

Supplementary Information:

The anion dependence of the interaction strength between ions in imidazolium-based ionic liquids probed by far infrared spectroscopy

Koichi Fumino,^a Kai Wittler,^a and Ralf Ludwig^{*ab}

^a Universität Rostock, Institut für Chemie, Abteilung für Physikalische Chemie, Dr.-Lorenz-Weg 1, 18059 Rostock, Germany. Fax: 49 381 498 6524; Tel: 49 381 498 6517; E-mail: ralf.ludwig@uni-rostock.de

^b Faculty of Interdisciplinary Research, Department „Science and Technology of Life, Light and Matter“, University of Rostock, Rostock, Germany.

^c Leibniz-Institut für Katalyse an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059

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1. Ionic Liquids (ILs) under investigation

The following imidazolium-based ionic liquids have been investigated:

1-ethyl-3-methyl-imidazolium dicyanamide	[C ₂ mim][N(CN) ₂]	(I)
1-ethyl-3-methyl-imidazolium thiocyanate	[C ₂ mim][SCN]	(II)
1-ethyl-3-methyl-imidazolium nitrate	[C ₂ mim][NO ₃]	(III)
1-ethyl-3-methyl-imidazolium acetate	[C ₂ mim][CH ₃ COO]	(IV)

2. FTIR measurements on imidazolium-based ionic liquids I-IV

The FTIR measurements were performed with a Bruker Vertex 70 FTIR spectrometer equipped with an extension for measurements in the FIR region that consists a multilayer mylar beam splitter and a room temperature DLATGS detector with preamplifier. The accessible spectral region for this configuration lies between 30 and 680 cm⁻¹ (0.3 and 20.3 THz). Further improvement could be achieved by using a high pressure mercury lamp and an silica beam splitter. This configuration allowed measurements down to 10 cm⁻¹ and significantly better signal-to-noise ratios.

Table 1. Masses of cations and anions, reduced masses and their square roots of ion-pairs in the ILs I-IV. The masses are all given in atomic mass units (AMUs). Additionally, the correction factors for the measured frequencies due to different reduced masses are given relative to IL II.

IL	cation	anion	μ	(μ) ^{1/2}	correction factor
I	111,09	66,01	41.406	6.435	1.043
II	111,09	57,97	38.092	6.172	1
III	111,09	62,01	39.796	6.308	1.022
IV	111,09	59,01	38.539	6.208	1.006

3. DFT calculation on ion-pair clusters for the ILs I-IV

The binding energies of ion-pair clusters n=1-4 for all four ILs were calculated at the DFT level B3LYP, using the internal stored 6-31+G* basis set of the Gaussian 09 program.^[SI1] Afterwards they were corrected for the basis set superposition error (BSSE).^[SI2]
*[SI2] = [50] in the manuscript

Table SI2. DFT calculated binding energies per ion of ion-pair monomers, dimers, trimers and tetramers of the ILs I-IV. The energies are given in kJmol⁻¹.

IL	monomer	dimer	trimer	tetramer
I	-159.5	-186.3	-191.2	-198.9
II	-170.4	-193.0	-199.6	-207.4
III	-180.7	-204.0	-215.0	-220.4
IV	-205.4	-221.5	-227.3	-232.5

4. DFT calculated Frequencies of ion-pair clusters of the ILs I-IV.

All optimized clusters were found to have only positive frequencies, demonstrating that they are all true equilibrium species on the B3LYP/6-31+G* potential-energy surface. The measured FIR spectra are nicely reproduced by the DFT (B3LYP/6-31+G*) calculated frequencies obtained for IL clusters including four ion-pairs. Here, we would like to focus in detail on the spectra for the IL [C₂mim][CH₃COO]. In Figure SI1 the measured and calculated spectra are shown between 20 and 600 cm⁻¹. All the spectral features are reproduced in the DFT calculated spectrum, the intramolecular frequencies above as well as the intermolecular frequencies below 150 cm⁻¹.

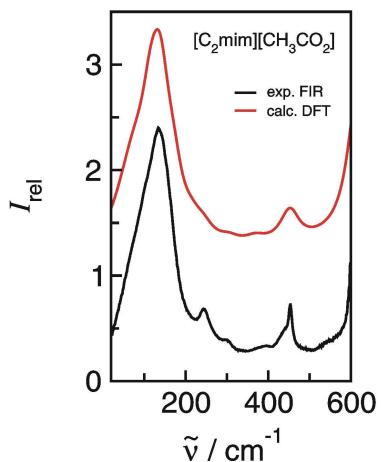


Fig. SI1 Recorded FIR (bottom) and calculated DFT (top) low frequency spectra between 20 and 600 cm⁻¹ of [C₂mim][CH₃COO]. The calculated spectrum of an ion-pair tetramer for this IL was obtained by using half-widths of about 20 cm⁻¹. The frequencies were not corrected for the harmonic approximation. All spectral features are reproduced by the DFT frequencies.

5. DFT calculated energies and far infrared frequencies of ion-pairs for IIs I-IV with and without including dispersion forces

B3LYP/6-31+G*				
Anion	SP Cation	SP Anion	Total	Energies per ion-pair in Hartrees (and per ion in kJ mol^{-1})
N(CN) ₂	-344.32739	-240.38113	-584.83193	-0.12341 (-162.08)
SCN	-344.32729	-491.00052	-835.45952	-0.13171 (-172.90)
NO ₃	-344.32696	-280.25536	-624.72301	-0.14069 (-184.69)
CO ₂ CH ₃	-344.32552	-228.41592	-572.90262	-0.16118 (-211.69)

Table SI3: Energies of cations, anions and ion-pairs along with binding energies calculated at B3LYP level of theory given per ion-pair in Hartrees and per ion in kJ mol^{-1} , respectively.

B3LYP-D3/6-31+G*				
Anion	SP Cation	SP Anion	Total	Energies per ion-pair in Hartrees (and per ion in kJ mol^{-1})
N(CN) ₂	-344.33758	-240.38243	-584.85729	-0.13728 (-180.21)
SCN	-344.33719	-491.00114	-835.48057	-0.14694 (-186.72)
NO ₃	-344.33848	-280.25567	-624.74109	-0.14694 (-192.90)
CO ₂ CH ₃	-344.33744	-228.41838	-572.92254	-0.16672 (-218.86)

Table SI4: Energies of cations, anions and ion-pairs along with binding energies calculated at B3LYP level of theory given per ion-pair in Hartrees and per ion in kJ mol^{-1} , respectively.

	N(CN) ₂	SCN	NO ₃	CO ₂ CH ₃
B3LYP-g09	149.1	173.5	165.4	189.2
B3LYP	148.9	176.4	165.0	190.3
B3LYP-D3	146.3	172.4	165.9	192.9

Table SI5: Calculated intermolecular frequencies in cm^{-1} of the various ion-pairs from three kinds of calculations: the conventional B3LYP/6-31+G* level of theory as implemented in GAUSSIAN09 [59] and TURBOMOLE,[60] and the B3LYP/6-31+G*/D3 as implemented in TURBOMOLE.[60,61]

6. Literature

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7. Geometries of the DFT calculated ion-pair clusters for the ILs I-IV with Gaussian09

[C₂mim][N(CN)₂]

Monomer

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7	0	-.852276	1.716201	.043399
6	0	-2.178074	1.763543	-.345150
6	0	-2.593374	.474576	-.514149
7	0	-1.516823	-.343424	-.228283
6	0	-.475618	.430945	.108450
6	0	-1.514062	-1.826843	-.266801
6	0	-.000530	2.878862	.347544
7	0	2.712711	-.737984	.516648
6	0	2.888192	.507005	.138268
6	0	-1.858813	-2.436271	1.090572
1	0	-2.243001	-2.109997	-1.031213
1	0	-.519161	-2.141275	-.603620
1	0	-.223053	3.666260	-.375272
1	0	-.215484	3.230985	1.360090
1	0	1.052260	2.586960	.257148
1	0	.507360	.076030	.390607
1	0	-2.699218	2.699152	-.477122
1	0	-3.546491	.073738	-.822939
1	0	-1.854613	-3.527282	.997673
1	0	-1.112493	-2.164841	1.844404
1	0	-2.848447	-2.123707	1.443639
6	0	2.182981	-1.625981	-.293462
7	0	1.645793	-2.475906	-.910473
7	0	3.010327	1.660965	-.074865

Dimer

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7	0	2.722503	-1.376910	0.380611
6	0	3.541745	-0.963283	-.653521
6	0	3.538159	0.400448	-.646689
7	0	2.716084	0.800528	0.390427
6	0	2.235582	-0.292355	0.997893
6	0	2.365289	2.198378	0.724063
6	0	2.372367	-2.771256	0.684157
7	0	-0.201523	-0.270695	3.074120
6	0	-0.732401	-1.418977	2.712917
6	0	3.522428	2.940273	1.390164
1	0	2.057567	2.664291	-.216561
1	0	1.489927	2.157564	1.377386
1	0	1.998015	-3.230747	-0.234049
1	0	3.256986	-3.296911	1.053276
1	0	1.586806	-2.782192	1.441741
1	0	1.546453	-0.295771	1.840149
1	0	4.003409	-1.667560	-1.327224
1	0	3.997089	1.111431	-1.314937
1	0	3.207099	3.965346	1.612057
1	0	3.815372	2.462476	2.331450
1	0	4.400630	2.993127	0.736984
6	0	-0.757565	0.868999	2.722604
7	0	-1.141061	1.942120	2.422032
7	0	-1.088460	-2.498742	2.402188
7	0	-2.721957	-1.377632	-0.380307
6	0	-3.541437	-0.964103	0.653677
6	0	-3.538420	0.399628	0.646515
7	0	-2.716468	0.799804	-0.390663
6	0	-2.235522	-0.293019	-0.997873
6	0	-2.366113	2.197723	-0.724504
6	0	-2.371347	-2.771899	-0.683641
7	0	0.201659	-0.271403	-3.074049
6	0	0.733170	-1.419337	-2.712677
6	0	-3.523618	2.939248	-1.390378
1	0	-2.058279	2.663795	0.216005
1	0	-1.490914	2.157068	-1.378056
1	0	-1.997089	-3.231212	0.234688

1	0	-3.255711	-3.297840	-1.052966
1	0	-1.585576	-2.782680	-1.441013
1	0	-1.546319	-0.296430	-1.840063
1	0	-4.002854	-1.668413	1.327516
1	0	-3.997665	1.110576	1.314583
1	0	-3.208608	3.964375	-1.612471
1	0	-3.816696	2.461268	-2.331529
1	0	-4.401658	2.991961	-0.736967
6	0	0.757150	0.868646	-2.722794
7	0	1.140135	1.942034	-2.422527
7	0	1.089833	-2.498848	-2.401756

Trimer

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7	0	5.950538	-2.176823	0.574262
6	0	5.071677	-3.162256	0.994429
6	0	3.841410	-2.848635	0.491285
7	0	3.991595	-1.675061	-0.228513
6	0	5.272293	-1.291460	-0.166719
6	0	2.918683	-0.971756	-0.970519
6	0	7.382119	-2.078032	0.885588
6	0	2.916685	-1.341081	-2.453311
1	0	1.983383	-1.269159	-0.492216
1	0	3.067513	0.102053	-0.823781
1	0	7.744592	-1.112843	0.523450
1	0	7.517681	-2.141660	1.967976
1	0	7.920381	-2.894183	0.396130
1	0	5.718601	-0.402056	-0.596850
1	0	5.391162	-3.982272	1.618904
1	0	2.866117	-3.308554	0.599225
1	0	2.100298	-0.807851	-2.952031
1	0	3.854228	-1.053597	-2.942143
1	0	2.759162	-2.415962	-2.593737
7	0	5.739133	2.981404	-0.586824
6	0	6.549946	1.958768	-0.501107
6	0	4.449840	2.780737	-0.532339
7	0	3.274280	2.671607	-0.496386
7	0	7.321305	1.067319	-0.433795
7	0	-5.004102	-1.777888	0.517677
6	0	-5.732308	-1.615063	-0.645991
6	0	-4.896577	-1.905263	-1.683748
7	0	-3.670349	-2.239509	-1.138736
6	0	-3.759052	-2.151599	0.194485
6	0	-2.441887	-2.555629	-1.899678
6	0	-5.484448	-1.487762	1.873641
7	0	-1.233453	-2.316065	2.098376
6	0	-1.230290	-1.261233	2.888159
6	0	-2.576846	-3.848746	-2.700986
1	0	-2.248302	-1.688337	-2.538385
1	0	-1.632209	-2.633435	-1.169688
1	0	-5.782831	-0.436599	1.909888
1	0	-6.328107	-2.141851	2.108276
1	0	-4.671114	-1.671924	2.577111
1	0	-2.944987	-2.326247	0.898088
1	0	-6.751915	-1.263886	-0.633140
1	0	-5.052797	-1.856841	-2.749389
1	0	-1.636723	-4.037536	-3.229818
1	0	-2.779056	-4.705085	-2.048484
1	0	-3.373036	-3.783442	-3.450756
6	0	-0.195258	-2.643126	1.369357
7	0	0.648129	-3.026491	0.639301
7	0	-1.366330	-0.339628	3.606714
7	0	-1.595485	2.706219	1.837856
6	0	-0.269084	2.604938	2.218937
6	0	0.490463	2.807853	1.102368
7	0	-0.389232	3.020741	0.054456
6	0	-1.642962	2.958341	0.523203
6	0	-0.008729	3.285099	-1.351737
6	0	-2.752015	2.551870	2.730403
7	0	-4.179522	2.207334	-1.325933
6	0	-4.966852	1.790359	-0.360415
6	0	-0.099602	4.770089	-1.700866
1	0	1.016502	2.924119	-1.456470
1	0	-0.667731	2.682036	-1.983398
1	0	-2.590039	1.658509	3.337761

1	0	-2.840557	3.438363	3.364978
1	0	-3.655625	2.434398	2.128866
1	0	-2.544674	3.043344	-0.074998
1	0	0.006116	2.351567	3.230500
1	0	1.559550	2.792737	0.926191
1	0	0.207972	4.911846	-2.742541
1	0	-1.122395	5.148509	-1.594994
1	0	0.567098	5.363630	-1.066649
6	0	-3.537372	1.341704	-2.081113
7	0	-2.893278	0.652558	-2.787594
7	0	-5.658555	1.523353	0.556596

Tetramer

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7	0	1.898759	1.079970	-3.491070
6	0	1.925210	2.316074	-2.867262
6	0	3.113413	2.396078	-2.197403
7	0	3.790871	1.210742	-2.425277
6	0	3.037364	0.431242	-3.211665
6	0	5.134090	0.873209	-1.907784
6	0	0.804454	0.571357	-4.331873
7	0	3.206473	-2.834161	-2.933160
6	0	1.901539	-2.916943	-3.013199
6	0	6.245069	1.362191	-2.836976
1	0	5.201922	1.344112	-0.924149
1	0	5.164124	-0.212304	-1.780668
1	0	-0.091528	1.145327	-4.091826
1	0	1.056858	0.711408	-5.386796
1	0	0.649709	-0.488891	-4.118339
1	0	3.285493	-0.578056	-3.518831
1	0	1.071525	2.978525	-2.927653
1	0	3.517785	3.146175	-1.534090
1	0	7.215996	1.097590	-2.404208
1	0	6.176612	0.898412	-3.827441
1	0	6.213798	2.450548	-2.955429
6	0	3.822309	-2.824717	-1.774207
7	0	4.475435	-2.768437	-0.794785
7	0	0.738927	-2.942922	-3.209278
7	0	-4.281581	2.365486	1.219949
6	0	-3.606950	2.130635	2.405517
6	0	-2.396884	2.757694	2.311236
7	0	-2.353492	3.361172	1.065404
6	0	-3.504213	3.113296	0.425723
6	0	-1.231878	4.170456	0.540804
6	0	-5.633307	1.887771	0.897013
7	0	-3.667945	2.942135	-2.835707
6	0	-4.318392	1.803600	-2.789416
6	0	-1.389031	5.652803	0.877896
1	0	-0.327649	3.763408	0.997728
1	0	-1.188030	4.002279	-0.538853
1	0	-5.778571	0.933852	1.407448
1	0	-6.371602	2.617725	1.241602
1	0	-5.712723	1.752290	-0.183527
1	0	-3.744770	3.419084	-0.586401
1	0	-4.030724	1.494574	3.167815
1	0	-1.540662	2.800073	2.972284
1	0	-0.532559	6.204328	0.475336
1	0	-2.300318	6.070969	0.435828
1	0	-1.414924	5.810408	1.961076
6	0	-2.369015	2.985486	-3.001883
7	0	-1.205531	3.147618	-3.103472
7	0	-5.001212	0.848375	-2.687202
7	0	1.902525	-1.071646	3.496557
6	0	1.934078	-2.308563	2.874624
6	0	3.122049	-2.384129	2.203828
7	0	3.794252	-1.195340	2.429305
6	0	3.037935	-0.418097	3.215189
6	0	5.135775	-0.852772	1.910740
6	0	0.806432	-0.565962	4.336901
7	0	3.191804	2.842495	2.931632
6	0	1.886623	2.926258	3.007207
6	0	6.249230	-1.336405	2.839784
1	0	5.204935	-1.324192	0.927447
1	0	5.161345	0.232741	1.782661

1	0	-0.084081	-1.152625	4.107329
1	0	1.065241	-0.691372	5.392051
1	0	0.638495	0.489917	4.112176
1	0	3.281635	0.592858	3.520806
1	0	1.083794	-2.975202	2.937214
1	0	3.529287	-3.133364	1.541304
1	0	7.218854	-1.068334	2.406232
1	0	6.179457	-0.871929	3.829829
1	0	6.222371	-2.424760	2.959347
6	0	3.812292	2.838687	1.775153
7	0	4.469171	2.785782	0.798052
7	0	0.723440	2.952385	3.199729
7	0	-4.265193	-2.389009	-1.220386
6	0	-3.592877	-2.148714	-2.406216
6	0	-2.376627	-2.763471	-2.311439
7	0	-2.327278	-3.365060	-1.064787
6	0	-3.480350	-3.128154	-0.425393
6	0	-1.197221	-4.160757	-0.538138
6	0	-5.621533	-1.924618	-0.897568
7	0	-3.650080	-2.963690	2.831265
6	0	-4.306505	-1.828287	2.791632
6	0	-1.304472	-5.634571	-0.927591
1	0	-0.292500	-3.715331	-0.956661
1	0	-1.186102	-4.026976	0.547041
1	0	-5.775171	-0.970565	-1.405250
1	0	-6.352846	-2.660303	-1.244849
1	0	-5.703153	-1.793079	0.183278
1	0	-3.717202	-3.434237	0.587613
1	0	-4.022773	-1.517484	-3.169070
1	0	-1.520281	-2.798958	-2.972802
1	0	-0.444877	-6.176471	-0.518675
1	0	-2.216381	-6.090398	-0.525879
1	0	-1.295141	-5.756396	-2.015530
6	0	-2.352891	-3.002140	3.012423
7	0	-1.189800	-3.159531	3.124823
7	0	-4.993685	-0.875878	2.692344

[C₂mim] [SCN]

Monomer

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7	0	1.143830	0.839089	-0.281659
6	0	2.520934	0.693659	-0.299129
6	0	2.787178	-0.633182	-0.118106
7	0	1.567953	-1.275855	0.010623
6	0	0.592345	-0.365804	-0.092702
6	0	1.332798	-2.712863	0.221238
6	0	0.379123	2.100263	-0.413731
7	0	-1.972004	-2.086377	0.310699
6	0	-2.525828	-1.059190	0.097495
16	0	-3.153731	0.442704	-0.217965
1	0	1.728920	-3.271972	-0.630123
1	0	1.831925	-3.027591	1.141006
1	0	0.252159	-2.865515	0.305894
6	0	0.485117	2.970516	0.836611
1	0	0.762305	2.615248	-1.300270
1	0	-0.660925	1.808258	-0.596837
1	0	-0.465902	-0.601130	-0.028155
1	0	3.184733	1.532507	-0.440620
1	0	3.724170	-1.166693	-0.073786
1	0	-0.094641	3.886235	0.681077
1	0	0.067933	2.452821	1.706190
1	0	1.520558	3.256181	1.055370

Dimer

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7	0	-3.020306	-1.351266	0.547893
6	0	-3.712981	-0.239134	0.092830
6	0	-3.079754	0.865072	0.584802
7	0	-2.012692	0.409298	1.337886
6	0	-1.994600	-0.927079	1.298110

6	0	-1.041863	1.245574	2.059116
6	0	-3.323780	-2.763406	0.243733
6	0	0.991431	-2.165609	0.905925
16	0	0.589291	-3.364007	-0.171379
7	0	1.225320	-1.289080	1.667334
7	0	3.461903	0.694532	-0.151146
6	0	4.067670	-0.476637	-0.575148
6	0	3.263216	-1.018427	-1.532479
7	0	2.184290	-0.167153	-1.679851
6	0	2.318762	0.856482	-0.829140
6	0	1.029569	-0.368963	-2.561487
6	0	3.934279	1.584789	0.924577
7	0	-0.068004	2.706123	-0.925565
6	0	-1.054677	3.358599	-0.835369
16	0	-2.447959	4.224923	-0.659784
1	0	1.369423	-0.419679	-3.599397
1	0	0.535935	-1.301326	-2.273786
1	0	0.354680	0.479385	-2.432404
6	0	4.043816	0.861053	2.266617
1	0	4.896321	2.006157	0.612572
1	0	3.213447	2.404368	0.977138
1	0	1.586573	1.663183	-0.728585
1	0	4.992196	-0.833137	-0.149985
1	0	3.343203	-1.940813	-2.085527
1	0	-0.676943	2.012551	1.373536
1	0	-1.532107	1.703676	2.922033
1	0	-0.215005	0.605213	2.371433
1	0	-4.308184	-2.987717	0.668620
6	0	-3.277431	-3.059819	-1.253250
1	0	-2.572431	-3.359502	0.766717
1	0	-1.235879	-1.546346	1.753410
1	0	-4.576743	-0.322609	-0.547536
1	0	-3.248583	1.924479	0.417857
1	0	4.287415	1.590313	3.047243
1	0	3.103802	0.359339	2.514519
1	0	4.839311	0.107818	2.254404
1	0	-3.512220	-4.117654	-1.412883
1	0	-4.006610	-2.464709	-1.813719
1	0	-2.274438	-2.869798	-1.645938

Trimer

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7	0	-2.560472	-0.461550	2.240028
6	0	-1.183529	-0.519465	2.374327
6	0	-0.756712	-1.581526	1.630760
7	0	-1.879617	-2.154637	1.056610
6	0	-2.958490	-1.459923	1.440416
6	0	-1.890066	-3.331192	0.160364
6	0	-3.442590	0.539545	2.852468
7	0	-4.261738	-1.738063	-1.693967
6	0	-5.028164	-1.095748	-1.058125
16	0	-6.040363	-0.184816	-0.112957
6	0	-1.694475	-0.581245	-3.348732
7	0	-1.832709	0.671642	-2.591309
6	0	-3.014651	1.346501	-2.348250
6	0	-2.695005	2.454351	-1.619046
7	0	-1.324019	2.434463	-1.421800
6	0	-0.824785	1.342812	-2.018274
6	0	-0.533381	3.448886	-0.696668
7	0	1.626454	-0.547161	-1.955099
6	0	1.881864	-1.470350	-1.257825
16	0	2.277713	-2.741359	-0.272483
16	0	-0.196946	2.992887	3.135055
6	0	0.994827	2.350951	2.183770
7	0	1.836676	1.876242	1.497849
6	0	4.180746	0.246316	0.325965
7	0	5.042604	0.069270	-0.684342
6	0	6.182793	-0.541195	-0.189920
6	0	5.989932	-0.726788	1.146529
7	0	4.739961	-0.219729	1.448951
6	0	4.800916	0.467758	-2.087760
6	0	4.073233	-0.268579	2.754481
1	0	5.442558	1.330028	-2.301469
6	0	5.052287	-0.675612	-3.067125
1	0	3.754779	0.774547	-2.138668

1	0	3.238742	0.435544	2.732816
1	0	3.706892	-1.283211	2.932634
1	0	4.788198	0.018541	3.528790
1	0	3.205535	0.722568	0.289693
1	0	6.622587	-1.174524	1.897263
1	0	7.019875	-0.793877	-0.820559
6	0	-0.353393	4.728868	-1.510893
1	0	-1.038654	3.641884	0.253595
1	0	0.425004	2.987057	-0.450408
1	0	-2.460606	-1.276569	-2.994989
1	0	-1.833291	-0.373488	-4.413735
1	0	-0.690674	-0.972547	-3.174599
1	0	0.205502	0.993887	-1.998468
1	0	-3.969467	0.954588	-2.661557
1	0	-3.322851	3.226881	-1.203318
1	0	-2.651007	-3.137642	-0.601878
1	0	-0.907160	-3.355956	-0.317835
6	0	-2.161465	-4.629158	0.920332
1	0	-3.688574	0.239880	3.875141
1	0	-2.913734	1.494921	2.868502
1	0	-4.351059	0.612642	2.249920
1	0	-3.977552	-1.625202	1.120520
1	0	-0.645436	0.233934	2.932127
1	0	0.237058	-1.948984	1.408167
1	0	-2.138605	-5.467731	0.215905
1	0	-1.402843	-4.809369	1.689995
1	0	-3.148850	-4.614615	1.395050
1	0	4.813205	-0.329074	-4.077995
1	0	6.098407	-1.002407	-3.066411
1	0	4.408148	-1.528638	-2.837442
1	0	0.237997	5.442106	-0.926976
1	0	0.174389	4.532526	-2.451053
1	0	-1.314327	5.200332	-1.745805

Tetramer

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7	0	5.959271	-3.478380	-0.174097
6	0	4.822307	-4.198102	-0.510064
6	0	3.792473	-3.700900	0.234513
7	0	4.319034	-2.683753	1.011211
6	0	5.624753	-2.566499	0.748620
6	0	3.579337	-1.830480	1.952936
6	0	7.290923	-3.602484	-0.797623
7	0	6.355780	0.223179	1.814222
6	0	6.654643	0.619498	0.738592
16	0	7.035407	1.129131	-0.794660
6	0	0.715660	-1.976226	-0.208587
16	0	0.057595	-3.379729	0.388746
7	0	1.188541	-0.971183	-0.617333
6	0	1.953490	3.405424	-0.399719
7	0	3.066126	2.710380	-0.671257
6	0	4.097433	3.194293	0.112762
6	0	3.578322	4.204217	0.870102
7	0	2.240659	4.324748	0.533294
6	0	3.176774	1.608596	-1.644513
6	0	1.277703	5.283374	1.113720
6	0	-1.747992	-0.519291	-2.405996
6	0	-2.152484	0.763791	-2.633569
7	0	-3.533646	0.743963	-2.736616
6	0	-3.960768	-0.517217	-2.572464
7	0	-2.892074	-1.299172	-2.370337
6	0	-2.954717	-2.751697	-2.158265
6	0	-4.402495	1.918271	-2.963635
7	0	-6.395249	-1.853880	-1.488793
6	0	-7.012674	-2.321296	-0.592327
16	0	-7.851130	-2.950209	0.688784
16	0	-1.436547	4.213461	-1.434500
6	0	-1.999905	3.433666	-0.076656
7	0	-2.389984	2.869676	0.886055
6	0	-3.838671	0.353142	2.025563
7	0	-2.847513	-0.536739	2.162317
6	0	-3.397340	-1.805079	2.239401
6	0	-4.752217	-1.664331	2.144296
7	0	-5.004503	-0.309051	2.012542
6	0	-1.411989	-0.198340	2.245623

6	0	-6.335769	0.302949	1.910744
1	0	-2.691523	-3.268198	-3.085778
1	0	-2.247089	-3.027658	-1.372393
1	0	-3.974886	-3.007524	-1.865236
6	0	-5.360979	2.168074	-1.800841
1	0	-3.731364	2.769003	-3.099999
1	0	-4.947296	1.751647	-3.898432
1	0	-4.990854	-0.869100	-2.497241
1	0	-1.600319	1.692239	-2.673996
1	0	-0.763663	-0.921643	-2.213225
1	0	2.900106	1.978560	-2.635184
1	0	4.218997	1.282377	-1.652271
1	0	2.524331	0.782758	-1.346467
1	0	1.774375	6.258642	1.128388
1	0	0.433473	5.338530	0.421299
6	0	0.816156	4.870481	2.510718
1	0	0.979334	3.287571	-0.864530
1	0	4.042664	4.840187	1.607666
1	0	5.096090	2.779874	0.041202
6	0	-0.930629	-0.114227	3.693895
1	0	-0.874449	-0.972298	1.693877
1	0	-1.289784	0.755181	1.727332
1	0	-7.016686	-0.425767	1.464475
1	0	-6.691976	0.576784	2.907912
1	0	-6.270614	1.192741	1.282749
1	0	-3.681227	1.416867	1.877320
1	0	-5.557755	-2.387508	2.090001
1	0	-2.776192	-2.684930	2.311608
1	0	2.754616	-1.359008	1.414897
1	0	3.193511	-2.445787	2.769165
1	0	4.269068	-1.072020	2.328703
6	0	7.390764	-2.834780	-2.115788
1	0	8.015968	-3.226642	-0.071148
1	0	7.478885	-4.671831	-0.934422
1	0	6.264215	-1.803377	1.184665
1	0	4.843315	-4.989788	-1.243011
1	0	2.740817	-3.959233	0.273420
1	0	-5.979207	3.042626	-2.031395
1	0	-6.025999	1.312986	-1.637923
1	0	-4.801239	2.378402	-0.883940
1	0	0.136892	0.131899	3.702717
1	0	-1.464848	0.666265	4.246960
1	0	-1.061165	-1.067450	4.218071
1	0	0.128651	5.630090	2.897802
1	0	0.277746	3.918558	2.477667
1	0	1.657391	4.783275	3.207531
1	0	8.392005	-2.975815	-2.537843
1	0	6.658918	-3.199102	-2.845277
1	0	7.233813	-1.762321	-1.956734

[C₂mim] [NO₃]

Monomer

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C	2.748814	-1.009099	0.028816
N	1.414657	-1.398111	0.055169
C	0.652569	-0.317332	-0.141076
N	1.440808	0.751481	-0.293116
C	2.763388	0.338558	-0.185390
C	0.879045	-2.753356	0.259131
C	0.941347	2.134556	-0.489624
C	0.455601	2.758658	0.823090
O	-1.968883	0.875253	-0.223549
N	-2.656096	-0.152785	-0.585121
O	-3.877034	-0.088121	-0.720189
O	-2.017656	-1.246996	-0.794789
H	-0.212408	-2.685620	0.256602
H	1.219211	-3.402998	-0.551061
H	1.229311	-3.137867	1.220002
H	1.764267	2.696455	-0.938623
H	0.115181	2.069824	-1.198657
H	-0.445752	-0.311545	-0.149534
H	3.585788	1.032363	-0.276129

H	3.554081	-1.716042	0.161793
H	1.236666	2.728566	1.590775
H	0.185219	3.804903	0.644842
H	-0.437997	2.231722	1.175105

Dimer

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8	0	1.816967	-2.271332	1.240045
7	0	1.363987	-3.018643	0.317888
8	0	1.609515	-2.731771	-0.890133
8	0	0.654886	-4.012485	0.607593
6	0	-1.950868	-2.524642	0.025884
6	0	-2.662262	-2.047580	-1.035422
7	0	-3.054374	-0.756059	-0.723368
6	0	-2.597631	-0.454726	0.499796
7	0	-1.927897	-1.513953	0.973497
6	0	-3.827741	0.164896	-1.577351
6	0	-5.334581	0.039294	-1.353904
6	0	-1.265162	-1.579433	2.285041
8	0	-1.626323	2.349658	-0.504736
7	0	-1.649180	2.817466	0.680441
8	0	-2.504623	2.379319	1.499490
8	0	-0.819360	3.688140	1.027623
6	0	3.473581	1.853143	0.036936
7	0	2.345883	2.514164	-0.256804
6	0	1.404031	1.601018	-0.699755
6	0	1.994531	0.368072	-0.664578
7	0	3.284772	0.549394	-0.200199
6	0	2.135015	3.963128	-0.149899
6	0	4.265834	-0.532022	0.034276
6	0	4.802266	-1.116713	-1.270677
1	0	-3.460100	1.169712	-1.353095
1	0	-3.559893	-0.070585	-2.611745
1	0	-1.761534	-2.333815	2.900604
1	0	-0.212429	-1.843450	2.150204
1	0	-1.352740	-0.600282	2.758750
1	0	-2.705925	0.516951	0.986349
1	0	-1.393935	-3.442222	0.166719
1	0	-2.895379	-2.501579	-1.986111
1	0	2.278663	4.428659	-1.129220
1	0	1.114255	4.130570	0.204263
1	0	2.852643	4.374116	0.563068
1	0	3.740388	-1.291582	0.620665
1	0	5.067288	-0.098589	0.640456
1	0	4.381759	2.298214	0.413667
1	0	1.631862	-0.630773	-0.884468
1	0	0.387743	1.907616	-0.928123
1	0	5.542294	-1.889157	-1.034429
1	0	3.997608	-1.591233	-1.839511
1	0	-5.858269	0.732511	-2.021372
1	0	-5.692360	-0.974913	-1.564756
1	0	-5.601343	0.296656	-0.323466
1	0	5.286494	-0.352264	-1.889770

Trimer

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6	0	3.608707	2.024647	-0.244058
6	0	2.641412	2.522903	-1.068851
7	0	1.502099	2.710734	-0.303503
6	0	1.768749	2.335742	0.954675
7	0	3.040232	1.918764	1.013521
6	0	0.197180	3.207762	-0.785193
6	0	0.230363	4.701338	-1.104835
6	0	3.714636	1.419790	2.218625
8	0	0.547697	0.066740	2.899060
7	0	-0.609169	0.514852	2.687228
8	0	-1.590335	-0.265051	2.572783
8	0	-0.780484	1.769919	2.569629
6	0	-4.839394	-0.097035	2.042554
6	0	-5.143532	-1.221726	1.334132
7	0	-4.788734	-0.980879	0.017805

6	0	-4.288535	0.260783	-0.069804
7	0	-4.321058	0.816591	1.146599
6	0	-4.955670	-1.906671	-1.119402
6	0	-6.384950	-1.907402	-1.661245
6	0	-3.801340	2.148745	1.479502
8	0	-2.392308	-0.499998	-2.529428
7	0	-1.898564	0.669476	-2.562178
8	0	-2.598820	1.647892	-2.168093
8	0	-0.723804	0.845994	-2.959612
8	0	5.904811	0.095124	-1.116502
7	0	5.225239	-0.904246	-0.786519
8	0	4.778069	-1.007437	0.400320
8	0	4.949625	-1.807884	-1.626792
6	0	2.155861	-2.316466	-0.631933
7	0	1.230347	-2.019973	-1.554508
6	0	0.004482	-1.857183	-0.928957
6	0	0.212594	-2.060329	0.404903
7	0	1.559120	-2.346497	0.566908
6	0	1.487504	-1.852953	-2.989397
6	0	2.240084	-2.619580	1.846787
6	0	2.060864	-4.070660	2.293771
1	0	-0.081122	2.613350	-1.659773
1	0	-0.522569	2.987977	0.006502
1	0	4.355554	0.587422	1.920111
1	0	4.312239	2.221930	2.661647
1	0	2.950573	1.084005	2.921663
1	0	1.042632	2.305154	1.763196
1	0	4.613773	1.673023	-0.451764
1	0	2.657236	2.728391	-2.127816
1	0	-4.235324	-1.590087	-1.876964
1	0	-4.665161	-2.900187	-0.764018
1	0	-4.553213	2.685035	2.063946
1	0	-2.865815	2.041845	2.038146
1	0	-3.615983	2.681864	0.545737
1	0	-3.870774	0.727640	-0.963842
1	0	-4.911742	0.117581	3.096995
1	0	-5.558420	-2.165792	1.651687
1	0	1.150547	-2.741484	-3.531212
1	0	0.935091	-0.977539	-3.337668
1	0	2.560748	-1.715552	-3.134074
1	0	1.815470	-1.921245	2.572138
1	0	3.292496	-2.371528	1.690291
1	0	3.221224	-2.427133	-0.831055
1	0	-0.453768	-1.950617	1.249517
1	0	-0.878004	-1.566991	-1.486603
1	0	2.578499	-4.220881	3.247786
1	0	1.003521	-4.318411	2.440592
1	0	-0.758372	5.009398	-1.461199
1	0	0.954494	4.929231	-1.894865
1	0	-6.453064	-2.611646	-2.497521
1	0	-7.110956	-2.213016	-0.899297
1	0	-6.664494	-0.915169	-2.030907
1	0	0.482998	5.297213	-0.220405
1	0	2.485385	-4.768141	1.562990

Tetramer

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6	0	-0.717780	-3.767087	1.065074
6	0	-0.717355	-3.133453	2.275516
7	0	-2.013948	-2.695037	2.501522
6	0	-2.778030	-3.052251	1.460697
7	0	-2.014542	-3.709066	0.578757
6	0	-2.494678	-1.960604	3.687919
6	0	-2.969831	-2.903817	4.793697
6	0	-2.487845	-4.290483	-0.682402
8	0	-4.615946	-1.506142	-0.392402
7	0	-4.471741	-0.320971	0.023452
8	0	-4.617205	0.648512	-0.766085
8	0	-4.164216	-0.112318	1.234830
6	0	-2.800275	2.804092	0.996584
6	0	-2.836013	3.972457	0.294351
7	0	-1.583052	4.554900	0.397663
6	0	-0.804500	3.761796	1.146298
7	0	-1.522168	2.698341	1.523512
6	0	-1.145967	5.824745	-0.208441

6	0	-1.620731	7.041245	0.586610
6	0	-1.037090	1.598273	2.368711
8	0	0.458244	-0.628814	4.028699
7	0	1.532552	-0.574507	3.381425
8	0	2.115964	-1.642736	3.022446
8	0	2.029903	0.542883	3.063033
8	0	1.191499	3.470732	-1.249918
7	0	2.190809	3.974241	-0.641147
8	0	1.998922	4.697413	0.382095
8	0	3.352659	3.728584	-1.033097
6	0	4.266482	-0.580054	1.010376
7	0	4.785820	-1.483286	0.162872
6	0	5.667682	-0.836013	-0.683619
6	0	5.670357	0.481768	-0.328832
7	0	4.790032	0.620660	0.726141
6	0	4.487366	-2.938755	0.200897
6	0	4.683102	-3.614090	-1.150678
6	0	4.474560	1.889114	1.403797
8	0	1.399097	-4.044086	-1.320784
7	0	1.058270	-3.312412	-2.284331
8	0	-0.104380	-3.414609	-2.781569
8	0	1.861949	-2.464256	-2.762021
6	0	-0.511926	-0.451459	-3.393925
7	0	0.104523	0.703195	-3.113052
6	0	-0.835819	1.607548	-2.643210
6	0	-2.042127	0.966014	-2.648824
7	0	-1.816462	-0.316761	-3.119118
6	0	1.543687	0.954552	-3.278629
6	0	-2.843086	-1.357702	-3.326700
6	0	-3.642180	-1.120115	-4.608248
1	0	3.670922	1.698531	2.117214
1	0	5.366816	2.245213	1.926183
1	0	4.165496	2.612252	0.641762
1	0	5.136465	-3.380951	0.965973
1	0	3.450329	-3.034358	0.531576
1	0	3.536902	-0.791241	1.793158
1	0	6.197040	-1.352030	-1.467242
1	0	6.189476	1.329609	-0.748724
1	0	-1.656655	-1.347737	4.026197
1	0	-3.298200	-1.306151	3.341226
1	0	-1.704646	-4.176405	-1.436457
1	0	-2.713080	-5.351058	-0.534707
1	0	-3.389329	-3.756019	-0.986725
1	0	-3.804964	-2.755340	1.292572
1	0	0.084686	-4.185951	0.471971
1	0	0.094872	-2.897098	2.951384
1	0	-0.057199	5.776499	-0.263694
1	0	-1.537728	5.842201	-1.230144
1	0	-1.492928	1.670603	3.358398
1	0	-1.320222	0.650636	1.909335
1	0	0.048378	1.654761	2.464960
1	0	0.249172	3.947242	1.330422
1	0	-3.529819	2.014158	1.128164
1	0	-3.631862	4.421978	-0.279399
1	0	1.737706	1.280145	-4.305240
1	0	1.828451	1.743935	-2.580601
1	0	2.078464	0.026806	-3.075423
1	0	-3.499398	-1.350515	-2.451303
1	0	-2.306529	-2.308501	-3.357466
1	0	-0.024363	-1.373965	-3.685942
1	0	-3.018678	1.264760	-2.295053
1	0	-0.547655	2.594446	-2.309431
1	0	-4.387922	-1.915166	-4.718007
1	0	-4.175575	-0.164373	-4.571232
1	0	-3.305841	-2.312788	5.653019
1	0	-2.159239	-3.559277	5.130120
1	0	-1.282501	7.954110	0.084230
1	0	-2.713420	7.078088	0.661703
1	0	4.032564	-3.164378	-1.905008
1	0	5.730688	-3.590776	-1.476634
1	0	-1.202544	7.036558	1.598881
1	0	-3.808052	-3.525672	4.459330
1	0	4.385270	-4.662672	-1.053809
1	0	-2.995933	-1.130819	-5.493317

[C₂mim] [CH₃COO]

Monomer

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7	0	-1.367395	0.683440	-0.266099
6	0	-0.669920	-0.438006	-0.042123
7	0	-1.540823	-1.455565	0.046701
6	0	-2.828362	-0.972784	-0.124672
6	0	-2.717296	0.373115	-0.319621
6	0	-1.135373	-2.844251	0.281528
6	0	-0.754739	2.023366	-0.415081
6	0	-1.046332	2.920671	0.785848
1	0	-0.567394	3.892764	0.626906
8	0	2.023467	-1.162116	0.185030
6	0	2.702060	-0.104769	-0.050344
6	0	4.226357	-0.250534	-0.011514
8	0	2.207695	1.026695	-0.305366
1	0	-1.570485	-3.204068	1.217850
1	0	-1.470646	-3.472416	-0.548119
1	0	-0.045522	-2.868021	0.345875
1	0	0.322524	1.843486	-0.520230
1	0	-1.146763	2.453880	-1.342751
1	0	0.443507	-0.570811	0.044494
1	0	-3.473194	1.123238	-0.494758
1	0	-3.695121	-1.615568	-0.098025
1	0	-2.119965	3.091262	0.932974
1	0	-0.629784	2.487550	1.701198
1	0	4.544057	-1.011431	-0.734619
1	0	4.720276	0.698554	-0.236314
1	0	4.538369	-0.601005	0.979875

Dimer

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7	0	-0.089396	1.843392	0.964193
6	0	-1.375605	1.785056	0.596645
7	0	-1.622596	2.804947	-0.237183
6	0	-0.455472	3.535649	-0.402144
6	0	0.511071	2.926161	0.343792
6	0	-2.919520	3.050707	-0.877312
6	0	0.583509	0.899423	1.878791
6	0	0.786530	1.499546	3.269617
1	0	1.283499	0.762774	3.910563
8	0	-3.461202	0.016326	-0.060718
6	0	-4.074002	-1.104585	0.033782
6	0	-5.606996	-1.040489	0.007855
8	0	-3.526580	-2.230063	0.129561
8	0	2.930040	1.270794	-0.061459
6	0	3.884446	0.646021	-0.613223
6	0	5.186541	1.412379	-0.880801
8	0	3.851305	-0.566420	-0.987538
6	0	1.358038	-1.944283	-0.551388
7	0	0.029233	-1.927847	-0.729387
6	0	-0.572403	-2.765508	0.200687
6	0	0.437107	-3.299667	0.947682
7	0	1.628340	-2.775329	0.466632
6	0	-0.723025	-1.180070	-1.763062
6	0	0.144752	-0.173345	-2.508960
1	0	-0.491720	0.373997	-3.212541
6	0	2.980702	-3.050426	0.959449
1	0	-1.138212	-1.923459	-2.451923
1	0	-1.568050	-0.705048	-1.252170
1	0	3.011484	-2.894835	2.041290
1	0	3.254931	-4.084487	0.730631
1	0	3.664529	-2.356964	0.462707
1	0	2.143443	-1.337886	-1.023732
1	0	0.411377	-3.994514	1.773281
1	0	-1.661251	-2.821239	0.255332
1	0	-3.393184	3.929420	-0.429787
1	0	-2.762786	3.222408	-1.945216
1	0	-3.536665	2.159299	-0.730509
1	0	-0.048452	0.007928	1.923337
1	0	1.536158	0.654221	1.396969
1	0	-2.099575	0.991859	0.800926
1	0	1.576350	3.089340	0.421568

1	0	-0.408533	4.397399	-1.049925
1	0	0.615762	0.548250	-1.832934
1	0	0.938990	-0.657686	-3.087649
1	0	1.425114	2.388219	3.227194
1	0	-0.166618	1.772585	3.736910
1	0	-5.942419	-0.655191	-0.963501
1	0	-6.046753	-2.027554	0.172921
1	0	-5.967863	-0.342287	0.772630
1	0	5.221506	2.351827	-0.321397
1	0	6.053548	0.792053	-0.629150
1	0	5.253782	1.638930	-1.952850

Trimer

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7	0	-4.123833	0.507072	-1.917068
6	0	-4.018113	0.337181	-0.590157
7	0	-4.576065	-0.837456	-0.268613
6	0	-5.037184	-1.438691	-1.425886
6	0	-4.757223	-0.594876	-2.460539
6	0	-4.597015	-1.458047	1.079015
6	0	-4.782614	-0.430578	2.190465
1	0	-4.823048	-0.959458	3.148488
6	0	-3.638727	1.688913	-2.641578
8	0	-2.655521	2.701628	0.212057
6	0	-2.039874	3.491567	1.009066
8	0	-0.917388	3.261930	1.526876
6	0	-2.740731	4.817481	1.328061
8	0	-1.759972	-2.720086	0.798478
6	0	-1.379798	-3.256023	-0.293953
6	0	-2.164084	-4.482274	-0.787697
8	0	-0.394217	-2.882859	-0.986945
6	0	0.717102	-1.328047	1.840458
7	0	0.661281	-0.186354	2.540635
6	0	1.937808	0.344830	2.633631
6	0	2.776420	-0.506838	1.974789
7	0	1.994615	-1.542159	1.494249
6	0	-0.563129	0.433826	3.054668
6	0	2.497206	-2.713972	0.747677
6	0	2.926021	-3.842778	1.685865
8	0	4.761608	-0.650640	-0.309743
6	0	5.576403	0.138451	-0.885240
6	0	7.070264	-0.086686	-0.611833
8	0	5.255071	1.090764	-1.654135
6	0	2.342273	1.113423	-1.594721
7	0	1.471790	1.958883	-1.018853
6	0	0.222913	1.353873	-0.953086
6	0	0.356681	0.113086	-1.505896
7	0	1.679314	-0.011252	-1.898243
6	0	1.763171	3.331137	-0.551511
6	0	3.140565	3.460475	0.093724
1	0	3.218339	2.819062	0.977478
6	0	2.281457	-1.190279	-2.529237
1	0	-3.239513	2.389943	-1.904088
1	0	-2.853657	1.388532	-3.340334
1	0	-4.470130	2.142759	-3.187424
1	0	-5.432105	-2.164691	1.065872
1	0	-3.657801	-2.019226	1.182280
1	0	-3.530993	1.070933	0.057557
1	0	-5.510626	-2.408102	-1.413512
1	0	-4.951423	-0.682602	-3.518432
1	0	1.675866	4.002524	-1.414198
1	0	0.968824	3.576798	0.158831
1	0	1.659963	-2.054660	-2.289204
1	0	2.319964	-1.051622	-3.613994
1	0	3.289964	-1.310681	-2.126780
1	0	3.434081	1.236083	-1.713108
1	0	-0.312587	-0.735753	-1.560718
1	0	-0.620924	1.838775	-0.475292
1	0	-0.479267	0.552309	4.139018
1	0	-0.714117	1.406991	2.571392
1	0	-1.396282	-0.232761	2.826663
1	0	3.340117	-2.348750	0.156158
1	0	1.686256	-3.028053	0.084731
1	0	-0.151351	-1.923658	1.531596
1	0	3.825501	-0.449072	1.715437

1	0	2.123791	1.283695	3.131691
1	0	3.300709	-4.681840	1.088859
1	0	3.730384	-3.521084	2.356867
1	0	3.279927	4.499603	0.412208
1	0	3.954913	3.196213	-0.588041
1	0	-3.948868	0.276782	2.238559
1	0	-5.712368	0.137537	2.072608
1	0	-2.220845	-4.492787	-1.881188
1	0	-1.628507	-5.390098	-0.480722
1	0	-3.168035	-4.524708	-0.351969
1	0	-2.156474	5.416050	2.031785
1	0	-2.892430	5.388247	0.403486
1	0	-3.734730	4.622653	1.748815
1	0	7.337060	-1.127974	-0.828242
1	0	7.690770	0.585968	-1.210195
1	0	7.278312	0.082253	0.452590
1	0	2.086198	-4.204107	2.290508

Tetramer

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8	0	-5.769926	-2.462835	-0.808868
6	0	-4.707390	-3.063065	-1.144335
8	0	-3.544366	-2.550475	-1.159485
6	0	-4.851407	-4.520380	-1.604087
6	0	-5.355739	0.328012	-0.322773
7	0	-4.388041	1.141934	-0.764108
6	0	-4.499897	2.379813	-0.147775
6	0	-5.577071	2.295811	0.686418
7	0	-6.094144	1.012187	0.564300
6	0	-3.395383	0.763440	-1.778138
6	0	-7.266206	0.459998	1.262057
6	0	-8.584236	1.005689	0.712249
1	0	-2.481148	1.323819	-1.581675
1	0	-3.233190	-0.317132	-1.710176
1	0	-3.771493	1.027037	-2.771259
1	0	-7.155745	0.691976	2.326600
1	0	-7.212656	-0.625225	1.143903
1	0	-5.492635	-0.744801	-0.584872
1	0	-6.003261	3.023768	1.359608
1	0	-3.764810	3.163871	-0.323515
1	0	-9.420411	0.561235	1.263102
1	0	-8.647769	2.094279	0.818991
1	0	-3.941851	-5.097324	-1.405228
1	0	-5.711020	-4.997304	-1.124189
1	0	-5.025102	-4.532990	-2.688319
1	0	-8.698733	0.751960	-0.346582
7	0	-0.368612	-3.645688	0.123191
6	0	0.944941	-3.885066	0.245552
7	0	1.451249	-4.094705	-0.977025
6	0	0.424118	-3.972205	-1.901139
6	0	-0.721578	-3.690961	-1.213245
6	0	2.875596	-4.315160	-1.324503
6	0	3.699928	-4.822808	-0.147406
1	0	4.723521	-4.995324	-0.495131
6	0	-1.283925	-3.395476	1.243239
8	0	1.618821	-2.647230	2.797944
6	0	2.148623	-1.967812	3.739678
8	0	2.486319	-0.755651	3.651819
6	0	2.377562	-2.699894	5.068011
8	0	3.961483	-1.396940	-2.026559
6	0	4.361467	-0.537690	-2.873025
6	0	5.024421	-1.050201	-4.156991
8	0	4.275489	0.718959	-2.731145
6	0	4.187770	1.746380	0.024445
7	0	4.236066	0.985073	1.126624
6	0	3.755625	1.710174	2.201780
6	0	3.422051	2.944869	1.723100
7	0	3.696590	2.946744	0.364296
6	0	4.690975	-0.410406	1.169525
6	0	3.444709	4.057524	-0.579375
6	0	4.312834	5.277247	-0.274799
8	0	0.238643	4.511055	-0.884109
6	0	-1.003248	4.690075	-0.772638
6	0	-1.559051	6.109810	-0.935481

8	0	-1.853436	3.768388	-0.524510
6	0	-0.005281	1.429513	-0.090920
7	0	0.154928	0.624395	0.971569
6	0	1.054251	-0.380822	0.648425
6	0	1.442635	-0.166409	-0.641711
7	0	0.774218	0.966831	-1.078851
6	0	-0.496134	0.758018	2.289649
6	0	-0.719892	2.211457	2.698236
1	0	0.232231	2.748299	2.761093
6	0	0.912151	1.584574	-2.403673
1	0	-0.702850	-2.980389	2.069254
1	0	-2.060401	-2.710121	0.899135
1	0	-1.750396	-4.335991	1.551380
1	0	2.875246	-5.049504	-2.136552
1	0	3.279627	-3.368272	-1.705422
1	0	1.481128	-3.821941	1.187238
1	0	0.603634	-4.080733	-2.959602
1	0	-1.746091	-3.473868	-1.513682
1	0	-1.446903	0.212930	2.254996
1	0	0.166826	0.250495	2.995616
1	0	1.946463	1.455948	-2.735055
1	0	0.237237	1.093855	-3.112317
1	0	0.662510	2.644141	-2.310273
1	0	-0.644896	2.315791	-0.166815
1	0	2.198565	-0.662172	-1.246686
1	0	1.356769	-1.120259	1.386591
1	0	5.740063	-0.442288	1.479859
1	0	4.069602	-0.935439	1.897936
1	0	4.576722	-0.843439	0.171205
1	0	2.377174	4.299662	-0.542056
1	0	3.665915	3.662099	-1.573987
1	0	4.390612	1.399457	-0.999969
1	0	2.996083	3.803226	2.218403
1	0	3.628231	1.247807	3.170517
1	0	4.092505	6.061194	-1.007093
1	0	4.102767	5.685878	0.719977
1	0	-1.187225	2.229367	3.689113
1	0	-1.371632	2.747546	2.000956
1	0	3.748717	-4.089787	0.663979
1	0	3.310488	-5.765862	0.253674
1	0	4.774517	-0.404913	-5.005112
1	0	6.114604	-1.016150	-4.030442
1	0	4.738632	-2.084764	-4.370505
1	0	2.850766	-2.047058	5.806424
1	0	1.419500	-3.060936	5.461880
1	0	3.006398	-3.583251	4.902815
1	0	-0.771573	6.814304	-1.216128
1	0	-2.348342	6.118963	-1.696667
1	0	-2.016662	6.437038	0.006735
1	0	5.380460	5.037418	-0.334439