -0.308736

6 0.530694 -3.296789 0.275883
6 0.056946 -4.412233 -0.354241
6 0.072019 -0.793405 0.063993
1 -4.726521 -0.328141 -1.152262
1 -5.470094 0.237655 -2.683027
1 -3.839363 -0.482676 -2.698917
1 -3.614033 5.361038 -0.491361
1 -4.138377 4.232730 0.769922
1 -4.719015 1.927841 0.039084
1 -2.104130 4.092026 -2.493798
1 -2.760645 1.663156 -3.699549
1 -0.999208 0.048525 6.133569
1 -1.980591 -0.357431 4.711005
1 3.051703 1.722592 1.896418
1 3.330551 2.582704 3.437289
1 3.641563 0.817404 3.317631
1 1.880140 -0.404227 4.562724
1 0.621927 2.923983 2.298193
1 -1.622850 1.709492 3.439893
1 -1.969146 -4.196519 -3.042971
1 -0.907528 -5.562452 -2.670578
1 -0.767293 -0.489866 0.692339
1 1.016167 -0.693596 0.595230
1 0.085923 -0.189232 -0.842780
1 -1.511437 -2.035467 -1.921003
1 1.266326 -3.189574 1.062862
1 0.295343 -5.454589 -0.209604
1 2.011144 1.999094 -4.886918
1 0.576410 1.347668 -4.034874
1 1.536451 2.643028 -3.279375
1 4.452970 -0.983539 -0.084556

1 5.014246 0.652730 -0.409659
1 3.498551 1.950472 -1.840395
1 3.592131 -2.223673 -2.545361
1 1.697508 -1.045214 -4.222536
1 6.835625 -1.072158 -0.483801
1 6.031723 -1.896627 -1.802208
1 -1.185679 -2.328866 6.025027
1 0.483291 -1.953852 5.650631
1 -3.198489 -6.265465 -2.297673
1 -2.391771 -6.200847 -0.736818
1 -1.788517 3.537621 1.164414
1 -1.203339 4.662582 -0.056810
6 -5.046279 -5.424227 -0.394086
1 -3.469579 -3.953911 -0.286654
1 -4.260063 -4.034046 -1.856724
1 -0.938992 5.510768 2.274099
6 -1.998597 7.047238 1.200123
1 -2.679629 5.463013 2.519200
6 -0.328699 -4.174321 4.165773
1 -1.689467 -2.587401 3.572471
1 0.002783 -2.276788 3.196807
1 7.817693 -0.595492 -2.758304
1 6.319924 0.164195 -3.258026
6 7.461780 1.311907 -1.814415
1 -1.854115 7.786731 1.996418
1 -1.227503 7.223119 0.439743
1 -2.975525 7.252943 0.744351
1 -0.457332 -4.739012 3.235197
1 0.711976 -4.302067 4.484966
1 -0.981120 -4.628074 4.923315
1 -5.817527 -4.740548 -0.022633

1 -5.517359 -6.100229 -1.119067
1 -4.703936 -6.030189 0.454360
1 8.037737 1.863448 -2.566348
1 6.642170 1.965768 -1.492917
1 8.115126 1.149187 -0.947792

[C₄C₁mim][BF₄]

Monomer

6 1.589599 -2.104743 -1.107098
7 1.885142 -1.488904 0.094124
6 0.736627 -1.190903 0.731854
7 -0.279587 -1.626678 -0.039745
6 0.236134 -2.193334 -1.190508
6 3.230065 -1.087337 0.522454
6 -1.716310 -1.418437 0.220902
6 -2.347849 -0.431715 -0.770452
6 -3.823582 -0.136737 -0.450430
6 -4.047137 0.628020 0.861906
9 -0.294463 2.019267 0.488434
5 0.895957 2.066123 -0.298718
9 2.001027 1.778689 0.559458
9 1.043716 3.302075 -0.902051
9 0.819146 1.026709 -1.268707
1 3.456854 -1.516263 1.501750
1 3.942201 -1.474522 -0.207268
1 3.279338 0.003876 0.552755
1 -2.204616 -2.399396 0.174712
1 -1.802261 -1.053019 1.244594
6 0.606231 -0.519579 2.052979
1 -0.398241 -2.589030 -1.967422
1 2.361686 -2.402527 -1.798658
1 -1.763607 0.494149 -0.766161

1 -2.275561 -0.850813 -1.783007
1 -4.225562 0.458595 -1.279943
1 -4.401744 -1.073625 -0.441857
1 -5.101116 0.909109 0.971251
1 -3.782187 0.030445 1.743618
1 -3.446596 1.544738 0.887559
1 0.067240 0.426516 1.933166
1 0.078008 -1.162349 2.767506
1 1.589991 -0.279493 2.456486

Dimer

7 2.661206 -2.116366 1.187897
6 3.051371 -1.290164 0.199132
7 2.597192 -0.057964 0.497526
6 1.903412 -0.100797 1.695209
6 1.942307 -1.391378 2.122522
6 2.789141 1.160115 -0.312276
6 4.078209 1.905370 0.059098
6 4.297109 3.174798 -0.783931
6 3.320269 4.318232 -0.475554
6 2.839849 -3.570637 1.198701
9 0.823528 -1.707257 -2.054730
5 0.265219 -2.904887 -1.522265
9 0.083058 -2.738363 -0.125616
9 -0.983724 -3.133031 -2.132242
9 1.156837 -3.968833 -1.744709
6 -1.902277 0.027116 -2.008183
7 -2.897500 -0.061863 -1.049469
6 -3.324021 1.177654 -0.738952
7 -2.634660 2.048581 -1.499128
6 -1.739176 1.348132 -2.286386
6 -3.360568 -1.331147 -0.450974

6 -2.815559 -1.574721 0.959587
6 -3.296823 -2.926526 1.504570
6 -2.756935 -3.218767 2.909406
6 -2.758543 3.507342 -1.438978
9 -0.022924 2.826081 0.019957
5 -0.574326 2.691267 1.328144
9 -1.454030 3.760814 1.569760
9 -1.292265 1.471707 1.391593
9 0.477320 2.665388 2.265127
1 -4.456713 -1.323941 -0.463084
1 -3.021807 -2.119390 -1.127170
1 -2.036676 3.933889 -2.135276
1 -3.767838 3.809122 -1.734747
1 -2.525324 3.859300 -0.431937
6 -4.331791 1.552262 0.288494
1 -1.052720 1.850806 -2.948232
1 -1.387599 -0.849380 -2.372276
1 3.904771 -3.819959 1.215161
1 2.370097 -3.958554 2.103002
1 2.351611 -4.006827 0.324418
1 2.793544 0.855147 -1.362681
1 1.903392 1.777708 -0.153750
6 3.805465 -1.687632 -1.020995
1 1.425876 0.780923 2.102764
1 1.498723 -1.862164 2.985191
1 -1.722466 -1.559446 0.917743
1 -3.124770 -0.764395 1.631705
1 4.042684 2.171027 1.124146
1 4.935188 1.229227 -0.070278
1 -4.397317 -2.950968 1.524333
1 -2.976966 -3.723084 0.819668

1 5.323854 3.523552 -0.610434
1 4.243427 2.914497 -1.851854
1 3.550307 5.195890 -1.091714
1 2.276551 4.043490 -0.660537
1 3.392486 4.621199 0.576295
1 -3.120091 -4.184512 3.280869
1 -1.660760 -3.252354 2.903870
1 -3.065386 -2.446062 3.625330
1 4.403025 -2.582284 -0.829176
1 3.102618 -1.910643 -1.832381
1 4.479187 -0.888552 -1.340919
1 -4.983220 2.353390 -0.075176
1 -4.955976 0.696350 0.553221
1 -3.818671 1.904299 1.191531

[C₄mim][NO₃]

Monomer

6 -2.094215 -2.514116 -0.038880
7 -2.306678 -1.156805 0.138009
6 -1.153399 -0.504360 -0.065281
7 -0.208897 -1.403658 -0.367547
6 -0.775568 -2.667882 -0.354768
6 -3.569841 -0.492672 0.478907
6 1.203539 -1.063145 -0.647192
6 2.143116 -1.522904 0.473209
6 3.607262 -1.126714 0.206725
6 3.887583 0.377553 0.331867
8 0.552242 2.072853 -0.362950
7 -0.404479 2.868451 -0.090697
8 -1.541309 2.355103 0.205765
8 -0.249053 4.093391 -0.108399

1 -4.317103 -0.710396 -0.288393
1 -3.921210 -0.846796 1.451453
1 -3.385488 0.582423 0.519991
1 1.467855 -1.534401 -1.600407
1 1.222800 0.021409 -0.770041
1 -1.045270 0.589340 0.000308
1 -0.203223 -3.556224 -0.572942
1 -2.885531 -3.240081 0.069149
1 1.807930 -1.080836 1.420900
1 2.073635 -2.614278 0.584722
1 4.239555 -1.671389 0.920156
1 3.903648 -1.482587 -0.791445
1 4.946642 0.586890 0.141384
1 3.297819 0.979525 -0.367382
1 3.652416 0.736144 1.341340

Dimer

7 2.270022 2.488361 0.491767
6 1.343060 2.209323 -0.434850
7 0.150720 2.131516 0.170283
6 0.314699 2.360773 1.525744
6 1.645194 2.590017 1.725282
6 -1.130672 1.879943 -0.520250
6 -1.817001 3.187290 -0.938936
6 -3.171211 2.945951 -1.628890
6 -4.280709 2.457434 -0.686729
6 3.703595 2.633830 0.222157
8 1.251680 0.445401 -2.859659
7 2.285816 -0.234910 -2.575025
8 2.343704 -1.451980 -2.885959
8 3.240630 0.313973 -1.958666
6 -0.436767 -2.443766 -1.996711

7 -0.154706 -2.583909 -0.647445
6 -1.302906 -2.540346 0.045608
7 -2.312098 -2.389664 -0.822052
6 -1.791648 -2.328442 -2.104278
6 1.194597 -2.809315 -0.077305
6 1.555543 -1.826965 1.039669
6 2.942552 -2.144442 1.618265
6 3.339382 -1.193109 2.752777
6 -3.724240 -2.285468 -0.443575
8 -2.499603 -0.186824 1.582498
7 -1.832830 -0.432935 2.640186
8 -1.562303 -1.634812 2.927802
8 -1.438045 0.505642 3.365783
1 1.225811 -3.842026 0.288482
1 1.890710 -2.714335 -0.913985
1 -4.240365 -1.679426 -1.190783
1 -4.176842 -3.280352 -0.402498
1 -3.776398 -1.787585 0.526659
1 -1.410415 -2.532403 1.130112
1 -2.420331 -2.186244 -2.969469
1 0.359575 -2.360412 -2.726034
1 3.966176 3.693908 0.160759
1 4.264972 2.162082 1.031394
1 3.925087 2.122955 -0.716087
1 -0.895347 1.266877 -1.395394
1 -1.740725 1.292634 0.171139
1 1.525919 1.968848 -1.479056
1 -0.503608 2.248376 2.225736
1 2.197891 2.784070 2.631349
1 1.550037 -0.808471 0.630609
1 0.806168 -1.861350 1.840390

1 -1.963228 3.822322 -0.054155
1 -1.150508 3.733827 -1.619750
1 2.949565 -3.177323 1.995643
1 3.691575 -2.097359 0.816399
1 -3.488079 3.886442 -2.098261
1 -3.033585 2.229778 -2.452285
1 -5.217395 2.306053 -1.236756
1 -4.024607 1.514651 -0.190967
1 -4.475851 3.194851 0.102094
1 4.326392 -1.449817 3.155048
1 3.383325 -0.155741 2.397132
1 2.616311 -1.231500 3.576271

[PrAm][NO₃]

Monomer

6 -2.942796 0.106846 0.370401
6 -1.551363 0.177625 -0.268209
7 -0.559087 0.974606 0.488044
8 1.849669 0.831919 -0.583539
7 2.496807 -0.226034 -0.015292
8 1.883302 -0.869035 0.837160
8 3.624842 -0.426971 -0.413871
1 -0.436325 0.587531 1.424620
1 -0.882888 1.935363 0.604339
1 0.893249 0.881407 -0.139259
1 -1.616555 0.609353 -1.274320
1 -1.133494 -0.829626 -0.379579
6 -3.925784 -0.730834 -0.456642
1 -2.853285 -0.317389 1.380871
1 -3.337016 1.126377 0.493010
1 -4.910784 -0.768669 0.021576
1 -4.059112 -0.310940 -1.461476

1 -3.570680 -1.762531 -0.570336

Dimer

7 2.261906 -0.858971 -0.361145

6 2.972080 -1.458308 0.812430

6 3.787403 -0.423166 1.587850

8 1.967164 2.209824 -1.166649

7 0.818803 2.166557 -0.696136

8 0.546638 1.233250 0.180771

8 -0.090013 2.948044 -1.019618

7 -2.163098 0.796048 -0.000063

6 -2.913581 0.807337 1.294379

6 -4.425016 0.681213 1.099617

8 -1.803139 -1.612276 -1.361085

7 -0.700541 -1.908783 -0.816890

8 0.241161 -2.380749 -1.517709

8 -0.527257 -1.697263 0.411364

1 -2.492845 1.524652 -0.638973

1 -2.216770 -0.132759 -0.484502

1 -2.216770 -0.132759 -0.484502

1 -1.135118 0.986766 0.150672

1 -2.512036 -0.024914 1.879044

1 -2.658072 1.743002 1.800537

1 -4.886310 0.827599 2.084943

1 -4.780819 1.513934 0.474831

6 -4.884043 -0.659665 0.511616

1 2.910312 -0.494980 -1.062897

1 1.653077 -0.046531 -0.073548

1 1.621239 -1.556186 -0.816147

1 2.191176 -1.901667 1.434744

1 3.608021 -2.264514 0.431135

1 4.223174 -0.944880 2.449774
6 4.899636 0.250908 0.773030
1 3.109180 0.338083 1.994002
1 -5.976654 -0.688310 0.436920
1 -4.480397 -0.839208 -0.490904
1 -4.567140 -1.496640 1.144884
1 5.506525 0.896552 1.416823
1 5.572365 -0.489702 0.320296
1 4.496295 0.889188 -0.022116

Trimer

7 3.374674 -0.180813 1.282951
6 4.819541 0.046534 0.969297
6 5.121167 -0.277302 -0.493548
7 -1.423110 2.852525 0.647458
6 -2.156370 3.889029 -0.145126
6 -1.272780 4.557894 -1.198223
8 1.473092 1.555202 0.054605
7 0.937690 0.779205 -0.802331
8 -0.318967 0.874683 -1.005281
8 1.614017 -0.054569 -1.414917
8 0.777499 -1.508671 1.270532
7 1.262634 -2.549702 0.753746
8 0.517564 -3.388646 0.190029
8 2.518204 -2.740029 0.792970
7 -1.697145 -1.734257 -0.518221
6 -2.340000 -2.258318 -1.763262
6 -2.930072 -3.655705 -1.566742
8 -3.427680 -0.800904 1.590281
7 -3.306304 0.404181 1.260925
8 -3.115853 1.293729 2.149910
8 -3.332383 0.740013 0.045330

1 -0.961006 -2.382866 -0.162450
1 -2.391668 -1.560511 0.236092
1 -1.236402 -0.826859 -0.704815
1 -3.106935 -1.532778 -2.050251
1 -1.563761 -2.268878 -2.533669
1 -3.256984 -4.003201 -2.555731
1 -2.132414 -4.340534 -1.249130
6 -4.108606 -3.720020 -0.586134
1 3.073371 -1.179963 1.084154
1 2.746208 0.451750 0.738092
1 3.161803 -0.016844 2.269741
1 5.050583 1.091869 1.201004
1 5.402786 -0.590896 1.642141
6 6.599398 -0.044559 -0.825626
1 4.849094 -1.321058 -0.692626
1 4.483551 0.337770 -1.139362
1 -0.650427 3.248086 1.186276
1 -1.009483 2.117695 0.022418
1 -2.087181 2.354476 1.302111
1 -2.997402 3.362544 -0.601483
1 -2.553831 4.620286 0.567054
1 -1.917290 5.243475 -1.763366
6 -0.076126 5.330873 -0.627594
1 -0.925617 3.799435 -1.911345
1 -4.507384 -4.739596 -0.538471
1 -3.822151 -3.432673 0.431449
1 -4.921990 -3.053683 -0.898285
1 0.451134 5.865255 -1.425310
1 -0.396287 6.075182 0.113644
1 0.657557 4.665466 -0.155976
1 6.798273 -0.281485 -1.876003

1 6.889750 1.000796 -0.660217

1 7.254177 -0.677247 -0.213323

Tetramer

7 2.233941 -1.505434 -0.798957

6 3.539175 -2.177371 -1.074443

6 3.522312 -2.896403 -2.422681

8 3.210146 1.527163 2.863744

7 2.614632 0.537022 2.433270

8 2.299467 -0.437205 3.173921

8 2.271636 0.485598 1.187995

7 0.908290 2.807892 0.279749

6 1.430036 4.209913 0.229042

6 2.420209 4.424536 -0.916090

8 1.528778 0.830899 -2.213381

7 0.288794 0.774651 -2.462059

8 -0.465838 1.696034 -1.987861

8 -0.201596 -0.151065 -3.123459

7 -0.482985 -0.716478 2.641683

6 -1.281489 -1.377592 3.720858

6 -0.845240 -2.820736 3.976885

8 -0.711045 -1.308588 -0.120972

7 -0.960249 -2.366135 -0.794058

8 -2.081981 -2.504831 -1.327824

8 -0.062466 -3.237519 -0.914350

7 -2.921920 0.289284 -1.444337

6 -4.020649 0.560773 -2.421679

6 -5.267021 -0.281187 -2.144586

8 -2.935715 0.937706 1.387728

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8 -1.143897 1.979630 2.092070

8 -2.351902 2.843334 0.488991

1 -2.648884 -0.714052 -1.436517
1 -3.169394 0.544619 -0.471029
1 -2.067592 0.833876 -1.688099
1 -4.239707 1.631653 -2.365800
1 -3.611134 0.343637 -3.411988
1 -5.954870 -0.119339 -2.984661
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6 -5.979902 0.053963 -0.827741
1 1.442541 -2.182376 -0.774611
1 2.009161 -0.787711 -1.519701
1 2.241430 -0.976666 0.097271
1 4.314082 -1.405030 -1.043269
1 3.725062 -2.876713 -0.252867
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1 3.298771 -2.170686 -3.215611
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1 0.539804 -0.733601 2.844134
1 -0.766503 0.283490 2.531920
1 -1.152161 -0.767851 4.619701
1 -2.330311 -1.317672 3.415885
1 -1.402874 -3.167209 4.856702
6 -1.089762 -3.781211 2.805816
1 0.215331 -2.831508 4.262979
1 1.635812 2.106638 0.522346
1 0.483399 2.510416 -0.624833
1 0.164542 2.705778 0.999211
1 0.558269 4.861432 0.121218
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1 2.667145 5.494417 -0.922160
6 3.706313 3.596139 -0.807479

1 1.918343 4.216005 -1.870180
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1 4.398725 3.863978 -1.613376
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1 3.504976 2.523328 -0.893940
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1 -0.488863 -3.532011 1.923844
1 4.827382 -4.099274 -3.681097
1 5.686239 -2.872305 -2.737994
1 5.090624 -4.344545 -1.948427



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