

Coulombic interactions and crystal packing effects in the folding of donor-acceptor oligorotaxanes:

Supplementary Materials

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The contents of this document are as follows:

- A. XYZ coordinates for the molecules in Table 1 (Pages 1-10)
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- E. XYZ coordinates for the 3DNP-[3]Rotaxane in the pleated structure with 8Cl⁻ counterions with positions optimized through simulated annealing (pages 102-109)

A. XYZ coordinates for the molecules in Table 1, Figure 3.

1. Molecule 1, MM3 optimized. Total Charge: +4

C	-0.007691	0.435757	0.117018
C	-0.032266	0.180132	1.444952
C	1.175370	-0.106149	1.982558
C	2.296034	-0.053859	1.251651
N	2.276289	0.275323	0.008600
C	1.143185	0.474206	-0.566248
C	-1.176484	0.274930	2.198112
C	-1.187467	0.089606	3.537848
C	-2.285262	0.325693	4.267201
N	-3.376015	0.743613	3.729123
C	-3.438107	0.853770	2.449304
C	-2.370524	0.631522	1.672310
C	-4.483793	1.267408	4.583794
C	-4.278981	2.750579	4.884765
C	-3.562689	3.145338	5.953688
C	-3.311143	4.446312	6.172096
C	-3.768787	5.389254	5.327748
C	-4.512859	4.996796	4.277110
C	-4.764405	3.695822	4.058701
C	-3.402634	6.859057	5.522521
N	-2.130428	7.185673	4.810614
C	-2.150170	7.514873	3.567567
C	-1.029506	7.567160	2.836660
C	0.178127	7.280861	3.374261
C	0.153550	7.025217	4.702192
C	-0.997326	6.986769	5.385458
C	1.322344	7.186064	2.621099
C	2.516383	6.829459	3.146898
C	3.583964	6.607214	2.369902
N	3.521873	6.717385	1.090083
C	2.431122	7.135316	0.552009
C	1.333328	7.371401	1.281364
C	4.629650	6.193591	0.235408

C	4.424839	4.710420	-0.065562
C	4.910289	3.765177	0.760487
C	4.658743	2.464202	0.542082
C	3.914645	2.071744	-0.508539
C	3.456974	3.014685	-1.352874
C	3.708520	4.315660	-1.134468
C	3.548494	0.601940	-0.703309
H	-0.291904	-0.220372	4.095053
H	-4.401033	1.212339	2.051691
H	-2.511761	0.796465	0.594608
H	-2.299062	0.249501	5.366245
H	-0.918962	0.664490	-0.453826
H	3.297299	-0.214143	1.682550
H	1.300901	-0.352325	3.046623
H	1.195321	0.748672	-1.632009
H	1.064819	6.796465	5.273030
H	-3.151433	7.675173	3.136671
H	-1.155035	7.813353	1.772598
H	-1.049464	6.712287	6.451214
H	2.657619	6.664504	4.224599
H	2.444923	7.211519	-0.547035
H	0.437767	7.681389	0.724162
H	4.546889	6.248635	2.767510
H	-2.716368	4.730549	7.057808
H	-3.166764	2.401146	6.666746
H	-5.375525	3.412939	3.183749
H	-4.925129	5.742343	3.574810
H	3.312572	5.059852	-1.847515
H	2.862177	2.730448	-2.238571
H	5.071035	1.718655	1.244369
H	5.521431	4.048060	1.635426
H	3.399901	0.345980	-1.775708
H	4.331833	-0.080917	-0.306170
H	-4.503856	0.651112	5.509758
H	-5.435784	1.078009	4.040216
H	4.649708	6.809886	-0.690558
H	5.581642	6.382994	0.778982
H	-4.185973	7.541915	5.125381
H	-3.254041	7.115017	6.594920

2. Molecule 2, MM3 optimized. Total Charge: 0

C	0.057454	-0.426842	0.091044
C	0.116680	-0.319929	1.426616
C	1.288713	-0.147984	2.060507
C	2.408908	-0.085250	1.317940
C	2.349682	-0.192164	-0.017632
C	1.177649	-0.364109	-0.651522
O	1.248467	-0.049455	3.424660
O	1.217895	-0.462638	-2.015676
H	-0.815609	-0.374316	2.015720

H	3.396634	0.054734	1.786842
H	3.281971	-0.137777	-0.606735
H	-0.930272	-0.566827	-0.377858
C	2.470083	0.134154	4.143611
H	2.245361	0.192072	5.228221
H	3.156401	-0.723017	3.983160
H	2.965147	1.082065	3.847142
C	-0.003721	-0.646247	-2.734626
H	0.221001	-0.704165	-3.819237
H	-0.498785	-1.594158	-2.438157
H	-0.690039	0.210924	-2.574175

3. Molecule **3**, MM3 optimized. Total Charge: 0

C	0.020087	0.000000	0.093282
C	0.025257	0.000000	1.448891
C	1.197873	0.000000	2.131911
C	2.353395	0.000000	1.440331
C	2.350702	0.000000	0.103648
C	1.193587	0.000000	-0.565692
C	-1.130266	0.000000	2.140472
C	-1.127573	0.000000	3.477155
C	0.029542	0.000000	4.146495
C	1.203043	0.000000	3.487521
O	2.413813	0.000000	4.130391
C	2.466697	0.000000	5.558475
O	-1.190684	0.000000	-0.549589
C	-1.243568	0.000000	-1.977672
H	3.307044	0.000000	-0.448070
H	1.232866	0.000000	-1.667021
H	-2.103001	0.000000	1.619658
H	-2.083914	0.000000	4.028873
H	-0.009736	0.000000	5.247824
H	3.326131	0.000000	1.961145
H	-2.305255	0.000000	-2.298658
H	-0.763413	0.910658	-2.391897
H	-0.763413	-0.910658	-2.391897
H	3.528384	0.000000	5.879461
H	1.986542	0.910658	5.972699
H	1.986542	-0.910658	5.972699

4. Molecule **4**, MM3 optimized. Total Charge: 0

C	0.069184	0.000535	-0.024775
C	0.068691	0.000605	1.316961
C	1.216649	0.004184	2.010824
C	2.364502	-0.002439	1.316813
C	2.363836	-0.002509	-0.024923
C	1.216465	0.000696	-0.746680
N	1.216736	0.001297	3.413775
C	1.216378	0.001896	-2.119410

C	0.069005	0.002998	-2.841169
C	0.068343	0.005414	-4.182903
C	1.216212	0.010205	-4.876904
C	2.364153	0.002367	-4.183051
C	2.363657	-0.000047	-2.841317
N	1.216121	0.009769	-6.279858
H	-0.922065	-0.000488	-2.363737
H	3.354777	-0.006164	-2.364012
H	3.329041	-0.006010	-4.720150
H	-0.896633	-0.000403	-4.719878
H	-0.896216	-0.006151	1.854048
H	3.329458	-0.011754	1.853774
H	3.354894	-0.007790	-0.502364
H	-0.921947	-0.002118	-0.502087
H	0.388268	0.428949	-6.692466
H	2.045030	0.426750	-6.692573
H	2.045698	0.417557	3.827113
H	0.388936	0.419755	3.827220

5. Rotaxane **1•2**, MM3 optimized, Total Charge: +4

C	0.063345	0.525232	0.088388
C	0.069126	0.270869	1.416566
C	1.288612	-0.014184	1.926608
C	2.390942	0.028627	1.168096
N	2.342709	0.347712	-0.076800
C	1.197267	0.555862	-0.622759
C	-1.058386	0.360321	2.194458
C	-1.039123	0.176384	3.534080
C	-2.125447	0.394386	4.285627
N	-3.234923	0.790399	3.770194
C	-3.321896	0.907122	2.492415
C	-2.266601	0.704243	1.693981
C	-4.346896	1.268738	4.647432
C	-4.182765	2.752429	4.963130
C	-3.452145	3.151421	6.020102
C	-3.202901	4.453313	6.231658
C	-3.677567	5.391264	5.391938
C	-4.451818	4.996196	4.364381
C	-4.701188	3.693644	4.152718
C	-3.277505	6.854571	5.555123
N	-2.018577	7.143839	4.802619
C	-2.066810	7.462931	3.557725
C	-0.964480	7.505742	2.799213
C	0.255006	7.220683	3.309253
C	0.260787	6.966313	4.637429
C	-0.873136	6.935682	5.348576
C	1.382516	7.131231	2.531360
C	2.590732	6.787304	3.031833
C	3.646024	6.584426	2.233396
N	3.559049	6.701154	0.955617

C	2.449573	7.097172	0.440188
C	1.363251	7.315174	1.191738
C	4.671020	6.222816	0.078376
C	4.506889	4.739125	-0.237321
C	5.025318	3.797911	0.573089
C	4.775950	2.495359	0.361428
C	4.001695	2.100288	-0.666124
C	3.527023	3.038237	-1.505843
C	3.776265	4.340130	-1.294289
C	3.601636	0.636981	-0.829306
H	-0.127203	-0.117800	4.072662
H	-4.298988	1.248164	2.114522
H	-2.430590	0.870391	0.619800
H	-2.116523	0.314989	5.384402
H	-0.860131	0.759054	-0.460003
H	3.401379	-0.138243	1.574291
H	1.438267	-0.255203	2.988623
H	1.224669	0.825009	-1.690701
H	1.184262	6.732485	5.185818
H	-3.077246	7.629806	3.151531
H	-1.114135	7.746768	1.737199
H	-0.900538	6.666530	6.416516
H	2.754721	6.621151	4.106013
H	2.440648	7.176574	-0.658587
H	0.451332	7.609362	0.653159
H	4.623116	6.243379	2.611286
H	-2.582211	4.740856	7.098174
H	-3.028539	2.409519	6.719334
H	-5.325625	3.405324	3.289072
H	-4.878800	5.739256	3.668334
H	3.352654	5.082031	-1.993520
H	2.906329	2.750692	-2.372355
H	5.202938	1.752300	1.057473
H	5.649759	4.086234	1.436731
H	3.417250	0.368801	-1.893094
H	4.381653	-0.056102	-0.443642
H	-4.334081	0.640743	5.565594
H	-5.300189	1.056730	4.114691
H	4.658201	6.850811	-0.839786
H	5.624314	6.434826	0.611113
H	-4.057521	7.547655	5.169461
H	-3.093119	7.122747	6.618912
C	-0.830098	4.071654	1.526404
C	-1.070197	3.905078	2.834363
C	-0.087409	3.577966	3.689508
C	1.154223	3.419903	3.199406
C	1.394322	3.586484	1.891449
C	0.411533	3.913590	1.036302
O	-0.429376	3.429742	5.004518
O	0.753498	4.061806	-0.278709
H	-2.096558	4.040259	3.211649

H	1.996524	3.151612	3.858055
H	2.420680	3.451288	1.514159
H	-1.672401	4.339936	0.867754
C	-0.252356	4.409250	-1.231819
H	0.213059	4.483287	-2.235774
H	-1.039869	3.628751	-1.276637
H	-0.701824	5.394503	-0.989708
C	0.576478	3.082293	5.957627
H	0.111061	3.008251	6.961581
H	1.025946	2.097041	5.715512
H	1.363991	3.862792	6.002449

6. Rotaxane **1•3**, MM3 optimized, Total Charge: +4

C	0.655524	0.327122	0.174612
C	0.461485	0.122811	1.497479
C	1.592723	-0.133341	2.193238
C	2.796303	-0.115411	1.605579
N	2.935929	0.148109	0.354339
C	1.883171	0.331951	-0.361496
C	-0.771907	0.227406	2.094340
C	-0.958369	0.069852	3.424671
C	-2.149595	0.289776	3.996656
N	-3.171222	0.665726	3.311486
C	-3.058224	0.764921	2.034016
C	-1.891366	0.556250	1.410185
C	-4.417763	1.128573	4.000582
C	-4.347569	2.619142	4.320086
C	-3.818351	3.055088	5.478597
C	-3.606024	4.365351	5.687752
C	-3.917490	5.273150	4.743739
C	-4.517604	4.842936	3.618598
C	-4.729799	3.533490	3.409574
C	-3.509138	6.735676	4.895631
N	-2.148320	6.978031	4.319105
C	-2.008693	7.241551	3.067866
C	-0.805114	7.259481	2.480207
C	0.326124	7.003329	3.175965
C	0.132085	6.799019	4.498833
C	-1.095561	6.794190	5.034940
C	1.559517	6.898734	2.579105
C	2.678975	6.569890	3.263260
C	3.845834	6.361219	2.639429
N	3.958832	6.460414	1.361959
C	2.937205	6.836364	0.676790
C	1.745979	7.056288	1.248773
C	5.205373	5.997567	0.672863
C	5.135179	4.506998	0.353359
C	5.517408	3.592650	1.263871
C	5.305214	2.283204	1.054847
C	4.705099	1.852991	-0.070295

C	4.393634	2.760789	-1.014307
C	4.605960	4.071053	-0.805153
C	4.296748	0.390464	-0.222187
H	-0.138062	-0.208948	4.101242
H	-3.967217	1.091477	1.504143
H	-1.888634	0.706440	0.321239
H	-2.309810	0.224051	5.084687
H	-0.176453	0.533907	-0.513454
H	3.734469	-0.261938	2.164190
H	1.582844	-0.327636	3.275143
H	2.068652	0.553594	-1.424638
H	0.964062	6.592234	5.186899
H	-2.946859	7.388077	2.509254
H	-0.795234	7.453776	1.398301
H	-1.281043	6.572547	6.098083
H	2.676243	6.419700	4.352206
H	3.097420	6.902089	-0.411242
H	0.925672	7.335089	0.572203
H	4.754826	6.034663	3.169303
H	-3.138217	4.683993	6.635678
H	-3.518723	2.335898	6.260857
H	-5.193817	3.215351	2.459824
H	-4.813698	5.561058	2.834264
H	4.306333	4.790242	-1.587412
H	3.925827	2.442148	-1.962233
H	5.601307	1.565082	1.839180
H	5.981427	3.910789	2.213620
H	4.260815	0.075828	-1.288607
H	4.999894	-0.295186	0.300425
H	-4.533039	0.510110	4.918054
H	-5.271376	0.885701	3.329752
H	5.320649	6.616030	-0.244608
H	6.058985	6.240439	1.343693
H	-4.212284	7.421326	4.373018
H	-3.473206	7.050313	5.962051
C	-0.942717	3.960782	1.202025
C	-0.274537	3.670014	2.345242
C	1.062147	3.456126	2.328201
C	1.710238	3.538397	1.154885
C	1.059350	3.824459	0.023587
C	-0.259211	4.034533	0.046129
C	-0.922628	3.587743	3.518558
C	-0.271739	3.301681	4.649856
C	1.046822	3.091607	4.627314
C	1.730328	3.165358	3.471418
O	3.082999	2.957173	3.402415
C	3.818207	2.648701	4.588510
O	-2.295389	4.168967	1.271028
C	-3.030596	4.477440	0.084934
H	1.604311	3.888989	-0.933893
H	-0.761633	4.268006	-0.906437

H	-2.006349	3.756297	3.562801
H	-0.816701	3.237151	5.607337
H	1.549243	2.858134	5.579880
H	2.793959	3.369843	1.110643
H	-4.099937	4.608932	0.346759
H	-2.673314	5.426144	-0.366318
H	-2.961306	3.648960	-0.650006
H	4.887547	2.517210	4.326685
H	3.748916	3.477181	5.323449
H	3.460925	1.699997	5.039762

7. Rotaxane **1•4**, MM3 optimized, Total Charge: +4

C	0.223053	0.463947	0.243274
C	0.104251	0.224015	1.568397
C	1.265885	-0.071582	2.193185
C	2.432829	-0.056417	1.539222
N	2.502479	0.247946	0.292047
C	1.416868	0.467090	-0.360690
C	-1.087940	0.333487	2.236282
C	-1.193480	0.164603	3.573433
C	-2.343858	0.394163	4.216791
N	-3.396471	0.790082	3.593980
C	-3.364112	0.894668	2.312985
C	-2.240093	0.679873	1.620093
C	-4.577172	1.293078	4.358456
C	-4.413104	2.778514	4.665384
C	-3.805914	3.186202	5.794851
C	-3.564185	4.488608	6.013318
C	-3.923227	5.417004	5.107860
C	-4.568354	5.012833	3.998322
C	-4.810132	3.710756	3.779990
C	-3.539692	6.881650	5.295707
N	-2.213331	7.153597	4.664524
C	-2.140742	7.455947	3.416984
C	-0.971996	7.471768	2.765859
C	0.188695	7.178190	3.393580
C	0.066634	6.940475	4.718848
C	-1.128772	6.937030	5.319996
C	1.382770	7.067903	2.728424
C	2.533161	6.719137	3.346802
C	3.658464	6.502228	2.656278
N	3.694298	6.607671	1.375404
C	2.643734	7.006361	0.750763
C	1.492143	7.237642	1.391648
C	4.875795	6.103546	0.612841
C	4.708894	4.619371	0.301485
C	5.103935	3.683770	1.184216
C	4.859821	2.382806	0.961882
C	4.214175	1.983139	-0.148989
C	3.857004	2.914863	-1.051709
C	4.101286	4.216143	-0.829402

C	3.827813	0.519785	-0.341258
H	-0.336866	-0.123694	4.198996
H	-4.298052	1.238837	1.840749
H	-2.300646	0.839500	0.534223
H	-2.437038	0.328198	5.312565
H	-0.641458	0.709934	-0.389451
H	3.398324	-0.231536	2.040076
H	1.313975	-0.297972	3.267753
H	1.545904	0.725145	-1.423945
H	0.930115	6.697339	5.354047
H	-3.105412	7.628891	2.913786
H	-1.017757	7.696339	1.690826
H	-1.260440	6.681081	6.383435
H	2.590870	6.558579	4.432672
H	2.740124	7.073316	-0.344670
H	0.637641	7.528876	0.764591
H	4.590730	6.155688	3.130088
H	-3.051794	4.785243	6.945169
H	-3.484908	2.451013	6.553368
H	-5.330994	3.415430	2.852438
H	-4.897979	5.748022	3.243527
H	3.781976	4.953885	-1.586143
H	3.344031	2.621637	-1.984325
H	5.187763	1.644612	1.714471
H	5.625184	3.975156	2.112798
H	3.742120	0.244017	-1.415527
H	4.563686	-0.173655	0.122546
H	-4.657738	0.678155	5.281941
H	-5.480687	1.088422	3.742614
H	4.960421	6.720636	-0.308839
H	5.778155	6.304349	1.231628
H	-4.275663	7.572231	4.827821
H	-3.456924	7.161327	6.369200
C	-0.346901	3.503616	4.215605
C	0.166013	3.181488	5.411994
C	1.468863	2.897732	5.550927
C	2.242366	2.949723	4.456984
C	1.728285	3.272839	3.261454
C	0.413756	3.556138	3.095929
N	1.999492	2.526968	6.793647
C	-0.116698	3.862642	1.870288
C	-1.434703	4.127317	1.701609
C	-1.957478	4.403857	0.498195
C	-1.187901	4.434817	-0.599308
C	0.120931	4.183110	-0.454950
C	0.642218	3.905836	0.749032
N	-1.740062	4.690232	-1.861556
H	-2.147577	4.118616	2.538455
H	1.722787	3.706370	0.766439
H	0.775404	4.193344	-1.344241
H	-3.040682	4.598330	0.406594

H	-0.494830	3.137127	6.295508
H	3.317416	2.711567	4.541190
H	2.441125	3.281353	2.424577
H	-1.425650	3.712829	4.199848
H	-2.621404	5.193466	-1.890832
H	-1.118698	5.050822	-2.579094
H	2.997998	2.651402	6.929181
H	1.502783	2.834180	7.624237

B. XYZ coordinates for the minimum energy structures for the mDNP-[n]Rotaxanes in vacuum

1. 3DNP-[3]Rotaxane, MM3, Total Charge: 0

C	-14.675964	-0.142512	-6.238912
C	-15.479266	0.625807	-7.006433
C	-16.758685	0.701315	-6.585450
C	-17.162506	0.076544	-5.478257
N	-16.363646	-0.624557	-4.761501
C	-15.138476	-0.746794	-5.137186
C	-15.030829	1.317815	-8.096320
C	-15.841416	2.105651	-8.832560
C	-15.367149	2.844026	-9.837828
N	-14.125225	2.848863	-10.147726
C	-13.322495	2.074866	-9.507947
C	-13.739830	1.312712	-8.490902
C	-13.598043	3.865907	-11.110816
C	-13.243979	5.148128	-10.369712
C	-14.179910	6.090485	-10.156884
C	-13.942402	7.116861	-9.325743
C	-12.763001	7.224091	-8.688813
C	-11.799662	6.326847	-8.964233
C	-12.038070	5.301121	-9.795220
C	-12.562107	8.256576	-7.589203
N	-12.991840	7.725928	-6.254019
C	-12.174071	7.053531	-5.521929
C	-12.571500	6.431280	-4.406232
C	-13.860373	6.468053	-4.004885
C	-14.672811	7.212042	-4.787014
C	-14.217455	7.829344	-5.882122
C	-14.319039	5.767827	-2.921519
C	-15.627193	5.724725	-2.593240
C	-16.070746	4.962498	-1.589590
N	-15.278991	4.228678	-0.895533
C	-14.015354	4.278948	-1.135587
C	-13.515427	5.026842	-2.127358
C	-15.841977	3.215145	0.056619
C	-16.186730	1.927438	-0.677321
C	-15.273446	0.949740	-0.820639
C	-15.503142	-0.084594	-1.645562
C	-16.652329	-0.162832	-2.340607
C	-17.599880	0.766887	-2.126368
C	-17.369283	1.801985	-1.306005

C	-16.828375	-1.185326	-3.453540
Cl-	-17.867117	5.002990	-9.582524
Cl-	-20.591519	-0.010142	-4.675392
Cl-	-11.733315	9.963274	-5.175293
Cl-	-15.018446	5.861624	1.296939
O	-11.647292	3.502972	-6.439584
C	-12.647655	3.139738	-5.571872
C	-13.903499	3.595237	-5.802145
C	-14.925803	3.257704	-4.978449
C	-14.668383	2.456454	-3.932682
C	-13.434638	2.001144	-3.698915
C	-12.431105	2.340298	-4.511342
C	-16.183355	3.713823	-5.205049
C	-16.407399	4.474526	-6.287770
C	-15.401883	4.821596	-7.093034
C	-14.161995	4.388776	-6.853444
O	-17.183354	3.327017	-4.351698
C	-18.573530	3.462770	-4.674584
C	-19.122406	4.862822	-4.415900
O	-19.019905	5.182951	-3.034349
C	-19.795962	6.333032	-2.711437
C	-19.331500	6.927105	-1.386680
O	-18.049598	7.503669	-1.589753
C	-17.586006	8.260001	-0.479648
C	-16.219863	8.837725	-0.830957
O	-16.378661	9.695102	-1.952217
C	-15.141561	10.106853	-2.518182
C	-15.464065	10.903779	-3.776176
O	-16.259543	10.092710	-4.651449
C	-10.330003	2.974981	-6.240922
C	-9.410056	3.423252	-7.368918
O	-9.854528	2.829542	-8.581886
C	-8.827177	2.755386	-9.561901
C	-9.411133	2.177576	-10.844414
O	-9.917823	0.880489	-10.564038
C	-10.574477	0.294581	-11.678489
C	-11.185517	-1.031409	-11.245785
O	-12.182989	-0.775411	-10.264863
C	-12.977019	-1.911010	-9.945261
C	-14.111097	-2.055847	-10.951880
O	-14.907568	-3.180970	-10.569607
C	-15.891475	-3.630110	-11.409668
C	-16.524256	-4.784401	-11.089291
C	-17.494557	-5.280519	-11.896102
C	-17.811042	-4.613108	-13.022116
C	-17.181327	-3.479104	-13.343180
C	-16.231042	-2.987792	-12.542689
C	-16.205845	-5.455441	-9.965372
C	-16.838516	-6.588033	-9.642764
C	-17.793472	-7.075026	-10.441679
C	-18.128123	-6.433933	-11.576018

O	-19.092639	-6.888584	-12.432617
C	-19.860102	-8.059150	-12.137089
C	-20.731170	-8.370591	-13.346048
O	-21.616454	-7.283133	-13.585401
C	-22.377573	-7.497215	-14.767283
C	-23.165823	-6.242403	-15.114933
O	-22.262078	-5.206744	-15.484815
C	-22.933367	-4.117283	-16.102462
C	-21.938067	-3.012526	-16.435328
O	-21.423309	-2.426014	-15.244589
C	-20.630292	-1.281849	-15.536456
C	-19.927741	-0.763657	-14.286439
O	-20.870404	-0.298520	-13.309311
C	-21.217360	-1.062232	-12.224994
C	-21.878022	-0.461645	-11.204889
C	-22.225944	-1.158272	-10.096222
C	-21.889213	-2.457143	-10.022660
C	-21.228751	-3.052695	-11.020824
C	-20.894233	-2.361798	-12.112309
C	-22.899141	-0.553830	-9.085396
C	-23.195468	0.754255	-9.189177
C	-22.854856	1.444159	-10.278952
C	-22.205049	0.838623	-11.275983
O	-23.242639	-1.295882	-7.984452
C	-23.859562	-0.649233	-6.863181
C	-24.254167	-1.701896	-5.834598
O	-25.340283	-2.480163	-6.332690
C	-26.606773	-1.965333	-5.938434
C	-27.727311	-2.763755	-6.596310
O	-27.783495	-2.448791	-7.981979
C	-28.902823	-3.054180	-8.619851
C	-28.931010	-2.652714	-10.089478
O	-29.097824	-1.244827	-10.174335
C	-29.006504	-0.766615	-11.510393
C	-29.114775	0.752452	-11.463824
O	-28.101251	1.268779	-10.590978
C	-22.032025	2.634318	-14.544486
C	-20.863825	3.013260	-14.003207
C	-20.839713	3.774106	-12.894621
C	-22.005820	4.216696	-12.389696
C	-23.173420	3.836931	-12.930352
C	-23.199356	3.007615	-13.988634
C	-19.539305	4.014859	-12.142115
N	-19.238047	2.871139	-11.221021
C	-18.530800	1.879166	-11.629740
C	-18.416593	0.751944	-10.917805
C	-19.037042	0.606348	-9.727654
C	-19.716837	1.696878	-9.310590
C	-19.802109	2.795603	-10.068277
C	-24.511587	2.399091	-14.461377
N	-24.766980	1.086585	-13.781908

C	-24.302659	-0.002970	-14.282530
C	-24.354882	-1.160141	-13.616630
C	-24.895764	-1.241184	-12.383079
C	-25.401848	-0.080480	-11.915427
C	-25.334889	1.049257	-12.628669
C	-19.022217	-0.567071	-9.023128
C	-19.705986	-0.726160	-7.870868
C	-19.751258	-1.903529	-7.239962
N	-19.153734	-2.940601	-7.699637
C	-18.457899	-2.826961	-8.774444
C	-18.372934	-1.672636	-9.446556
C	-19.386139	-4.276772	-7.063437
C	-20.702845	-4.881871	-7.521294
C	-20.770254	-5.579528	-8.667752
C	-21.956480	-5.945491	-9.174904
C	-23.098609	-5.617456	-8.546498
C	-23.026601	-4.991014	-7.359469
C	-21.840083	-4.628062	-6.851038
C	-24.438527	-5.812634	-9.237086
N	-24.724113	-4.649154	-10.137513
C	-24.308809	-4.649840	-11.354488
C	-24.374126	-3.554513	-12.118298
C	-24.889714	-2.397208	-11.649993
C	-25.356921	-2.460657	-10.384583
C	-25.262577	-3.583333	-9.664573
Cl-	-26.996608	0.891786	-15.358172
Cl-	-16.686759	-3.080555	-6.193831
Cl-	-27.052840	-5.961120	-10.776424
Cl-	-15.335297	1.369364	-12.424979
H	-23.966618	-3.645753	-13.133318
H	-25.590707	-3.658260	-8.618266
H	-25.805474	-1.594618	-9.878133
H	-23.860708	-5.596035	-11.695796
H	-25.873964	-0.007113	-10.926827
H	-23.833817	0.098670	-15.273602
H	-23.908080	-2.027787	-14.115915
H	-25.714366	2.015042	-12.260035
H	-17.773752	-1.682932	-10.367224
H	-20.337412	-2.074612	-6.326256
H	-20.285147	0.086792	-7.414615
H	-17.978608	-3.755573	-9.110448
H	-17.817580	-0.050526	-11.370585
H	-20.395147	3.676825	-9.778243
H	-20.257004	1.724258	-8.353765
H	-18.078466	2.002041	-12.625369
H	-19.851650	-5.803968	-9.234266
H	-21.988441	-6.463550	-10.148441
H	-23.948218	-4.718682	-6.818019
H	-21.812584	-4.068189	-5.900679
H	-22.016220	4.853478	-11.487892
H	-24.115523	4.169777	-12.461012

H	-22.023414	1.964455	-15.421416
H	-19.922403	2.645265	-14.446412
H	-25.376087	3.063082	-14.238283
H	-24.494961	2.215027	-15.558403
H	-24.444199	-6.734246	-9.860175
H	-25.272959	-5.883750	-8.504562
H	-19.609277	4.937484	-11.529063
H	-18.670794	4.129881	-12.827535
H	-19.369496	-4.123323	-5.961372
H	-18.529326	-4.933704	-7.330854
H	-16.912858	2.215114	-8.623385
H	-12.268379	2.134186	-9.815191
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H	-15.984242	3.529676	-10.431367
H	-13.612546	-0.293260	-6.472838
H	-18.181994	0.154918	-5.089522
H	-17.518630	1.300662	-7.103916
H	-14.505933	-1.360189	-4.476446
H	-15.742611	7.337511	-4.570930
H	-11.140006	7.009932	-5.898321
H	-11.802179	5.869180	-3.858279
H	-14.864348	8.418517	-6.550647
H	-16.390318	6.281258	-3.152789
H	-13.394166	3.631688	-0.496817
H	-12.426226	4.989060	-2.270348
H	-17.134363	4.871089	-1.327282
H	-14.753751	7.838350	-9.126679
H	-15.181056	5.996423	-10.611550
H	-11.247823	4.550238	-9.954214
H	-10.818129	6.395619	-8.464425
H	-14.299238	1.021496	-0.306294
H	-14.711962	-0.840403	-1.792250
H	-18.558867	0.721133	-2.669128
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H	-17.890792	-1.488893	-3.581914
H	-14.380274	4.040385	-11.881461
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H	-15.082358	3.038729	0.849855
H	-16.740773	3.665541	0.533630
H	-11.490120	8.541716	-7.510242
H	-13.146472	9.183760	-7.781621
H	-13.358262	4.683838	-7.543045
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H	-9.924138	3.339144	-5.273326
H	-9.404173	4.527932	-7.466768
H	-8.373104	3.099371	-7.140266
H	-7.997997	2.113524	-9.197888

H	-8.416810	3.768568	-9.755494
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H	-11.367354	0.970821	-12.060623
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H	-15.422238	-5.083228	-9.283178
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H	-19.187262	-8.921284	-11.946691
H	-20.087432	-8.544891	-14.233615
H	-21.315474	-9.296707	-13.163757
H	-23.073207	-8.347744	-14.608167
H	-21.711539	-7.762516	-15.614844
H	-23.850250	-6.467075	-15.959838
H	-23.788193	-5.918296	-14.256388
H	-23.735354	-3.734180	-15.442115
H	-23.417174	-4.466308	-17.039009
H	-21.106539	-3.419287	-17.047776
H	-22.450548	-2.235034	-17.040559
H	-21.270141	-0.483720	-15.966841
H	-19.865379	-1.542143	-16.298119
H	-19.220071	-1.499001	-13.863187
H	-19.299032	0.103904	-14.577861
H	-23.726701	1.291838	-8.388201
H	-23.115247	2.513876	-10.347844
H	-21.938235	1.426174	-12.163612
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H	-20.955069	-4.118460	-10.958374
H	-20.358151	-2.895951	-12.911658
H	-19.138779	2.743346	-4.047497
H	-18.754415	3.150941	-5.723724
H	-18.588053	5.629689	-5.009560
H	-20.188086	4.889966	-4.727644
H	-20.865213	6.042307	-2.644515
H	-19.708315	7.099929	-3.509679
H	-20.048039	7.708879	-1.058712
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H	-17.510319	7.608672	0.415213
H	-15.507022	8.021532	-1.064021

H	-15.808745	9.412097	0.024762
H	-14.578702	10.730555	-1.793573
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H	-16.015305	11.834312	-3.525458
H	-14.533677	11.202092	-4.300530
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H	-16.980947	9.771903	-4.120284
H	-24.763311	-0.091224	-7.181627
H	-23.146157	0.069945	-6.409913
H	-23.393641	-2.369907	-5.633006
H	-24.519248	-1.232382	-4.865241
H	-26.702555	-2.038181	-4.834536
H	-26.695193	-0.893809	-6.211776
H	-28.693189	-2.501739	-6.115468
H	-27.564524	-3.852523	-6.456216
H	-28.830727	-4.158369	-8.532285
H	-29.843754	-2.736451	-8.124201
H	-27.993847	-2.962315	-10.592109
H	-29.771827	-3.159968	-10.606746
H	-28.042728	-1.072009	-11.965892
H	-29.825203	-1.193554	-12.125731
H	-28.977343	1.184079	-12.476474
H	-30.115937	1.067881	-11.102110
H	-28.206821	0.800030	-9.769859

2. 3DNP-[3]Rotaxane, OPLS-AA, Total Charge: 0

O	-4.149967	6.306652	22.034443
O	-6.147690	4.086122	22.136274
O	-5.745809	1.458631	23.499912
O	-3.245804	1.032992	24.473619
O	-1.137015	-0.332419	23.163106
O	1.356370	2.264086	18.312043
O	3.921538	1.050105	17.275049
O	6.105824	0.581111	18.953815
O	7.670406	2.451622	20.783221
O	8.867861	5.157066	22.950801
H	8.107525	5.387854	23.472334
C	-1.165240	8.953465	23.209565
H	-0.453792	9.314502	22.481694
C	-2.196812	8.086973	22.811867
H	-2.281301	7.798657	21.775797
C	-3.103617	7.584556	23.763366
C	-4.100623	6.671853	23.361022
C	-5.009610	6.175039	24.322692
H	-5.776684	5.471424	24.037801
C	-5.447534	6.353087	21.435987
H	-6.184268	6.868201	22.054958
H	-5.354586	6.960182	20.535222
C	-5.955319	4.962577	21.023767

H	-5.224963	4.539133	20.338241
H	-6.899917	5.099892	20.495716
C	-6.677704	2.855301	21.645872
H	-7.627458	3.029015	21.137508
H	-5.990866	2.399179	20.936647
C	-6.920023	1.850986	22.788691
H	-7.347256	0.942473	22.363796
H	-7.665186	2.228571	23.490013
C	-5.157465	2.551995	24.208688
H	-4.725421	3.273798	23.517893
H	-5.897919	3.063597	24.825326
C	-4.041996	2.026655	25.129865
H	-4.482044	1.590793	26.027666
H	-3.442409	2.882017	25.439010
C	-2.079912	0.767908	25.251843
H	-1.516070	1.690330	25.363131
H	-2.362912	0.439805	26.252418
C	-1.184118	-0.315257	24.601637
H	-1.595333	-1.278565	24.895202
H	-0.169966	-0.295770	25.001094
C	-0.384135	0.626121	22.514806
C	-0.260435	0.497672	21.115895
C	-0.840814	-0.602645	20.470731
H	-1.363660	-1.334469	21.059150
C	-0.786067	-0.713275	19.071189
H	-1.269041	-1.543473	18.577414
C	-0.093737	0.249451	18.313293
H	-0.076012	0.128433	17.241616
C	0.576192	1.320254	18.953777
C	0.436710	1.459651	20.349429
C	1.000365	2.570472	20.991384
H	1.517871	3.311190	20.409780
C	0.928329	2.689342	22.387873
H	1.403246	3.524972	22.880221
C	0.263737	1.709774	23.147715
H	0.264130	1.820814	24.217027
C	1.686084	2.039713	16.933704
H	0.775910	1.950546	16.339985
H	2.170626	2.948238	16.576590
C	2.642668	0.850556	16.669879
H	2.764382	0.741968	15.591100
H	2.196520	-0.064982	17.043597
C	4.732029	-0.104664	17.028879
H	4.252979	-0.974620	17.475956
H	4.832920	-0.292148	15.958592
C	6.140953	0.013997	17.643477
H	6.786526	0.623533	17.010079
H	6.555013	-0.995707	17.670167
C	7.331815	0.330785	19.647036
H	7.426376	-0.742196	19.820959
H	8.180804	0.652255	19.041824

C	7.415911	1.064659	20.998067
H	8.232956	0.617480	21.566861
H	6.493360	0.937786	21.557553
C	7.932964	3.119391	22.015973
H	7.052515	3.089197	22.657650
H	8.746051	2.611144	22.537507
C	8.383835	4.569480	21.762824
H	7.570584	5.170575	21.358750
H	9.191537	4.581608	21.029857
O	-1.998086	9.327969	26.831642
O	-1.388758	10.507130	29.526877
O	0.498159	10.681383	31.665624
O	3.244582	10.616883	30.807134
O	3.964432	7.878151	30.632629
O	1.380667	3.016507	28.220912
O	3.373041	1.526358	27.114638
O	6.234061	1.896976	27.278668
O	8.408409	3.342280	27.095802
O	9.454071	2.240895	29.209768
H	8.744844	2.821999	28.972423
C	-4.926240	6.596814	25.663662
H	-5.626404	6.215393	26.391940
C	-3.935275	7.515739	26.058202
H	-3.879938	7.834608	27.088881
C	-3.010146	8.003746	25.115213
C	-2.004163	8.909219	25.515093
C	-1.063743	9.357197	24.552819
H	-0.251953	10.014779	24.823880
C	-1.409128	10.618008	27.047216
H	-1.722121	11.303764	26.257625
H	-0.325017	10.534811	27.009087
C	-1.846207	11.238095	28.383348
H	-1.450014	12.254542	28.410935
H	-2.935427	11.298729	28.408718
C	-1.787084	11.172454	30.721035
H	-2.846612	11.006159	30.918589
H	-1.647951	12.250279	30.620029
C	-0.908756	10.736984	31.918178
H	-1.084383	11.422770	32.747590
H	-1.214146	9.747881	32.259837
C	1.002323	11.779833	30.901682
H	0.623109	12.725468	31.291835
H	0.651911	11.666983	29.881690
C	2.546806	11.861751	30.928364
H	2.877334	12.514664	30.121097
H	2.883394	12.354063	31.841962
C	3.053247	9.771671	31.940961
H	2.042623	9.383465	31.982987
H	3.250876	10.315726	32.865629
C	4.065250	8.614899	31.856429
H	5.061603	9.054591	31.875993

H	4.023884	7.967951	32.730534
C	3.041889	6.853729	30.599670
C	3.139365	5.965747	29.511839
C	4.152896	6.145374	28.561216
H	4.849880	6.953595	28.676213
C	4.225476	5.309911	27.436410
H	4.991878	5.481527	26.701586
C	3.298244	4.268128	27.266590
H	3.380769	3.658208	26.381350
C	2.299299	4.041700	28.244817
C	2.221684	4.906003	29.351985
C	1.201475	4.724573	30.296453
H	0.507867	3.911654	30.170750
C	1.080695	5.606367	31.382779
H	0.295914	5.466666	32.110581
C	1.983607	6.674507	31.525279
H	1.864087	7.307620	32.388713
C	1.093473	2.468730	26.932380
H	1.045944	3.262483	26.186559
H	0.092525	2.043493	26.971622
C	2.088447	1.369022	26.507960
H	1.696435	0.396237	26.789430
H	2.171906	1.391710	25.422001
C	4.252043	0.520016	26.609685
H	4.337093	0.666982	25.539600
H	3.843390	-0.476658	26.784791
C	5.652303	0.590513	27.252566
H	5.565009	0.272519	28.291490
H	6.337523	-0.120767	26.791637
C	6.442643	2.402052	25.952453
H	5.515919	2.715493	25.471032
H	6.903788	1.635213	25.330906
C	7.456363	3.556094	26.043787
H	7.944910	3.749401	25.089423
H	6.929842	4.465739	26.315598
C	9.218603	2.191127	26.869538
H	9.756195	2.277677	25.924599
H	8.625583	1.276086	26.853885
C	10.213159	2.108903	28.029410
H	10.770052	1.171749	28.023920
H	10.926917	2.931948	27.985040
N	7.049643	4.416171	30.609154
N	0.916979	1.242997	31.388126
N	-1.679390	6.557772	28.672737
N	4.504696	9.374242	27.077406
C	6.610875	4.256078	31.929167
H	7.070636	4.759068	32.767586
C	5.519242	3.377837	32.102162
H	5.204585	3.222982	33.119150
C	4.826357	2.769160	31.028561
C	5.387886	2.957966	29.743872

H	4.918144	2.567607	28.860591
C	6.524621	3.748972	29.500112
H	6.890752	3.910431	28.505149
C	3.564616	2.111297	31.204367
C	2.842952	2.177497	32.422516
H	3.267020	2.625357	33.303565
C	1.500473	1.760333	32.549775
H	0.951054	1.893250	33.470513
C	1.572487	1.036608	30.170755
H	1.090105	0.636890	29.295707
C	2.909156	1.470439	30.126496
H	3.398012	1.326824	29.183921
C	-0.541178	0.924814	31.411020
H	-0.873591	0.680542	32.421527
H	-0.744154	0.036251	30.804175
C	-1.343078	2.102319	30.874821
C	-1.646781	3.200757	31.708208
H	-1.387123	3.172987	32.756297
C	-2.194815	4.378699	31.158832
H	-2.355046	5.238508	31.792561
C	-2.448103	4.466231	29.773469
C	-2.226109	3.336109	28.957175
H	-2.421448	3.383233	27.896215
C	-1.671702	2.164054	29.503513
H	-1.442763	1.339288	28.848441
C	-2.865173	5.789328	29.147510
H	-3.534311	5.593959	28.307759
H	-3.446467	6.371404	29.864953
C	-1.066506	6.101193	27.505984
H	-1.441191	5.234996	26.993645
C	0.097669	6.787140	27.101431
H	0.582727	6.395395	26.222841
C	0.643172	7.871685	27.830811
C	-0.088848	8.285429	28.973805
H	0.234310	9.098953	29.597734
C	-1.283031	7.677138	29.404257
H	-1.799387	8.009731	30.292607
C	1.896121	8.474046	27.481129
C	2.648801	8.082300	26.343914
H	2.265384	7.366206	25.635771
C	3.973413	8.516723	26.108756
H	4.559963	8.130457	25.289108
C	3.791890	9.949276	28.133724
H	4.230104	10.640182	28.838139
C	2.490743	9.452761	28.312989
H	1.993760	9.837311	29.180551
C	5.965852	9.658959	27.023017
H	6.323924	9.610843	25.992195
H	6.171055	10.674366	27.368331
C	6.722719	8.655265	27.887326
C	7.376549	7.555400	27.291217

H	7.432215	7.473608	26.215706
C	7.903471	6.522943	28.093754
H	8.378984	5.675884	27.624453
C	7.749849	6.554605	29.497513
C	7.155575	7.685137	30.096819
H	7.038511	7.727481	31.169631
C	6.658563	8.735708	29.297387
H	6.154341	9.565287	29.770005
C	8.178120	5.362546	30.347941
H	8.606895	5.729702	31.282508
H	8.985516	4.832471	29.838491
N	1.679854	-3.242257	22.403325
N	4.415614	2.998684	20.874653
N	-1.493331	5.280858	19.611037
N	-4.265408	-0.971906	21.068867
C	1.798003	-2.332388	23.457854
H	1.326270	-2.486205	24.417935
C	2.495888	-1.143370	23.160089
H	2.525257	-0.417038	23.953581
C	3.034194	-0.858954	21.881106
C	2.955969	-1.897182	20.922285
H	3.406910	-1.796296	19.949808
C	2.284918	-3.115043	21.149864
H	2.203451	-3.877131	20.389648
C	3.586348	0.421851	21.556627
C	3.838731	1.410759	22.537422
H	3.680444	1.211195	23.579869
C	4.267185	2.718315	22.233920
H	4.381405	3.457866	23.007845
C	4.288357	2.075619	19.834312
H	4.442803	2.342780	18.801382
C	3.849877	0.792817	20.217729
H	3.655826	0.115591	19.408115
C	4.713388	4.406279	20.492789
H	5.211904	4.932329	21.305977
H	5.410662	4.432762	19.653094
C	3.424954	5.132523	20.140978
C	2.682379	5.779715	21.152852
H	3.070540	5.839315	22.158761
C	1.389408	6.268480	20.880285
H	0.805059	6.705010	21.676964
C	0.827343	6.111990	19.594670
C	1.593546	5.519856	18.568495
H	1.165729	5.379036	17.586671
C	2.888560	5.035980	18.838865
H	3.435849	4.522188	18.062333
C	-0.630697	6.464793	19.350613
H	-0.757605	6.818039	18.325783
H	-0.920556	7.297339	19.993648
C	-1.853308	4.489776	18.518030
H	-1.571430	4.732630	17.503861

C	-2.517726	3.287608	18.831147
H	-2.736090	2.652398	17.989200
C	-2.829085	2.894499	20.155545
C	-2.516798	3.828012	21.178167
H	-2.758330	3.655512	22.211737
C	-1.842388	5.038723	20.942516
H	-1.550066	5.689166	21.750032
C	-3.393084	1.610130	20.447099
C	-3.799138	0.697724	19.441807
H	-3.748136	0.952671	18.396674
C	-4.260716	-0.606230	19.718765
H	-4.508220	-1.296426	18.925401
C	-3.970345	-0.121172	22.141593
H	-3.996904	-0.442832	23.171378
C	-3.518634	1.160079	21.778533
H	-3.183730	1.774937	22.586582
C	-4.544856	-2.398857	21.401197
H	-5.044640	-2.903518	20.571981
H	-5.233282	-2.454107	22.247337
C	-3.249790	-3.129339	21.737671
C	-2.448508	-3.680061	20.712132
H	-2.794297	-3.663728	19.688973
C	-1.149413	-4.151691	20.999631
H	-0.519248	-4.500616	20.194462
C	-0.645415	-4.091161	22.318185
C	-1.477980	-3.618679	23.353375
H	-1.102487	-3.564202	24.364597
C	-2.770363	-3.138286	23.065278
H	-3.365469	-2.713055	23.860196
C	0.809231	-4.434271	22.610715
H	0.905118	-4.800163	23.635450
H	1.123322	-5.260198	21.968083
Cl-	1.585232	12.631775	27.441039
Cl-	-1.094150	4.572390	24.437243
Cl-	-0.428075	-1.092162	27.870867
Cl-	5.659822	5.726085	23.958922
Cl-	-5.859288	2.987297	18.048995
Cl-	3.670436	5.261202	34.141943
Cl-	6.076016	-0.861408	23.913693
Cl-	1.714546	-2.789642	17.843233

3. 6DNP-[4]Rotaxane, MM3, Total Charge: 0

C	-3.384621	-7.419001	2.009568
C	-4.172122	-6.325032	2.075301
C	-5.377288	-6.466079	1.481421
C	-5.718246	-7.599574	0.856913
N	-4.919765	-8.603915	0.789362
C	-3.783661	-8.524622	1.375621
C	-3.756640	-5.154643	2.650598
C	-2.535818	-5.014108	3.210108
C	-2.125966	-3.842633	3.705002

N	-2.860654	-2.789643	3.655531
C	-4.041288	-2.882359	3.152487
C	-4.510903	-4.034380	2.658622
C	-2.289893	-1.459849	4.035854
C	-1.460062	-0.892567	2.892672
C	-0.192497	-1.302679	2.709919
C	0.477191	-0.987043	1.591671
C	-0.106265	-0.248771	0.632389
C	-1.341027	0.236544	0.855198
C	-2.012651	-0.084115	1.971696
C	0.548593	-0.105521	-0.733304
N	0.218617	-1.285224	-1.594355
C	1.007464	-2.297188	-1.671923
C	0.644586	-3.422382	-2.299951
C	-0.566144	-3.546567	-2.885186
C	-1.343578	-2.447004	-2.803703
C	-0.927145	-1.350088	-2.166343
C	-0.998928	-4.708594	-3.463820
C	-0.247864	-5.830663	-3.513362
C	-0.731219	-6.974480	-4.014447
N	-1.932034	-7.057772	-4.469305
C	-2.665801	-6.005460	-4.468067
C	-2.237443	-4.837517	-3.984643
C	-2.524221	-8.372345	-4.878142
C	-3.318005	-8.979934	-3.732967
C	-4.604746	-8.636255	-3.546980
C	-5.240972	-8.967463	-2.414430
C	-4.606444	-9.650716	-1.446829
C	-3.352469	-10.080265	-1.676749
C	-2.714074	-9.747764	-2.809251
C	-5.230468	-9.794393	-0.067483
Cl-	0.225712	-3.047620	6.247996
Cl-	-0.826609	-10.152797	1.608062
Cl-	-5.510147	-5.641021	-6.421050
Cl-	-3.701190	0.918231	-2.099945
C	-7.930717	-6.464284	10.275044
C	-7.785996	-5.200118	9.833658
C	-7.883292	-4.959287	8.501529
C	-8.121539	-5.971881	7.633779
C	-8.252005	-7.224040	8.106236
C	-8.159725	-7.466356	9.418485
C	-7.533066	-4.184547	10.696634
C	-7.384713	-2.936778	10.213103
C	-7.474031	-2.698629	8.901483
C	-7.722366	-3.699917	8.053241
O	-7.456824	-4.468572	12.035918
C	-7.352627	-3.398917	12.984473
C	-7.443906	-3.969384	14.394086
O	-6.280122	-4.738964	14.659631
C	-6.319817	-5.339267	15.948038
C	-5.088615	-6.218127	16.119944

O	-5.168711	-7.275688	15.177485
C	-4.076309	-8.179414	15.251040
C	-4.140969	-9.080824	14.025880
O	-3.919764	-8.280187	12.872585
C	-4.200932	-8.980746	11.670858
C	-4.168773	-7.980085	10.520466
O	-2.827667	-7.577006	10.197977
C	-2.121840	-8.279537	9.254350
C	-1.045999	-7.705273	8.665633
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H	-7.446320	-0.614411	-5.365976
H	-8.811296	0.116774	-4.492693
H	-7.603941	-0.453708	-2.270981
H	-8.020712	-1.883234	-3.252774
H	2.052314	-5.538413	0.056966
H	1.516128	-6.300839	1.599030
H	3.599217	-4.885665	1.811041
H	2.621895	-3.433910	1.412575
H	4.030390	-4.553446	4.013505
H	2.708382	-4.266610	5.152797
H	2.378560	-1.930191	4.131169
H	3.898147	-2.189802	5.033896
H	4.743596	-0.353151	3.818740
H	3.337543	-0.215910	2.715126
H	5.518233	0.620031	1.704844
H	6.198967	-1.031049	1.862901
H	6.472284	-1.139937	-0.456913
H	5.744929	0.483655	-0.689142
H	3.845839	-0.599455	-1.987506
H	5.464631	-0.798658	-2.757254
H	1.838713	-8.248683	10.356134
H	-1.383717	-7.579574	13.851199
H	-1.235998	-9.797213	12.870315
H	1.530206	-6.121560	11.483881
H	-1.150163	-11.468786	11.960679

H	1.664418	-11.921822	8.098565
H	1.811223	-9.858067	9.348800
H	-1.143453	-13.443445	10.561983
H	-1.754185	-6.006194	5.869832
H	-5.323442	-4.939342	8.885068
H	-5.498095	-7.020450	7.640490
H	-1.823255	-3.980400	7.201384
H	-1.785942	-7.642237	4.895736
H	-5.174639	-10.926101	5.798309
H	-5.415274	-8.752132	6.844404
H	-1.761667	-9.857889	3.942313
H	-4.280844	-4.617936	11.157185
H	-2.921036	-5.547967	12.912755
H	0.501978	-3.648980	11.264282
H	-0.855656	-2.741080	9.491866
H	-3.963694	-13.357770	6.440111
H	-2.515833	-14.241366	8.135061
H	0.869275	-12.836378	5.988856
H	-0.585238	-11.966323	4.277618
H	-0.276898	-14.734716	8.994795
H	1.163715	-14.174892	8.094645
H	0.750306	-4.916847	13.288846
H	-0.701766	-5.515940	14.164660
H	-4.291329	-12.284636	4.260052
H	-2.880912	-11.738736	3.297133
H	-4.478653	-2.925078	9.229005
H	-2.966356	-2.436872	8.394579
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H	1.967700	-2.184277	-1.146258
H	1.367704	-4.247653	-2.283294
H	-1.549158	-0.456436	-2.040839
H	0.778009	-5.863316	-3.123200
H	-3.681079	-6.156226	-4.848056
H	-2.964909	-4.013904	-4.003329
H	-0.154517	-7.912142	-4.037935
H	-5.524753	-4.006987	2.235294
H	-1.122079	-3.697399	4.123850
H	-1.810071	-5.837622	3.256532
H	-4.616558	-1.943433	3.131204
H	-6.118763	-5.655291	1.456531
H	-3.161866	-9.419357	1.265145
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H	-6.672850	-7.727882	0.330194
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H	1.489882	-1.396901	1.441731
H	-1.845903	0.850402	0.090553
H	-3.050175	0.273539	2.091368
H	-2.805620	-10.647429	-0.903327
H	-1.660216	-10.051458	-2.936147
H	-5.130308	-8.018176	-4.294962
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H	-1.687714	-9.033994	-5.194150
H	-3.163580	-8.183716	-5.769186
H	0.192734	0.803022	-1.267598
H	1.656596	-0.042597	-0.660584
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H	-1.696457	-1.606179	4.961607
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4. 12DNP-[7]Rotaxane, MM3, Total Charge: 0

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C	-18.521178	-5.270196	-20.932913
O	-18.084677	-6.144324	-21.967821
C	-16.678582	-6.354253	-21.989742
C	-16.373290	-7.558258	-22.866464
O	-17.065425	-8.685698	-22.347330
C	-16.670772	-9.886286	-22.994593
C	-17.711707	-10.967953	-22.754142
O	-17.771233	-11.293274	-21.361250
C	-18.616308	-12.295073	-20.955998
C	-18.573491	-12.691297	-19.661190
C	-19.368989	-13.694388	-19.219531
C	-20.208375	-14.278701	-20.088387
C	-20.261995	-13.891373	-21.365170
C	-19.466867	-12.910473	-21.798014
C	-19.317119	-14.104720	-17.929081
C	-18.483066	-13.475672	-17.084362
C	-17.699529	-12.484497	-17.512566
C	-17.739922	-12.100507	-18.790265
O	-20.141201	-15.128043	-17.536500
C	-20.260126	-15.485399	-16.154911
C	-19.112671	-16.378119	-15.689280
O	-19.270379	-17.690773	-16.207149
C	-18.247059	-18.549767	-15.717847
C	-18.532767	-19.978293	-16.157020
O	-17.484792	-20.804181	-15.666557
C	-17.707019	-22.196743	-15.848358
C	-17.494716	-22.631926	-17.293414
O	-16.134971	-22.429418	-17.659430
C	-15.881367	-22.935499	-18.965267
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C	-10.624892	-7.154191	-26.614974
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H -6.541487 -13.847539 -13.444671
H -15.073473 -16.574062 -13.797661

H	-15.016627	-18.537134	-15.163368
H	-13.865296	-20.856064	-11.791919
H	-13.929381	-18.880098	-10.422007
H	-7.865455	-12.812720	-18.048676
H	-7.878078	-14.691139	-19.565825
H	-5.156623	-16.741264	-17.036645
H	-5.139773	-14.867765	-15.528651
H	-6.893450	-16.847368	-20.304550
H	-5.713496	-17.680488	-19.235981
H	-13.881312	-21.918143	-13.941100
H	-14.987109	-21.216613	-15.161263
H	-6.754125	-11.621941	-16.143092
H	-5.664424	-12.547535	-15.058133
H	-15.189623	-15.682523	-11.282870
H	-14.129600	-16.543216	-10.139196
Cl-	-15.417515	-13.837120	-15.149023
Cl-	-6.684807	-10.486182	-13.505343
Cl-	-6.819985	-19.914616	-20.476364
Cl-	-12.252937	-11.018149	-22.470255

C. XYZ coordinates for the minimum energy structures for the mDNP-[n]Rotaxanes in a high dielectric medium

1. 3DNP-[3]Rotaxane, MM3, Total Charge: 0

Cl-	-6.128409	5.069186	-0.319095
Cl-	9.201006	-5.058219	4.305861
Cl-	4.598106	-0.023078	7.177255
Cl-	-0.109599	-5.567052	-2.537007
Cl-	1.174884	6.491378	3.875994
Cl-	8.781583	-13.099091	3.894550
Cl-	5.205464	1.741615	3.192236
Cl-	-4.138778	-2.381866	9.092296
C	1.007994	-6.794674	1.702392
C	1.837980	-5.749233	1.910798
C	1.788767	-5.228016	3.155488
C	1.003416	-5.759433	4.099434
N	0.270693	-6.787165	3.870405
C	0.248170	-7.287223	2.688931
C	2.703635	-5.293441	0.954732
C	2.779671	-5.839701	-0.277626
C	3.710873	-5.447797	-1.154964
N	4.570967	-4.540134	-0.867540
C	4.501249	-3.952698	0.271210
C	3.592555	-4.304156	1.189555
C	5.716850	-4.267434	-1.791764
C	6.886458	-5.194263	-1.496407
C	7.790746	-4.883859	-0.552659
C	8.683139	-5.795004	-0.138204

C	8.689149	-7.033446	-0.659893
C	7.839615	-7.314909	-1.661459
C	6.947954	-6.404640	-2.074740
C	9.529515	-8.137792	-0.034338
N	8.793241	-8.820106	1.078452
C	7.976237	-9.777329	0.824447
C	7.194213	-10.307553	1.773549
C	7.230186	-9.855714	3.046609
C	8.138891	-8.881974	3.273654
C	8.896025	-8.391874	2.283818
C	6.373912	-10.307232	4.015187
C	6.359514	-9.801211	5.267790
C	5.434395	-10.177481	6.159992
N	4.524589	-11.034971	5.869044
C	4.539874	-11.591696	4.712384
C	5.437857	-11.252378	3.778396
C	3.384512	-11.282008	6.810614
C	2.220023	-10.345965	6.514387
C	2.210934	-9.096072	7.007907
C	1.312399	-8.198802	6.579112
C	0.402167	-8.532002	5.648561
C	0.360043	-9.803277	5.215378
C	1.259340	-10.700985	5.643963
C	-0.456584	-7.459800	4.992811
O	-2.359503	-5.001715	7.364917
C	-3.449136	-5.880434	7.110070
C	-4.421322	-5.228111	6.140301
O	-3.813142	-5.114950	4.849241
C	-4.538388	-4.583087	3.813634
C	-5.795807	-4.127051	3.966462
C	-6.466683	-3.612744	2.932679
C	-5.893730	-3.541102	1.729357
C	-4.641374	-3.995984	1.537361
C	-3.963565	-4.522492	2.588081
C	-2.712567	-4.977378	2.389948
C	-2.144666	-4.908358	1.182976
C	-2.808725	-4.375864	0.155203
C	-4.064396	-3.928514	0.314641
O	-4.774176	-3.355708	-0.702253
C	-4.119849	-2.935966	-1.904785
C	-5.117617	-2.096204	-2.685099
O	-5.425630	-0.954586	-1.896039
C	-6.646598	-0.332039	-2.265174
C	-6.918396	0.794242	-1.282022
O	-7.000529	0.239248	0.024717
C	-7.269478	1.221813	1.013503
C	-7.139470	0.594809	2.392706
O	-5.795345	0.176474	2.603921
C	-5.587449	-0.259673	3.940356
C	-4.191603	-0.841422	4.106734
O	-3.194978	0.179964	3.966565

C	-2.426163	0.320457	2.842955
C	-1.333815	1.118670	2.921393
C	-0.512668	1.283747	1.856640
C	-0.804186	0.630724	0.720162
C	-1.874369	-0.165299	0.639841
C	-2.678873	-0.324232	1.692192
C	0.576886	2.087495	1.944249
C	0.817627	2.729826	3.101507
C	0.015968	2.565217	4.152433
C	-1.046995	1.766095	4.061399
O	1.381491	2.250681	0.843919
C	2.374011	3.285466	0.877744
C	3.190198	3.277355	-0.402500
O	3.962421	2.084627	-0.451723
C	4.934379	2.123832	-1.487255
C	5.691350	0.806263	-1.524471
O	6.376873	0.622703	-0.292965
C	7.319479	-0.438363	-0.364455
C	7.847594	-0.737778	1.029315
O	6.811850	-1.340043	1.793245
C	7.227620	-1.641132	3.118028
C	6.129324	-2.426155	3.814834
O	4.963920	-1.604992	3.950792
C	-1.547788	-5.480590	8.429760
C	-0.457258	-4.470451	8.747728
O	0.496121	-4.432582	7.693857
C	1.593759	-3.592048	8.026373
C	2.647809	-3.652037	6.933656
O	3.178890	-4.970329	6.878352
C	4.435385	-5.019157	6.217954
C	4.907313	-6.467922	6.152752
O	4.218586	-7.192733	5.124003
C	4.668520	-7.151280	3.829122
C	4.140094	-8.012885	2.926266
C	4.568804	-8.021229	1.640849
C	5.539739	-7.165670	1.283284
C	6.073909	-6.325254	2.171325
C	5.646629	-6.320643	3.433363
C	4.029288	-8.875589	0.736957
C	3.085311	-9.742224	1.145610
C	2.663360	-9.740735	2.410880
C	3.182144	-8.879662	3.288249
O	4.489348	-8.844502	-0.555266
C	4.081758	-9.869381	-1.469519
C	4.667851	-9.594113	-2.846498
O	3.986469	-8.493096	-3.435315
C	4.415905	-8.246688	-4.768934
C	3.471510	-7.254234	-5.430160
O	3.596795	-5.977541	-4.817899
C	2.686312	-5.039612	-5.378704
C	2.858805	-3.689459	-4.701130

O	4.121543	-3.144778	-5.058574
C	4.318418	-1.846337	-4.515054
C	5.677831	-1.325157	-4.951841
O	6.706710	-2.115605	-4.342720
C	-1.031568	-0.159250	-2.819840
C	-0.514341	1.074573	-2.945557
C	0.795540	1.250795	-2.709200
C	1.550733	0.236856	-2.267708
C	1.014117	-0.974904	-2.056161
C	-0.274027	-1.174820	-2.380340
C	1.806344	-2.042774	-1.318192
N	1.592830	-1.957425	0.161027
C	0.609575	-2.575934	0.704807
C	0.307110	-2.419468	1.998886
C	1.027516	-1.601446	2.794468
C	2.078217	-1.006737	2.187583
C	2.332385	-1.199618	0.886801
C	0.677775	-1.346038	4.092793
C	1.362722	-0.481308	4.871788
C	0.928162	-0.155216	6.095271
N	-0.152630	-0.646620	6.582719
C	-0.802144	-1.521782	5.904010
C	-0.415637	-1.887609	4.674961
C	-0.710437	-0.108324	7.865176
C	-1.566303	1.125761	7.614054
C	-1.012329	2.350058	7.588357
C	-1.712919	3.408308	7.155075
C	-2.983266	3.265052	6.741219
C	-3.561510	2.056312	6.845513
C	-2.860001	0.998179	7.274768
C	-3.700728	4.402958	6.027464
N	-3.507443	4.324139	4.543083
C	-2.511882	4.906232	3.978068
C	-2.227315	4.719157	2.681405
C	-2.976625	3.901777	1.909778
C	-4.040380	3.357168	2.537791
C	-4.279497	3.584353	3.834193
C	-1.414662	2.277834	-3.187094
N	-1.915269	2.837346	-1.889557
C	-2.985289	2.370089	-1.357751
C	-3.372068	2.725738	-0.126889
C	-2.655506	3.600008	0.612992
C	-1.567135	4.103551	-0.009181
C	-1.226739	3.708228	-1.243568
H	-0.894618	4.825791	0.476755
H	-3.524401	1.620725	-1.956891
H	-4.276794	2.234109	0.256210
H	-0.316769	4.063033	-1.750821
H	-4.736037	2.677034	2.029864
H	-1.885745	5.520491	4.642613
H	-1.332894	5.230340	2.296664

H	-5.112734	3.111738	4.375373
H	2.746005	-0.311205	2.715462
H	0.014681	-3.201645	0.023933
H	-0.574687	-2.962687	2.364556
H	3.154247	-0.692473	0.359258
H	2.274943	0.027246	4.527225
H	-1.720604	-1.902458	6.375984
H	-1.061902	-2.612800	4.158837
H	1.433439	0.592254	6.725094
H	2.603943	0.421550	-2.007009
H	1.240393	2.254060	-2.806322
H	-2.105970	-0.326699	-3.002740
H	-0.737172	-2.160745	-2.210362
H	-3.334177	0.003448	7.276207
H	-4.600215	1.910709	6.506320
H	-1.213063	4.387626	7.069298
H	0.050741	2.479342	7.851510
H	-4.797369	4.384300	6.214659
H	-3.329659	5.399988	6.352620
H	-0.883097	3.100613	-3.714430
H	-2.307095	2.016578	-3.797829
H	-1.291198	-0.928559	8.341020
H	0.154722	0.109939	8.529723
H	1.512935	-3.068501	-1.630017
H	2.900163	-1.946875	-1.491742
H	-1.690304	1.652751	4.942874
H	0.235442	3.094816	5.093600
H	-3.550034	-0.987543	1.579735
H	-0.161385	0.740111	-0.164386
H	-4.104135	-1.254759	5.133370
H	-4.008148	-1.696899	3.432077
H	-6.340345	-1.030922	4.203418
H	-5.729005	0.589864	4.639631
H	-7.426638	1.340658	3.163475
H	-7.826036	-0.271995	2.488447
H	-8.296478	1.618253	0.871577
H	-6.568268	2.073363	0.913667
H	-6.106904	1.548837	-1.329169
H	-7.871057	1.302539	-1.538782
H	-7.478141	-1.066700	-2.236582
H	-6.571213	0.063419	-3.299342
H	-4.691695	-1.773868	-3.657525
H	-6.030314	-2.692728	-2.891716
H	-3.810633	-3.819127	-2.501480
H	-3.220642	-2.330961	-1.669560
H	1.679090	3.402871	3.225337
H	-2.099975	-0.697010	-0.297550
H	-1.119626	-5.282515	1.033157
H	-2.128139	-5.411891	3.217295
H	-7.495508	-3.240356	3.074344
H	-6.477552	-3.103466	0.902024

H	-2.304911	-4.321823	-0.822227
H	-6.305907	-4.158660	4.941998
H	-5.334449	-5.856657	6.070529
H	-4.710233	-4.225808	6.519880
H	-3.982295	-6.102329	8.058489
H	-3.077730	-6.843210	6.702736
H	-1.102698	-6.461468	8.163821
H	-2.173447	-5.632392	9.334508
H	-0.896005	-3.463065	8.902150
H	0.044457	-4.765831	9.693246
H	2.041590	-3.909864	8.991108
H	1.239882	-2.548282	8.151929
H	2.221211	-3.371196	5.949533
H	3.453374	-2.926057	7.168287
H	5.173892	-4.416110	6.786656
H	4.347633	-4.578034	5.205404
H	6.005132	-6.541732	6.020392
H	4.698938	-6.961053	7.124562
H	2.629684	-10.469522	0.456139
H	1.883787	-10.452655	2.728576
H	2.814386	-8.898871	4.321979
H	5.915298	-7.146554	0.251011
H	6.872577	-5.630124	1.870419
H	6.121501	-5.615612	4.131240
H	1.878016	4.272758	0.992948
H	3.064377	3.137683	1.732240
H	2.531646	3.348856	-1.290612
H	3.861961	4.161341	-0.411371
H	5.641355	2.961859	-1.314147
H	4.436335	2.298120	-2.464065
H	4.997203	-0.041444	-1.698105
H	6.418221	0.825253	-2.363294
H	6.849332	-1.344883	-0.795569
H	8.156574	-0.143820	-1.031404
H	8.198846	0.193559	1.519964
H	8.710901	-1.432365	0.959823
H	8.156462	-2.248018	3.091906
H	7.449536	-0.705642	3.671803
H	5.880521	-3.337728	3.234387
H	6.472652	-2.750616	4.819852
H	4.303768	-2.097129	4.420497
H	4.440445	-10.854853	-1.103426
H	2.975472	-9.904430	-1.551833
H	5.754269	-9.385020	-2.776500
H	4.539420	-10.494596	-3.483193
H	4.407231	-9.193894	-5.348108
H	5.456457	-7.862758	-4.772256
H	3.715662	-7.171860	-6.510149
H	2.425580	-7.617301	-5.349099
H	2.857975	-4.943092	-6.470998
H	1.646000	-5.397981	-5.232768

H	2.786395	-3.798897	-3.600249
H	2.048791	-3.003254	-5.026055
H	3.521415	-1.163054	-4.875981
H	4.258907	-1.880383	-3.408403
H	5.774434	-1.364139	-6.057216
H	5.795288	-0.264886	-4.643492
H	7.547499	-1.767724	-4.609173
H	3.640784	-3.773496	2.151084
H	3.830153	-5.918007	-2.141518
H	2.116616	-6.653987	-0.603388
H	5.270477	-3.189123	0.457736
H	0.944583	-7.313368	0.734665
H	0.975649	-5.383005	5.131615
H	2.406913	-4.371496	3.460855
H	-0.396576	-8.169836	2.560417
H	8.277133	-8.424636	4.264231
H	7.929763	-10.093581	-0.228688
H	6.501588	-11.097601	1.448225
H	9.609437	-7.567649	2.432593
H	7.069900	-9.029926	5.599336
H	3.731499	-12.314524	4.524264
H	5.341668	-11.754844	2.804734
H	5.364304	-9.734208	7.164855
H	9.365134	-5.543268	0.691090
H	7.753526	-3.900258	-0.055666
H	6.210617	-6.681970	-2.844448
H	7.822775	-8.325593	-2.101084
H	1.251686	-11.717365	5.216199
H	-0.371028	-10.098298	4.444259
H	1.371837	-7.160800	6.944847
H	2.992609	-8.778684	7.717622
H	-1.396830	-7.875922	4.568083
H	-0.746107	-6.664067	5.712209
H	5.987123	-3.196798	-1.671173
H	5.337391	-4.397253	-2.828551
H	3.100402	-12.352239	6.702752
H	3.774897	-11.147214	7.843543
H	9.801575	-8.924366	-0.772755
H	10.479659	-7.746164	0.391596

2. 6DNP-[4]Rotaxane, MM3, Total Charge: 0

C	-45.534737	-4.848202	-2.259082
C	-45.744827	-3.759983	-1.494879
C	-46.504691	-3.880713	-0.378676
C	-47.055218	-5.072871	-0.052210
C	-46.806805	-6.145020	-0.823706
C	-46.057242	-6.030778	-1.923248
C	-46.699296	-2.799334	0.397771
C	-46.167506	-1.620726	0.069027
C	-45.429459	-1.500878	-1.036679

C	-45.208324	-2.562946	-1.830958
O	-44.459079	-2.488703	-2.973773
C	-43.867540	-1.246809	-3.368080
C	-43.094888	-1.471674	-4.657406
O	-44.004547	-1.794929	-5.701437
C	-43.326538	-2.043120	-6.925364
C	-44.336854	-2.316266	-8.027933
O	-45.101613	-1.140193	-8.258656
C	-45.871624	-1.223831	-9.450049
C	-46.641328	0.075602	-9.636360
O	-47.738940	0.113961	-8.734598
C	-48.373183	1.386385	-8.721264
C	-49.809782	1.263288	-8.237515
O	-49.871795	0.799754	-6.879770
C	-50.231652	-0.490911	-6.595224
C	-50.729217	-0.767169	-5.365194
C	-51.141512	-2.017718	-5.050108
C	-51.047748	-2.978882	-5.982934
C	-50.566634	-2.710573	-7.198448
C	-50.171549	-1.475582	-7.506775
C	-50.828658	0.193767	-4.433521
C	-51.319128	-0.068271	-3.220271
C	-51.729776	-1.300535	-2.917323
C	-51.644616	-2.289741	-3.821916
O	-52.081098	-3.560650	-3.563359
C	-52.783482	-3.855496	-2.349827
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H	-49.894380	5.969832	3.462291
H	-48.974519	6.027636	4.996164
H	-47.885563	3.843132	4.475890
H	-47.560511	5.075740	3.215568
H	-47.384578	3.526150	1.275799
H	-47.131327	2.485251	2.711675
H	-49.314419	2.020428	0.571647
H	-47.740575	1.155852	0.681695
H	-50.675126	5.642767	6.623639
H	-63.246014	4.478227	0.826887
H	-61.612324	4.052547	1.454296
H	-62.549925	1.768248	2.135398
H	-63.241581	3.169428	3.014416

H	-64.625878	0.584172	2.711294
H	-65.235607	2.079687	3.489739
H	-67.081699	2.198660	1.739183
H	-67.172753	0.760226	2.806769
H	-68.429443	-0.325209	1.113213
H	-68.248978	1.046075	-0.029485
H	-67.096103	-1.794326	-0.460273
H	-68.615618	-1.177881	-1.188617
H	-66.259815	-2.075255	-2.686045
H	-67.725131	-1.338137	-3.415506
H	-65.820445	-1.001390	-4.949339
H	-66.286375	0.586303	-4.278683
H	-64.570536	0.319692	-2.750332
H	-51.371783	-4.005262	-5.761810
H	-50.499271	-3.504887	-7.958067
H	-52.136541	-1.479532	-1.911328
H	-50.502178	1.217487	-4.657079
H	-53.599548	-3.123919	-2.187142
H	-52.086497	-3.815620	-1.487570
H	-54.112085	-5.254325	-3.321485
H	-52.581705	-5.974055	-2.720085
H	-53.909640	-7.635261	-1.815577
H	-55.481327	-6.838656	-2.138820
H	-55.858947	-6.633447	0.365214
H	-55.695504	-8.330288	-0.188129
H	-54.811412	-9.160148	1.853139
H	-55.178456	-7.546185	2.544325
H	-53.369967	-8.835799	3.809948
H	-52.340980	-8.764735	2.341975
H	-50.685427	-7.277176	3.305819
H	-51.567291	-7.676236	4.813825
H	-52.085223	-5.227201	5.149614
H	-50.324440	-5.617601	5.176338
H	-49.790065	-1.299020	-8.523558
H	-51.389635	0.734544	-2.469009
H	-50.034159	-1.296246	6.286693
H	-49.434309	0.169687	4.481177
H	-50.077929	-2.511081	-0.607547
H	-50.677039	-3.985578	1.194296
H	-50.771662	-3.536723	5.866342
H	-49.334549	-0.259983	-0.171417
H	-50.273559	2.270691	-8.269032
H	-50.424906	0.642718	-8.916713
H	-48.379009	1.820650	-9.743219
H	-47.799085	2.078115	-8.070966
H	-45.970528	0.944173	-9.469153
H	-47.022465	0.138254	-10.677411
H	-46.567500	-2.087135	-9.401664
H	-45.004601	-3.158121	-7.753612
H	-43.796122	-2.604681	-8.953634
H	-42.696243	-1.171008	-7.198051

H	-42.655778	-2.919931	-6.807652
H	-42.357432	-2.290327	-4.523004
H	-42.534632	-0.550470	-4.922021
H	-43.171278	-0.892178	-2.579063
H	-44.647994	-0.473802	-3.524265
H	-45.196447	-1.380193	-10.317428
H	-53.447532	-1.360087	-8.728979
H	-54.847081	-4.494225	-5.372771
H	-54.810437	-2.150129	-4.761722
H	-53.553843	-3.746227	-9.116474
H	-54.563241	-0.311510	-4.311719
H	-52.782141	2.730119	-7.578290
H	-53.214063	0.458798	-8.285565
H	-54.055679	2.007410	-3.817425
H	-47.041057	-2.527458	-6.510640
H	-49.102840	-5.441316	-3.295803
H	-48.665508	-3.158123	-2.615985
H	-47.560289	-4.841341	-6.978706
H	-46.831914	-0.687149	-6.132395
H	-48.224862	1.079082	-1.890531
H	-48.369527	-1.321644	-2.206161
H	-46.775412	1.673044	-5.608694
H	-49.526255	-6.064544	-8.091552
H	-51.766884	-5.674266	-8.914570
H	-53.333144	-6.613969	-5.099286
H	-51.087940	-6.990593	-4.269303
H	-49.834944	3.090913	-2.036940
H	-52.111740	3.456033	-2.783914
H	-50.729398	4.077931	-6.727081
H	-48.455152	3.691533	-5.993322
H	-53.705727	4.122488	-4.505351
H	-53.135579	4.440541	-6.172672
H	-54.236785	-5.801698	-8.576441
H	-54.878599	-6.129785	-6.935914
H	-47.421685	3.103175	-2.481136
H	-46.817260	3.370656	-4.147068
H	-48.683470	-7.199520	-4.651033
H	-48.017015	-6.924911	-6.288928
H	-43.329213	-0.820743	1.180982
H	-42.813528	0.888913	1.039912
H	-44.011156	1.402957	3.227122
H	-45.112722	0.838073	1.933038
H	-46.718438	-0.097296	3.510936
H	-45.687326	0.683287	4.753889
H	-45.205306	-1.603195	5.748051
H	-46.931750	-1.129327	5.840092
H	-47.270636	-3.512275	6.073460
H	-45.578440	-3.946186	5.664035
H	-47.222565	-5.765671	5.062659
H	-48.066146	-4.619719	3.969251
H	-46.393452	-7.234393	3.341245

H	-45.596253	-6.520693	1.924747
H	-47.935486	-7.230858	1.348210
H	-48.588986	-6.249434	2.652611
H	-45.872329	-6.913903	-2.558067
H	-44.923724	-4.790965	-3.174837
H	-46.340500	-0.744295	0.713339
H	-47.296919	-2.859057	1.322397
H	-47.228474	-7.132996	-0.581120
H	-45.010829	-0.510878	-1.273811
H	-41.238014	-0.437229	2.098478

3. 12DNP-[7]Rotaxane, MM3, Total Charge: 0

Cl-	2.960524	-21.993087	-2.773685
Cl-	-4.250679	-8.596389	4.223375
Cl-	6.155508	-12.344783	8.925854
Cl-	-3.207472	-11.944652	2.325336
Cl-	4.818868	-5.076262	-3.053267
Cl-	2.455760	-18.337266	17.323342
Cl-	9.966270	-11.056767	-4.611337
Cl-	-10.169403	-22.225294	-2.318603
Cl-	6.791032	-24.480409	14.774737
Cl-	8.445177	-16.558393	7.484764
Cl-	8.217936	-26.247682	1.779844
Cl-	1.088494	-30.944203	2.391748
Cl-	-4.035445	-12.107139	10.641006
Cl-	-5.461581	-28.764616	6.401027
Cl-	-0.361653	-22.892446	4.380551
Cl-	4.867497	-29.777881	10.842572
Cl-	1.945759	-18.701130	-9.058339
Cl-	4.265578	-19.667007	-5.828967
Cl-	-2.334102	-6.106164	-7.372551
Cl-	0.296229	-28.997304	-1.068545
Cl-	3.863418	-7.749329	-7.289538
Cl-	10.429360	-8.878919	1.959785
Cl-	14.136650	-16.413132	-0.113329
Cl-	-7.192292	-21.238931	9.321682
C	8.101309	-17.763014	-4.379118
C	7.059501	-17.902245	-3.561562
C	7.236360	-18.280279	-2.285002
C	8.493230	-18.552941	-1.854704
C	9.556916	-18.408883	-2.682967
C	9.337781	-18.007771	-3.944147
C	8.713677	-18.974177	-0.600163
C	9.948279	-19.256887	-0.178217
C	10.990020	-19.113048	-0.996259
C	10.815424	-18.666261	-2.250546
O	11.859998	-18.515886	-3.125252
C	13.114319	-19.151175	-2.847134
C	14.126480	-18.742279	-3.905248
O	14.468560	-17.377366	-3.703630

C	15.385695	-16.898092	-4.677126
C	15.872780	-15.516726	-4.268646
O	14.771683	-14.619868	-4.224502
C	15.183156	-13.275297	-4.014412
C	13.951165	-12.405934	-3.802320
O	13.325247	-12.712719	-2.560255
C	13.855368	-11.968666	-1.470552
C	13.159872	-12.390318	-0.185651
O	11.767750	-12.085252	-0.304359
C	10.904453	-12.364089	0.720112
C	9.577616	-12.325356	0.456542
C	8.673866	-12.607313	1.426955
C	9.119871	-12.930054	2.655685
C	10.429644	-12.991053	2.911181
C	11.316479	-12.718872	1.949798
C	7.346915	-12.574204	1.156666
C	6.940253	-12.291340	-0.093292
C	7.829979	-12.007804	-1.047443
C	9.135447	-12.015609	-0.775089
O	6.479079	-12.867822	2.171633
C	5.076657	-13.029033	1.936343
C	4.381496	-13.049571	3.286338
O	4.826659	-14.167982	4.044283
C	4.499869	-14.013548	5.418207
C	4.968601	-15.215033	6.225517
O	4.068467	-16.307774	6.098469
C	4.359295	-17.201757	5.035994
C	3.360361	-18.345960	5.101906
O	3.565959	-19.052374	6.318452
C	2.551839	-20.012289	6.572143
C	2.825899	-20.674218	7.920369
O	3.894494	-21.624289	7.836574
C	3.645650	-22.899334	7.405191
C	4.624724	-23.828879	7.518855
C	4.419453	-25.102878	7.108147
C	3.218758	-25.429796	6.605454
C	2.245238	-24.523019	6.515239
C	2.452986	-23.269813	6.912793
C	5.404677	-26.027747	7.201984
C	6.582047	-25.670956	7.744964
C	6.785879	-24.419646	8.161120
C	5.818380	-23.507946	8.041422
O	6.178550	-18.445643	-1.426284
C	4.852402	-18.450947	-1.972091
C	3.842236	-18.742437	-0.875442
O	3.695004	-17.596530	-0.048416
C	2.772815	-17.825620	1.009569
C	2.363143	-16.495105	1.620398
O	1.576572	-15.808167	0.659604
C	1.037717	-14.563720	1.077548
C	-0.095378	-14.739521	2.077694

O	-1.074424	-15.589190	1.502558
C	-2.210964	-15.779208	2.334487
C	-2.959806	-16.993236	1.812259
O	-2.105622	-18.126386	2.003419
C	-2.295536	-19.274340	1.290000
C	-1.279909	-20.167865	1.242653
C	-1.398109	-21.298642	0.504192
C	-2.534838	-21.509178	-0.186568
C	-3.532236	-20.622691	-0.142238
C	-3.416864	-19.513393	0.590481
C	-0.137947	-19.947907	1.921669
C	0.867566	-20.825240	1.867996
C	0.748229	-21.937942	1.139617
C	-0.383125	-22.193373	0.458298
O	-0.550111	-23.314861	-0.307261
C	0.533248	-24.232961	-0.478501
C	0.140692	-25.248946	-1.536764
O	-0.086708	-24.558673	-2.757288
C	-0.203551	-25.435601	-3.867876
C	-0.591164	-24.616800	-5.089668
O	-1.943833	-24.200849	-4.955249
C	-2.324703	-23.274996	-5.964126
C	-3.838941	-23.143444	-5.976169
O	-4.285939	-22.626905	-4.730035
C	-5.692137	-22.417718	-4.724742
C	-6.129937	-21.960839	-3.342904
O	-5.911525	-23.031138	-2.419173
C	-6.298254	-22.902418	-1.112511
C	-6.879930	-21.791473	-0.632482
C	-7.241729	-21.715234	0.648717
C	-7.040458	-22.747288	1.471445
C	-6.464038	-23.876739	1.024348
C	-6.087473	-23.945479	-0.277300
C	-5.508155	-25.070162	-0.730010
C	-5.324811	-26.110330	0.082130
C	-5.714069	-26.050080	1.357576
C	-6.267529	-24.929694	1.853662
O	-6.699272	-24.836947	3.152242
C	-6.905167	-26.044256	3.895659
C	-7.582804	-25.719836	5.219336
O	-6.618093	-25.195671	6.119375
C	-7.170645	-24.898187	7.395256
C	-6.034387	-24.690976	8.384819
O	-5.381528	-25.936304	8.585353
C	-4.178703	-25.817034	9.331937
C	-3.785513	-27.201172	9.822787
O	-2.557907	-27.104209	10.530119
C	-2.300284	-28.248974	11.332598
C	-0.898434	-28.130245	11.907490
O	-0.819666	-26.898581	12.630965
O	5.150174	-27.298351	6.754610

C	6.122561	-28.328515	6.959462
C	5.631260	-29.621212	6.324811
O	5.726081	-29.521448	4.908116
C	5.359842	-30.738327	4.269176
C	5.735949	-30.691570	2.795637
O	4.927029	-29.749536	2.101829
C	5.129385	-29.834631	0.695622
C	4.248192	-28.824303	-0.023061
O	4.741496	-27.512224	0.208892
C	3.941801	-26.522366	-0.425793
C	4.628081	-25.172142	-0.291437
O	5.830329	-25.155011	-1.070460
C	0.649128	-12.207792	4.843823
C	1.558460	-11.457369	5.468311
C	1.196129	-10.613560	6.448860
C	-0.110114	-10.530010	6.795337
C	-1.039497	-11.287138	6.158835
C	-0.638711	-12.126115	5.185368
C	-0.507050	-9.697986	7.776130
C	-1.793331	-9.621810	8.125356
C	-2.704926	-10.370401	7.499386
C	-2.346683	-11.201416	6.504123
O	-3.247148	-11.994847	5.842912
C	-4.595611	-12.098346	6.313555
C	-5.385238	-12.993190	5.370612
O	-4.826741	-14.299377	5.386029
C	-5.523091	-15.235031	4.570382
C	-6.768101	-15.756928	5.272503
O	-6.377636	-16.440199	6.456941
C	-7.487393	-16.726330	7.296237
C	-7.014577	-17.495868	8.518641
O	-6.084524	-16.703486	9.245628
C	-5.790438	-17.254143	10.523312
C	-4.658281	-16.460294	11.158969
O	-3.450852	-16.751589	10.448817
C	-2.263130	-16.191273	10.835327
C	-1.122289	-16.675966	10.292276
C	0.086633	-16.167889	10.635519
C	0.125093	-15.176386	11.538020
C	-0.996517	-14.706865	12.093014
C	-2.182378	-15.214009	11.751712
C	1.224086	-16.652492	10.077250
C	1.121267	-17.641837	9.174178
C	-0.062434	-18.152542	8.846168
C	-1.174492	-17.674738	9.399531
O	2.446463	-16.131816	10.434125
C	3.607881	-16.692375	9.802526
C	4.885467	-16.033898	10.291530
O	5.126242	-16.406750	11.640779
C	6.442203	-16.065378	12.057256
C	6.582830	-16.323627	13.548959

O	6.390079	-17.707064	13.806332
C	6.472817	-18.004306	15.193932
C	6.230987	-19.491072	15.392227
O	4.886871	-19.786322	15.039164
C	4.616397	-21.178970	15.094045
C	3.163064	-21.410346	14.716696
O	2.960134	-22.820213	14.584244
C	1.744029	-23.301381	14.182942
C	1.660719	-24.603090	13.818767
C	0.479274	-25.123227	13.404499
C	-0.601279	-24.321806	13.345780
C	-0.515480	-23.034764	13.690281
C	0.648583	-22.525768	14.100799
C	0.391898	-26.428675	13.056134
C	1.498134	-27.192532	13.085293
C	2.664445	-26.682374	13.489290
C	2.744475	-25.401262	13.858852
O	2.101402	-9.843104	7.127749
C	3.500687	-9.984764	6.859982
C	4.270722	-9.096866	7.823337
O	3.952112	-7.740536	7.551606
C	4.640749	-6.843402	8.411785
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O	4.738397	-5.197125	6.690785
C	4.391964	-3.910625	6.201894
C	4.789703	-3.824290	4.737380
O	4.079693	-4.818589	4.009725
C	4.268969	-4.725017	2.602041
C	3.129953	-3.922915	1.978786
O	1.905394	-4.669421	1.997152
C	1.642389	-5.623619	1.048583
C	0.430212	-6.230551	1.058450
C	0.118303	-7.164439	0.129907
C	1.037680	-7.486206	-0.792864
C	2.230119	-6.890724	-0.812529
C	2.527756	-5.959696	0.094569
C	-0.490103	-5.919937	1.984696
C	-1.682769	-6.519532	2.001882
C	-1.981845	-7.443080	1.087320
C	-1.097185	-7.761445	0.128406
O	-1.342658	-8.712690	-0.822667
C	-2.408128	-9.656786	-0.677439
C	-3.716483	-9.138949	-1.251361
O	-3.555437	-8.933401	-2.647770
C	-4.803710	-8.846141	-3.319476
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O	-5.777234	-8.500679	-5.466612
C	-5.693573	-7.968517	-6.781111
C	-6.914499	-8.421937	-7.564350
O	-6.866791	-9.836315	-7.700015
C	-7.988880	-10.348951	-8.403263

C	-7.877545	-11.863579	-8.487409
O	-7.970938	-12.406750	-7.165097
C	-8.084667	-13.760280	-6.986059
C	-7.944931	-14.638318	-7.995416
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C	-8.081613	-28.114002	-0.201658
H	-8.631670	-26.152718	-0.604072
H	-8.748371	-29.994911	2.283121
H	-9.998804	-28.046109	2.971778
H	-7.454309	-28.212657	-1.100813
H	-10.732175	-26.406851	3.562272
H	-10.244463	-22.435591	0.903103
H	-9.434505	-24.519054	-0.041094
H	-11.468757	-24.229033	4.304435
H	-2.826605	-24.097486	1.585311
H	-2.769820	-27.768461	4.686439
H	-3.520379	-25.627894	5.511365
H	-2.098332	-26.331843	0.974443

H	-3.760033	-22.494839	2.071049
H	-5.267644	-21.877289	6.589463
H	-4.055147	-23.909103	6.079106
H	-4.980592	-20.523950	2.800513
H	-2.833645	-28.834272	-0.244775
H	-4.963114	-29.605883	-1.098866
H	-6.300851	-30.283722	2.860967
H	-4.172540	-29.524630	3.709330
H	-7.686923	-21.854227	6.177089
H	-9.826683	-22.660823	5.411630
H	-9.745144	-19.863667	2.234327
H	-7.590966	-19.057452	3.004133
H	-11.947194	-22.104321	3.982235
H	-11.624159	-21.351558	2.388825
H	-7.189875	-30.467819	-0.777788
H	-7.605956	-31.179130	0.813253
H	-6.002005	-19.854730	6.113894
H	-5.704943	-19.155156	4.488884
H	-1.705853	-29.030928	3.204197
H	-1.316936	-28.377384	1.583942

D. XYZ coordinates for the 3DNP-[3]Rotaxane in the experimentally determined crystal structure and associated Mulliken charges obtained at a B3LYP/DZP level.

1. XYZ coordinates, Total Charge: +8

O	-0.933692	1.774188	25.199094
O	-2.409063	-0.667549	24.556166
O	-0.099282	-2.470578	23.995218
O	0.374244	-3.412975	21.204906
O	1.021180	-1.224228	19.360522
O	0.589618	4.477325	17.778232
O	1.242243	6.732438	15.938586
O	2.227998	6.076092	13.258014
O	4.905013	4.875563	12.413877
O	7.723297	5.071463	12.165275
H	7.139826	5.783674	12.401897
C	3.054889	2.137296	25.631246
H	3.657454	1.242105	25.864137
C	1.729478	2.033396	25.485475
H	1.271940	1.036598	25.605032
C	0.982503	3.112456	25.185285
C	-0.359839	3.004353	25.026497
C	-1.077410	4.105504	24.742794
H	-2.172021	4.067969	24.621477
C	-2.356175	1.627025	25.271732
H	-2.768350	2.310106	26.039654
H	-2.831354	1.869897	24.300050
C	-2.648250	0.185699	25.669012
H	-3.702654	0.080856	25.996176
H	-2.003359	-0.096893	26.525113
C	-2.292248	-2.033048	24.943957
H	-2.928549	-2.239724	25.827249

H	-2.683366	-2.673776	24.131585
C	-0.830167	-2.375795	25.215605
H	-0.753237	-3.319057	25.790212
H	-0.361331	-1.589831	25.841666
C	0.091043	-3.815262	23.572670
H	0.531366	-4.409053	24.399339
H	-0.881398	-4.279320	23.317065
C	1.038200	-3.861435	22.378191
H	1.376075	-4.908549	22.234033
H	1.935997	-3.241002	22.572159
C	1.184254	-3.530377	20.039325
H	1.879891	-4.387900	20.127517
H	0.526231	-3.752409	19.176525
C	1.945259	-2.237454	19.777992
H	2.690912	-2.410669	18.974503
H	2.481629	-1.922222	20.696328
C	1.479070	0.042563	19.101054
C	0.595272	0.991584	18.700615
C	-0.706808	0.696648	18.545895
H	-1.075382	-0.322399	18.735680
C	-1.579146	1.630198	18.153898
H	-2.646730	1.387269	18.025214
C	-1.165631	2.873968	17.903472
H	-1.920312	3.605693	17.576490
C	0.128746	3.209466	18.041326
C	1.008306	2.258789	18.446428
C	2.309682	2.551808	18.600906
H	2.671796	3.571012	18.407546
C	3.185949	1.617983	18.984210
H	4.254904	1.860240	19.100590
C	2.775443	0.373306	19.231854
H	3.533467	-0.362294	19.544745
C	-0.330086	5.487529	17.340576
H	-0.845605	5.169298	16.415450
H	-1.096293	5.654712	18.125574
C	0.412077	6.795301	17.093728
H	1.050299	7.021541	17.969425
H	-0.297068	7.641549	17.012491
C	0.548068	7.022862	14.732566
H	-0.136594	6.190393	14.475866
H	-0.068630	7.935552	14.864781
C	1.540805	7.273554	13.600869
H	2.271118	8.055738	13.891701
H	0.985195	7.653584	12.719052
C	2.891642	6.177251	12.005966
H	2.140172	6.338356	11.207343
H	3.567738	7.053591	11.996807
C	3.669203	4.896963	11.709052
H	3.867900	4.841959	10.619303
H	3.066081	4.008668	11.982292
C	5.693276	3.755447	12.021447

H	5.206282	2.819723	12.365873
H	5.774939	3.708730	10.917421
C	7.085991	3.873830	12.627334
H	7.705731	3.001486	12.333437
H	7.039221	3.880850	13.733410
O	3.513856	5.651526	25.026822
O	4.983731	8.094651	25.671507
O	2.677435	9.906849	26.230025
O	2.202536	10.876048	29.011516
O	1.564006	8.700630	30.874346
O	2.054112	2.994441	32.405173
O	1.464242	0.680676	34.163219
O	0.572618	1.243339	36.887710
O	-2.028437	2.518628	37.789070
O	-4.769921	2.321321	38.187505
H	-4.174592	1.628973	37.921853
C	-0.473919	5.288535	24.596212
H	-1.076475	6.184188	24.365137
C	0.851528	5.392113	24.741228
H	1.309158	6.388955	24.622548
C	1.598421	4.312860	25.040800
C	2.940692	4.421138	25.199610
C	3.658379	3.320286	25.484130
H	4.752874	3.358031	25.606435
C	4.936186	5.799665	24.955086
H	5.349025	5.117603	24.186439
H	5.411143	5.556380	25.926784
C	5.226722	7.241698	24.559310
H	6.281633	7.348248	24.234295
H	4.582810	7.523589	23.702263
C	4.869015	9.460040	25.282750
H	5.507290	9.665929	24.400601
H	5.260036	10.099860	26.095476
C	3.407764	9.806105	25.010019
H	3.333688	10.748714	24.434056
H	2.936357	9.020156	24.385812
C	2.480608	11.254612	26.639437
H	2.036386	11.838058	25.807565
H	3.450739	11.726393	26.889620
C	1.534560	11.307139	27.834122
H	1.190215	12.353389	27.966986
H	0.640621	10.678878	27.647687
C	1.391420	10.998525	30.175520
H	0.692991	11.853216	30.081403
H	2.049001	11.228417	31.036569
C	0.635460	9.704321	30.445197
H	-0.113396	9.879918	31.244633
H	0.103488	9.378036	29.528191
C	1.115514	7.430423	31.131802
C	2.009333	6.486746	31.521554
C	3.309632	6.791811	31.671522

H	3.667775	7.815596	31.488534
C	4.193083	5.862957	32.049354
H	5.259099	6.113721	32.173362
C	3.793272	4.612992	32.289040
H	4.557177	3.884318	32.602041
C	2.500295	4.269366	32.158998
C	1.608780	5.214538	31.768386
C	0.308797	4.911101	31.619995
H	-0.044665	3.887929	31.809544
C	-0.577638	5.840257	31.248538
H	-1.645511	5.590253	31.138297
C	-0.178865	7.089867	31.005891
H	-0.945032	7.821215	30.702770
C	2.995851	1.975711	32.767461
H	3.544156	2.257969	33.685607
H	3.733034	1.845596	31.948094
C	2.263870	0.658601	32.985420
H	1.602302	0.463235	32.119946
H	2.976710	-0.187746	33.016947
C	2.195977	0.346854	35.335506
H	2.888973	1.168773	35.603818
H	2.805004	-0.561437	35.151490
C	1.238704	0.054623	36.485165
H	0.494778	-0.711549	36.185409
H	1.818102	-0.358378	37.337161
C	-0.106941	1.081015	38.123641
H	0.623913	0.820763	38.913495
H	-0.830327	0.245496	38.061686
C	-0.810563	2.378131	38.506876
H	-1.024250	2.363398	39.594755
H	-0.153222	3.245933	38.305570
C	-2.763798	3.650423	38.245631
H	-2.281422	4.580869	37.881470
H	-2.778949	3.685633	39.353509
C	-4.190504	3.545808	37.723012
H	-4.801308	4.397066	38.088218
H	-4.217056	3.574851	36.616438
N	3.870838	8.760492	34.640063
N	-1.077933	4.127828	34.729884
N	-0.155205	2.907707	28.614084
N	4.776845	7.552207	28.580097
C	2.673287	9.073296	34.300297
H	2.566377	10.068883	33.853248
C	1.652874	8.221529	34.432651
H	0.676737	8.572357	34.073075
C	1.840797	6.975974	34.916958
C	3.103650	6.712719	35.312899
H	3.386348	5.751177	35.757331
C	4.084168	7.609353	35.166666
H	5.123339	7.401052	35.448599
C	0.845346	6.037123	34.937221

C	-0.424768	6.315209	34.579439
H	-0.751432	7.329027	34.322804
C	-1.351964	5.358096	34.493429
H	-2.378745	5.555032	34.163816
C	0.106201	3.823007	35.117916
H	0.276175	2.753401	35.285053
C	1.068521	4.742172	35.245403
H	2.054827	4.375517	35.555193
C	-2.095409	3.062292	34.461758
H	-3.082970	3.475287	34.751714
H	-1.876211	2.221862	35.154904
C	-2.087265	2.610339	33.011965
C	-2.763112	3.289442	32.070409
H	-3.439602	4.114790	32.349676
C	-2.564703	3.025382	30.770927
H	-3.084871	3.645286	30.024758
C	-1.689164	2.079722	30.387202
C	-1.095264	1.333904	31.332368
H	-0.392092	0.533145	31.050321
C	-1.296076	1.595679	32.630946
H	-0.757989	1.004305	33.387379
C	-1.260775	1.950179	28.933635
H	-0.889346	0.929506	28.694754
H	-2.094277	2.164753	28.234423
C	1.069650	2.553266	28.746661
H	1.224635	1.497769	28.997372
C	2.069543	3.432526	28.647598
H	3.078920	3.036794	28.816363
C	1.833946	4.738052	28.398720
C	0.535031	5.051787	28.211481
H	0.197047	6.073043	27.991638
C	-0.422175	4.127568	28.321919
H	-1.488083	4.364445	28.229183
C	2.827540	5.675494	28.391909
C	4.124582	5.361878	28.586424
H	4.469320	4.328450	28.702325
C	5.063781	6.306207	28.674390
H	6.117548	6.077030	28.867639
C	3.563305	7.894562	28.352494
H	3.396637	8.976310	28.291967
C	2.583529	6.993973	28.246766
H	1.575248	7.392656	28.081567
C	5.821114	8.598940	28.812772
H	6.797335	8.177111	28.497113
H	5.594885	9.439948	28.125229
C	5.826029	9.055410	30.259934
C	6.482705	8.358290	31.201110
H	7.138835	7.516727	30.923513
C	6.286006	8.624654	32.499651
H	6.789610	7.997412	33.250446
C	5.427662	9.585167	32.881079

C	4.853657	10.349392	31.937628
H	4.164340	11.163207	32.218492
C	5.053518	10.086392	30.639361
H	4.523961	10.689546	29.884907
C	4.996509	9.699184	34.333755
H	4.638814	10.721477	34.588444
H	5.826605	9.457855	35.029572
N	-1.257170	-1.345195	15.611869
N	3.677796	3.301029	15.496589
N	2.752398	4.572703	21.591916
N	-2.184921	-0.066094	21.651112
C	-0.056455	-1.661482	15.937702
H	0.054439	-2.662712	16.373294
C	0.961098	-0.805859	15.804690
H	1.941213	-1.157352	16.152897
C	0.766559	0.443226	15.331449
C	-0.500603	0.708369	14.950813
H	-0.789701	1.672620	14.517120
C	-1.478981	-0.189231	15.100626
H	-2.522967	0.021200	14.837121
C	1.758981	1.385260	15.305784
C	3.034832	1.111604	15.647100
H	3.364620	0.097148	15.894710
C	3.962513	2.070284	15.724661
H	4.995994	1.871484	16.038218
C	2.486785	3.600884	15.126693
H	2.309128	4.669743	14.967588
C	1.526138	2.680074	15.006363
H	0.534656	3.045756	14.710679
C	4.689747	4.375612	15.750010
H	5.675370	3.970951	15.446452
H	4.455827	5.210277	15.054555
C	4.694277	4.837251	17.197473
C	5.359196	4.154309	18.144322
H	6.022761	3.316145	17.872297
C	5.162335	4.428919	19.442064
H	5.672483	3.806412	20.192885
C	4.296716	5.386354	19.819231
C	3.716738	6.136460	18.869017
H	3.021829	6.946906	19.143901
C	3.920048	5.867265	17.572521
H	3.395721	6.465863	16.812650
C	3.862615	5.524481	21.270398
H	3.493249	6.547352	21.502621
H	4.693211	5.310984	21.973816
C	1.528444	4.929165	21.454568
H	1.377797	5.983454	21.196521
C	0.525485	4.053191	21.558004
H	-0.483264	4.449489	21.383315
C	0.757999	2.748782	21.817078
C	2.055831	2.433507	22.009093

H	2.391562	1.413441	22.237984
C	3.015249	3.354420	21.893477
H	4.080060	3.115596	21.990765
C	-0.236452	1.812270	21.829285
C	-1.533359	2.125334	21.633481
H	-1.877937	3.158847	21.513581
C	-2.471698	1.179550	21.549554
H	-3.525391	1.406470	21.353860
C	-0.971692	-0.407458	21.881671
H	-0.803820	-1.488871	21.948475
C	0.007335	0.494418	21.981872
H	1.015429	0.096448	22.148709
C	-3.229271	-1.113846	21.422629
H	-4.207051	-0.687956	21.727395
H	-3.008691	-1.948652	22.119638
C	-3.226871	-1.584064	19.980003
C	-3.865566	-0.886499	19.026900
H	-4.512099	-0.033634	19.291595
C	-3.662480	-1.168172	17.732672
H	-4.149190	-0.540135	16.971389
C	-2.817290	-2.146574	17.367859
C	-2.259355	-2.907557	18.323145
H	-1.578246	-3.732410	18.054698
C	-2.465428	-2.629019	19.617069
H	-1.950561	-3.232342	20.381501
C	-2.379591	-2.285026	15.919606
H	-2.012397	-3.308144	15.684355
H	-3.204285	-2.060298	15.211935

2. Associated Mulliken charges, Total Charge: +8

Atom	Charge
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1 O	-0.6565
2 O	-0.6866
3 O	-0.6997
4 O	-0.7090
5 O	-0.6569
6 O	-0.6586
7 O	-0.7027
8 O	-0.7169
9 O	-0.6970
10 O	-0.4896
11 H	0.1708
12 C	0.0309
13 H	0.0083
14 C	0.0188
15 H	0.0164
16 C	-0.1093
17 C	0.3841
18 C	-0.0557

19 H	0.0010
20 C	0.3542
21 H	-0.0291
22 H	0.0198
23 C	0.4150
24 H	0.0149
25 H	-0.0418
26 C	0.3544
27 H	-0.0005
28 H	0.0112
29 C	0.4005
30 H	-0.0098
31 H	-0.0267
32 C	0.3647
33 H	0.0201
34 H	-0.0060
35 C	0.3793
36 H	0.0282
37 H	-0.0313
38 C	0.3973
39 H	0.0135
40 H	0.0269
41 C	0.3381
42 H	0.0024
43 H	-0.0290
44 C	0.3653
45 C	-0.0965
46 C	0.0277
47 H	0.0526
48 C	0.0298
49 H	0.0137
50 C	-0.0333
51 H	0.0005
52 C	0.3764
53 C	-0.0928
54 C	0.0310
55 H	0.0591
56 C	0.0166
57 H	0.0053
58 C	-0.0435
59 H	-0.0030
60 C	0.3406
61 H	-0.0080
62 H	-0.0179
63 C	0.4093
64 H	0.0053
65 H	0.0012
66 C	0.3587
67 H	-0.0340
68 H	0.0201
69 C	0.3908

70 H	0.0004
71 H	0.0148
72 C	0.3771
73 H	0.0068
74 H	0.0069
75 C	0.3910
76 H	0.0229
77 H	-0.0455
78 C	0.3320
79 H	-0.0544
80 H	0.0304
81 C	0.4524
82 H	0.0366
83 H	-0.0776
84 O	-0.6564
85 O	-0.6860
86 O	-0.6995
87 O	-0.7094
88 O	-0.6572
89 O	-0.6578
90 O	-0.6999
91 O	-0.7154
92 O	-0.7020
93 O	-0.4931
94 H	0.1712
95 C	0.0313
96 H	0.0080
97 C	0.0200
98 H	0.0163
99 C	-0.1089
100 C	0.3841
101 C	-0.0560
102 H	0.0008
103 C	0.3550
104 H	-0.0291
105 H	0.0194
106 C	0.4147
107 H	0.0145
108 H	-0.0420
109 C	0.3542
110 H	-0.0011
111 H	0.0126
112 C	0.4007
113 H	-0.0101
114 H	-0.0268
115 C	0.3631
116 H	0.0204
117 H	-0.0053
118 C	0.3799
119 H	0.0286
120 H	-0.0319

121 C	0.3970
122 H	0.0143
123 H	0.0269
124 C	0.3382
125 H	0.0033
126 H	-0.0300
127 C	0.3647
128 C	-0.0964
129 C	0.0267
130 H	0.0527
131 C	0.0310
132 H	0.0147
133 C	-0.0336
134 H	0.0002
135 C	0.3790
136 C	-0.0935
137 C	0.0308
138 H	0.0589
139 C	0.0160
140 H	0.0055
141 C	-0.0445
142 H	-0.0028
143 C	0.3423
144 H	-0.0058
145 H	-0.0220
146 C	0.4105
147 H	0.0032
148 H	-0.0021
149 C	0.3645
150 H	-0.0335
151 H	0.0156
152 C	0.3923
153 H	-0.0026
154 H	0.0143
155 C	0.3812
156 H	0.0069
157 H	0.0016
158 C	0.3892
159 H	0.0234
160 H	-0.0416
161 C	0.3303
162 H	-0.0507
163 H	0.0291
164 C	0.4508
165 H	0.0369
166 H	-0.0741
167 N	-0.4509
168 N	-0.4340
169 N	-0.4211
170 N	-0.4053
171 C	0.3892

172 H	0.0275
173 C	0.0882
174 H	0.0370
175 C	-0.0553
176 C	0.0879
177 H	0.0458
178 C	0.3850
179 H	0.0353
180 C	-0.0810
181 C	0.0945
182 H	0.0419
183 C	0.3605
184 H	0.0249
185 C	0.3691
186 H	0.0777
187 C	0.0819
188 H	0.0363
189 C	0.1252
190 H	0.0833
191 H	0.1004
192 C	-0.1274
193 C	0.0702
194 H	0.0064
195 C	0.0685
196 H	-0.0147
197 C	-0.1325
198 C	0.0786
199 H	-0.0172
200 C	0.0944
201 H	0.0508
202 C	0.1321
203 H	0.0415
204 H	0.0681
205 C	0.3511
206 H	0.0156
207 C	0.1022
208 H	0.0454
209 C	-0.0687
210 C	0.1103
211 H	0.0499
212 C	0.3473
213 H	0.0206
214 C	-0.0719
215 C	0.0781
216 H	0.0336
217 C	0.3240
218 H	0.0223
219 C	0.3600
220 H	0.0715
221 C	0.0970
222 H	0.0434

223 C	0.1254
224 H	0.0687
225 H	0.0834
226 C	-0.1360
227 C	0.0735
228 H	0.0012
229 C	0.0843
230 H	0.0106
231 C	-0.1438
232 C	0.0814
233 H	-0.0013
234 C	0.0856
235 H	0.0253
236 C	0.1368
237 H	0.0944
238 H	0.0905
239 N	-0.4498
240 N	-0.4351
241 N	-0.4218
242 N	-0.4061
243 C	0.3885
244 H	0.0271
245 C	0.0870
246 H	0.0366
247 C	-0.0560
248 C	0.0897
249 H	0.0458
250 C	0.3840
251 H	0.0349
252 C	-0.0800
253 C	0.0936
254 H	0.0413
255 C	0.3579
256 H	0.0258
257 C	0.3701
258 H	0.0790
259 C	0.0830
260 H	0.0348
261 C	0.1238
262 H	0.0896
263 H	0.1013
264 C	-0.1304
265 C	0.0700
266 H	0.0061
267 C	0.0680
268 H	-0.0152
269 C	-0.1326
270 C	0.0789
271 H	-0.0176
272 C	0.0955
273 H	0.0517

274 C	0.1325
275 H	0.0408
276 H	0.0679
277 C	0.3509
278 H	0.0165
279 C	0.1006
280 H	0.0463
281 C	-0.0686
282 C	0.1108
283 H	0.0505
284 C	0.3474
285 H	0.0200
286 C	-0.0728
287 C	0.0785
288 H	0.0347
289 C	0.3219
290 H	0.0224
291 C	0.3606
292 H	0.0720
293 C	0.0965
294 H	0.0432
295 C	0.1245
296 H	0.0687
297 H	0.0854
298 C	-0.1365
299 C	0.0739
300 H	0.0003
301 C	0.0832
302 H	0.0092
303 C	-0.1428
304 C	0.0826
305 H	-0.0012
306 C	0.0871
307 H	0.0254
308 C	0.1369
309 H	0.0920
310 H	0.0926

E. XYZ coordinates for the 3DNP-[3]Rotaxane in the pleated solid-state structure with 8Cl⁻ counterions with positions that have been optimized through simulated annealing

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.342925
C	1.176387	0.000000	1.990264
C	2.324132	-0.101475	1.306163
C	2.317552	-0.208203	-0.032967
C	1.147264	-0.105735	-0.683263
C	-1.305308	-0.158693	2.100070
N	-1.592901	-1.599800	2.384955
C	-1.224015	-2.136814	3.489365
C	-1.365308	-3.444762	3.715944

C	-1.904150	-4.263566	2.789917
C	-2.323951	-3.644384	1.667497
C	-2.150424	-2.332278	1.493772
C	-1.967754	-5.618553	2.951477
C	-1.450661	-6.247677	4.028270
C	-1.438715	-7.580565	4.113251
N	-1.911807	-8.320430	3.179025
C	-2.462460	-7.763840	2.163529
C	-2.503546	-6.437089	2.022194
C	-1.703026	-9.802882	3.203226
C	-0.434497	-10.187555	2.457393
C	-0.430506	-10.324197	1.119654
C	0.723195	-10.425330	0.443602
C	1.897240	-10.395201	1.096105
C	1.886144	-10.375003	2.437928
C	0.734233	-10.265598	3.113084
C	3.210192	-10.236646	0.348241
N	3.509787	-8.807040	0.017391
C	3.022488	-8.266505	-1.040048
C	3.153078	-6.958614	-1.280971
C	3.820108	-6.145126	-0.436880
C	4.374417	-6.771653	0.621712
C	4.188962	-8.078968	0.826040
C	3.869415	-4.787233	-0.600231
C	3.164820	-4.143125	-1.554530
C	3.131249	-2.808479	-1.607365
N	3.773120	-2.078932	-0.768507
C	4.505094	-2.648319	0.118531
C	4.570730	-3.978883	0.221709
C	3.582340	-0.595261	-0.780166
Cl	5.930542	-1.751426	-2.438693
O	-4.425966	-0.807496	2.829170
C	-5.049829	-0.038774	1.805218
C	-5.704409	-0.963655	0.782933
O	-4.718548	-1.589349	-0.035056
C	-4.578911	-0.961234	-1.303488
C	-3.659819	-1.785160	-2.199275
O	-2.307516	-1.633174	-1.790952
C	-1.396205	-2.302990	-2.656595
C	-1.108250	-3.710903	-2.152671
O	-0.327576	-3.630366	-0.953133
C	0.024283	-4.782606	-0.297170
C	0.768740	-4.693533	0.834175
C	1.125971	-5.810096	1.517323
C	0.725661	-7.003369	1.049183
C	0.001878	-7.097172	-0.070698
C	-0.345951	-5.996820	-0.739503
C	1.874195	-5.725767	2.646291
C	2.249944	-4.510839	3.081880
C	1.900280	-3.408431	2.416220
C	1.169102	-3.498563	1.301138

O	2.229034	-6.881316	3.300419
C	3.027561	-6.804131	4.489665
C	3.308439	-8.204889	5.019750
O	4.214082	-8.922789	4.187939
C	5.578702	-8.653911	4.481583
C	6.476019	-9.688372	3.807917
O	6.448777	-9.535505	2.393849
C	7.512842	-10.229492	1.757901
C	7.407022	-10.093913	0.240562
O	6.442301	-10.997345	-0.286303
C	6.452005	-10.975542	-1.710892
C	5.568965	-12.096279	-2.244708
O	6.062276	-13.365925	-1.799036
C	-5.297249	-1.039563	3.929479
C	-4.746208	-2.178361	4.778038
O	-4.980768	-3.398572	4.066380
C	-4.745039	-4.612806	4.651591
C	-5.189443	-5.726022	4.017528
C	-4.995287	-6.953050	4.563334
C	-4.357707	-7.042452	5.745653
C	-3.929673	-5.944153	6.377388
C	-4.125844	-4.737296	5.838626
C	-5.439660	-8.066325	3.929466
C	-6.059633	-7.942063	2.742835
C	-6.256326	-6.735200	2.204224
C	-5.827637	-5.636777	2.835455
O	-5.203549	-9.280156	4.515208
C	-5.438757	-10.500774	3.804657
C	-4.888678	-11.638639	4.655060
O	-5.758519	-11.867576	5.757112
C	-5.134238	-12.637942	6.779554
C	-4.478296	-11.715777	7.803638
O	-5.462956	-11.094146	8.625808
C	-5.588002	-11.720057	9.896801
C	-6.506517	-10.900801	10.796907
O	-7.860819	-11.066153	10.400911
C	-8.769535	-10.398626	11.270658
C	-9.066847	-8.993230	10.765055
O	-9.858164	-9.082125	9.573553
C	-10.210807	-7.935454	8.908991
C	-10.946442	-8.036671	7.773235
C	-11.300310	-6.927617	7.077062
C	-10.907862	-5.728584	7.537883
C	-10.193869	-5.622834	8.663097
C	-9.847322	-6.716431	9.343812
C	-12.036488	-7.026048	5.941686
C	-12.403094	-8.245485	5.511158
C	-12.059568	-9.339851	6.192379
C	-11.340204	-9.236795	7.313944
O	-12.379641	-5.879328	5.269083
C	-13.112376	-5.975334	4.040336

C	-13.369441	-4.579492	3.489313
O	-14.310601	-3.859016	4.278132
C	-15.658698	-4.134216	3.920320
C	-16.588253	-3.101007	4.546333
O	-16.624565	-3.260010	5.957771
C	-17.679569	-2.517685	6.550726
C	-17.670835	-2.714362	8.062581
O	-16.678168	-1.898389	8.668388
C	-16.759661	-1.963446	10.089405
C	-15.946333	-0.816954	10.675596
O	-16.459775	0.423360	10.176750
N	-8.589250	-11.124397	6.238350
C	-8.951256	-10.587954	5.131589
C	-8.805666	-9.280558	4.905518
C	-8.267985	-8.461836	5.832396
C	-7.855200	-9.080545	6.957475
C	-8.034408	-10.391984	7.131289
C	-8.880987	-12.564461	6.523642
C	-10.194611	-12.720214	7.267147
C	-11.363634	-12.735776	6.606725
C	-12.519513	-12.629713	7.276459
C	-12.528785	-12.500282	8.613616
C	-11.365602	-12.590947	9.278753
C	-10.210165	-12.701517	8.609911
C	-8.199576	-7.107432	5.668134
C	-8.707759	-6.480976	4.585937
C	-8.716775	-5.148899	4.495459
N	-8.248426	-4.406664	5.429917
C	-7.705610	-4.960126	6.451545
C	-7.668432	-6.286681	6.598138
C	-8.457374	-2.924577	5.398041
C	-9.730981	-2.539036	6.134545
C	-9.740967	-2.386831	7.470516
C	-10.897756	-2.277960	8.139645
C	-12.068584	-2.319578	7.482447
C	-12.053088	-2.363051	6.141343
C	-10.897344	-2.475147	5.472878
C	-13.382468	-2.462072	8.230533
N	-13.698904	-3.889295	8.555214
C	-13.206156	-4.438660	9.604004
C	-13.344981	-5.744486	9.846289
C	-14.027137	-6.549373	9.006437
C	-14.587590	-5.914399	7.955541
C	-14.394632	-4.607375	7.751499
C	-14.082827	-7.907262	9.167090
C	-13.369771	-8.555370	10.111960
C	-13.338086	-9.889881	10.160400
N	-13.991930	-10.617893	9.329796
C	-14.735849	-10.043459	8.455409
C	-14.797446	-8.712103	8.353198
C	-13.803425	-12.103315	9.339186

Cl	-16.141610	-10.933028	11.014095
Cl	1.422446	-1.713910	5.294485
Cl	-11.584222	-11.018539	3.302465
Cl	-1.742117	-9.582933	6.688136
Cl	-8.447152	-3.124635	1.910096
Cl	0.311240	-8.891938	-2.891644
Cl	-10.495480	-3.790272	11.468744
H	6.087456	-13.315855	-0.850073
H	-6.766318	-6.649020	1.228944
H	-6.000923	-4.660544	2.351531
H	-3.762962	-3.859503	6.397283
H	-5.274841	-2.200256	5.750797
H	-3.664699	-2.033636	4.973844
H	-5.384781	-0.114096	4.534164
H	-6.313665	-1.304357	3.575311
H	-5.783968	0.665784	2.243895
H	-4.286111	0.588772	1.308856
H	-6.428616	-0.403209	0.160631
H	-6.283486	-1.756754	1.297873
H	-5.571153	-0.878196	-1.791765
H	-4.185738	0.066894	-1.182273
H	-3.772176	-1.430070	-3.244586
H	-3.950873	-2.854367	-2.173136
H	-1.782727	-2.325658	-3.694440
H	-0.453499	-1.722523	-2.689451
H	-0.538487	-4.264772	-2.927394
H	-2.060756	-4.246889	-1.963320
H	0.904243	-2.573121	0.768478
H	2.230114	-2.428142	2.797735
H	2.858343	-4.385792	3.990778
H	0.995444	-7.924114	1.584660
H	-0.316600	-8.079184	-0.456862
H	-0.942244	-6.123351	-1.657127
H	3.981262	-6.283389	4.284310
H	2.479274	-6.231955	5.266352
H	2.358634	-8.771145	5.070589
H	3.689555	-8.164093	6.058359
H	5.845737	-7.630119	4.152642
H	5.744733	-8.708082	5.577165
H	6.157433	-10.714846	4.081060
H	7.512521	-9.555406	4.180353
H	8.478709	-9.801789	2.093506
H	7.509954	-11.296023	2.053981
H	8.397067	-10.311624	-0.209408
H	7.137845	-9.055072	-0.034825
H	6.079934	-9.993638	-2.069779
H	7.484124	-11.106966	-2.091919
H	5.563938	-12.082896	-3.354317
H	4.520278	-11.968208	-1.913810
H	-16.456611	0.349287	9.228681
H	-3.421375	-6.030491	7.353525

H	-4.185306	-8.018724	6.229777
H	-6.423409	-8.819826	2.184712
H	-4.909401	-10.480104	2.832125
H	-6.520298	-10.645079	3.608660
H	-4.803024	-12.565367	4.052015
H	-3.871713	-11.374240	5.007892
H	-4.401766	-13.343487	6.339483
H	-5.898429	-13.264837	7.275344
H	-3.753555	-12.278171	8.423473
H	-3.900405	-10.920512	7.290635
H	-4.591583	-11.794159	10.377853
H	-5.974160	-12.751516	9.781487
H	-6.382017	-11.251182	11.842181
H	-6.224854	-9.829255	10.764490
H	-8.377180	-10.372496	12.306290
H	-9.709170	-10.983650	11.309412
H	-9.631604	-8.438574	11.542309
H	-8.118453	-8.453916	10.564945
H	-11.078713	-10.156251	7.858104
H	-12.383288	-10.324070	5.816654
H	-12.999694	-8.380907	4.595616
H	-11.176636	-4.812633	6.993327
H	-9.882787	-4.636435	9.044217
H	-9.259220	-6.579994	10.265380
H	-14.072886	-6.500788	4.197240
H	-12.518325	-6.550052	3.299705
H	-12.418970	-4.012596	3.478466
H	-13.703743	-4.627507	2.435095
H	-15.940530	-5.157185	4.239523
H	-15.772549	-4.081189	2.818506
H	-16.255312	-2.074269	4.290872
H	-17.607090	-3.235387	4.126710
H	-18.648617	-2.869751	6.147313
H	-17.590826	-1.444655	6.293918
H	-18.667117	-2.442638	8.466251
H	-17.486563	-3.777435	8.310814
H	-16.368489	-2.940171	10.441574
H	-17.812726	-1.877266	10.424801
H	-16.015204	-0.818362	11.783004
H	-14.874301	-0.908995	10.414198
H	-12.720663	-10.447322	10.874909
H	-12.741778	-8.027186	10.841252
H	-15.447348	-8.314514	7.564812
H	-15.280451	-10.714572	7.780304
H	-12.856403	-6.122794	10.751039
H	-12.620548	-3.774569	10.250342
H	-14.770400	-4.079070	6.867998
H	-15.172806	-6.445339	7.194733
H	-13.364445	-1.906513	9.190191
H	-14.236246	-2.066243	7.639598
H	-10.873370	-2.219225	9.240909

H	-8.803202	-2.415585	8.046185
H	-10.921174	-2.570127	4.374868
H	-13.000140	-2.364887	5.580503
H	-8.482266	-2.620227	4.328672
H	-7.559074	-2.455873	5.848639
H	-9.166910	-4.610085	3.654026
H	-9.167864	-7.024690	3.751309
H	-7.211296	-6.657369	7.525039
H	-7.331543	-4.268885	7.215173
H	-9.166689	-8.916789	3.937227
H	-9.417633	-11.265605	4.408005
H	-7.759616	-10.921067	8.051169
H	-7.398275	-8.539186	7.794744
H	-8.873208	-13.107918	5.556593
H	-8.030861	-12.954600	7.120523
H	-11.387633	-12.768460	5.504840
H	-13.459123	-12.583005	6.705763
H	-11.341633	-12.514922	10.378746
H	-9.265030	-12.713403	9.175602
H	-13.796608	-12.418145	10.406299
H	-14.702083	-12.553396	8.868758
H	2.522942	-2.251702	-2.331562
H	2.546638	-4.674989	-2.289645
H	5.212282	-4.372184	1.018686
H	5.033549	-1.973143	0.802997
H	2.672277	-6.583135	-2.190387
H	2.450378	-8.936111	-1.695975
H	4.558730	-8.600081	1.715449
H	4.947192	-6.234844	1.388493
H	3.206972	-10.796858	-0.607532
H	4.068659	-10.617579	0.942350
H	0.692674	-10.465421	-0.658349
H	-1.370880	-10.285481	0.548957
H	0.764687	-10.183666	4.212012
H	2.834526	-10.388781	2.995623
H	-1.671845	-10.110782	4.271332
H	-2.604534	-10.269553	2.756270
H	-0.982738	-8.122727	4.949285
H	-0.984892	-5.705339	4.861379
H	-2.968679	-6.064536	1.099970
H	-2.841010	-8.452633	1.400255
H	-1.000436	-3.809083	4.683104
H	-0.755620	-1.458095	4.210477
H	-2.431466	-1.803796	0.575175
H	-2.782320	-4.185865	0.831336
H	-1.301578	0.382581	3.068226
H	-2.162186	0.233002	1.513799
H	1.212418	0.017092	3.092016
H	3.270022	-0.162959	1.865075
H	1.111458	-0.167478	-1.783836
H	-0.951341	0.024517	-0.554790

H	3.554494	-0.285726	-1.848041
H	4.488428	-0.140451	-0.328973