Using Density Functional Theory to Interpret the Infrared Spectra of Flexible Cyclic Phosphazenes

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Supporting Information

Contents

Table S01. Complete citation for 'Gaussian 03' Software (Reference 14)

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

Table S02. PZ-T3 Structure 01 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.302293	-0.952688	-0.001450
2	7	0	-1.466749	0.636648	-0.044879
3	15	0	-0.184775	1.591901	-0.043474
4	7	0	1.275251	0.940605	-0.003385
5	15	0	1.460590	-0.647015	0.036299
6	7	0	0.165436	-1.584704	0.040595
7	6	0	-3.415419	-1.153970	1.573669
8	6	0	-2.141979	-2.911678	-1.564477
9	6	0	3.574073	-0.476005	-1.544600
10	6	0	2.699040	-2.291796	1.693700
11	6	0	-1.389777	3.255501	-1.706796
12	6	0	0.620024	3.551254	1.539430
13	6	0	4.296707	-1.320130	-2.582197
14	1	0	4.230675	-0.362776	-0.676407
15	1	0	3.353655	0.504607	-1.974929
16	6	0	3.889485	-2.249777	2.638407
17	6	0	-1.000242	4.359888	-2.676327
18	6	0	-3.235799	-3.158515	-2.590924
19	6	0	0.044164	4.480164	2.596094
20	6	0	-3.969864	-2.104243	2.622860
21	9	0	3.564081	-1.496886	-3.699442
22	9	0	4.616902	-2.542501	-2.103342
23	9	0	5.447276	-0.698248	-2.932492
24	9	0	-4.455360	-2.814003	-2.120510
25	9	0	-3.030066	-2.475040	-3.733849
26	9	0	-3.266693	-4.477750	-2.893699
27	9	0	-3.236556	-2.103970	3.753382
28	9	0	-5.228842	-1.722373	2.942376
29	9	0	-4.026404	-3.376774	2.170402
30	9	0	4.982074	-1.715792	2.046728
31	9	0	3.636385	-1.533776	3.751291
32	9	0	4.199260	-3.512304	3.015862
33	9	0	-2.115678	5.022189	-3.063344
34	9	0	-0.396048	3.882641	-3.781862
35	9	0	-0.164056	5.256885	-2.106378
36	9	0	-0.340301	3.818489	3.705298
37	9	0	0.990471	5.380029	2.954447
38	9	0	-1.025353	5.166151	2.136119
39	1	0	1.849194	-2.744977	2.210793
40	1	0	2.973366	-2.900012	0.826349
41	1	0	-2.080652	2.570221	-2.204857
42	1	0	-1.881093	3.716740	-0.844487
43	1	0	0.917595	4.155645	0.676882
44	1	0	1.492733	3.039252	1.953541
45	1	0	-3.406240	-0.139549	1.981154
46	1	0	-4.066854	-1.195969	0.695198
47	1	0	-1.181314	-3.216263	-1.988233
48	1	0	-2.363940	-3.511913	-0.676664
49	8	0	2.364966	-1.159062	-1.204495
50	8	0	-0.191206	2.572900	-1.330990
51	8	0	-0.399860	2.610043	1.196117
52	8	0	-2.087236	-1.584227	1.265877
53	8	0	-2.139611	-1.513085	-1.268492

54	8	0	2.397967	-0.944406	1.322334

Table S03. PZ-T3 Structure 02 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.037861	-3.231835	2.119099
2	9	0	-4.357503	-3.372614	2.388268
3	6	0	-2.874246	-2.319630	0.914029
4	8	0	-1.474446	-2.224935	0.636020
5	15	0	-0.908935	-1.064238	-0.338313
6	8	0	-1.576044	-1.420784	-1.773217
7	6	0	-1.154207	-2.579069	-2.497151
8	6	0	-2.336476	-3.069566	-3.317986
9	9	0	-1.961285	-4.153755	-4.035337
10	7	0	-1.495683	0.359150	0.095689
11	15	0	-0.541474	1.649573	0.227754
12	8	0	-0.853415	2.742390	-0.907357
13	6	0	-2.184748	3.208891	-1.136220
14	6	0	-2.186388	3.958150	-2.459457
15	9	0	-1.346494	5.012771	-2.450728
16	7	0	1.035309	1.395506	0.236076
17	15	0	1.655832	-0.037930	-0.104806
18	8	0	2.666168	-0.368049	1.115887
19	6	0	3.315677	-1.640242	1.186094
20	6	0	4.131356	-1.663722	2.468611
21	9	0	4.764126	-2.857095	2.564682
22	7	0	0.676101	-1.271810	-0.381238
23	8	0	2.636441	0.040809	-1.390246
24	6	0	3.598788	1.093639	-1.496345
25	6	0	4.708935	0.606304	-2.413602
26	9	0	5.332588	-0.484266	-1.909324
27	8	0	-0.998279	2.492187	1.527686
28	6	0	-0.835602	1.943758	2.833776
29	6	0	-1.451457	2.919868	3.823615
30	9	0	-0.855771	4.128005	3.786681
31	9	0	-2.442664	-2.727749	3.221450
32	9	0	-2.525886	-4.460165	1.901804
33	9	0	-3.375156	-3.437834	-2.528702
34	9	0	-2.789482	-2.137971	-4.177360
35	9	0	-1.310952	2.423207	5.075340
36	9	0	-2.770125	3.105350	3.598207
37	9	0	5.070771	-0.694770	2.491636
38	9	0	3.360673	-1.513762	3.565190
39	9	0	-1.838585	3.164894	-3.493575
40	9	0	-3.436745	4.424800	-2.695607
41	9	0	4.257210	0.285470	-3.641640
42	9	0	5.634073	1.583943	-2.551286
43	1	0	-3.412392	-2.756550	0.068193
44	1	0	-3.294474	-1.340120	1.159538
45	1	0	-0.334457	-2.321923	-3.172699
46	1	0	-0.841865	-3.390198	-1.833128
47	1	0	-1.355107	0.985088	2.927236
48	1	0	0.225097	1.824229	3.074150
49	1	0	-2.492109	3.896237	-0.343377
50	1	0	-2.887478	2.373831	-1.209526

51	1	0	3.139504	1.984645	-1.931820
52	1	0	4.041516	1.342254	-0.527344
53	1	0	2.580827	-2.449280	1.220918
54	1	0	3.994332	-1.787579	0.340376

Table S04. PZ-T3 Structure 03 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.457116	0.307613	-2.530962
2	9	0	-5.786167	0.315472	-2.273698
3	6	0	-3.697348	0.105757	-1.228776
4	8	0	-2.303778	0.079140	-1.538605
5	15	0	-1.204763	0.584802	-0.462954
6	8	0	-1.553510	2.159946	-0.290404
7	6	0	-1.272461	3.079753	-1.349417
8	6	0	-1.604752	4.471968	-0.837886
9	9	0	-1.330296	5.375099	-1.808033
10	7	0	-1.461463	-0.057940	0.981215
11	15	0	-0.326124	-0.922592	1.725514
12	8	0	-0.248570	-0.414866	3.268421
13	6	0	-0.305133	0.959805	3.637849
14	6	0	1.070162	1.475715	4.043044
15	9	0	1.625312	0.736548	5.023429
16	7	0	1.108872	-1.005962	1.041135
17	15	0	1.381385	-0.418607	-0.418524
18	8	0	1.892004	-1.660213	-1.319009
19	6	0	2.146799	-1.479780	-2.714656
20	6	0	2.864453	-2.724261	-3.212461
21	9	0	3.111852	-2.587992	-4.537705
22	7	0	0.213299	0.382746	-1.167390
23	8	0	2.649676	0.583175	-0.401781
24	6	0	3.855226	0.216683	0.275724
25	6	0	4.973237	1.072905	-0.297047
26	9	0	5.160895	0.834334	-1.615832
27	8	0	-0.807467	-2.433643	1.997684
28	6	0	-2.030615	-2.703722	2.678998
29	6	0	-2.660165	-3.939248	2.053107
30	9	0	-2.958010	-3.749076	0.749124
31	9	0	-4.212673	-0.667949	-3.425703
32	9	0	-4.143149	1.488013	-3.115101
33	9	0	-2.910985	4.596689	-0.515327
34	9	0	-0.882282	4.800578	0.252736
35	9	0	-3.818212	-4.216467	2.703404
36	9	0	-1.866838	-5.022604	2.140142
37	9	0	4.048461	-2.907432	-2.588462
38	9	0	2.132836	-3.842024	-3.040964
39	9	0	1.939119	1.493646	3.004940
40	9	0	0.947661	2.745765	4.496127
41	9	0	4.736935	2.391371	-0.152434
42	9	0	6.129853	0.783502	0.343334
43	1	0	-3.953704	0.930038	-0.556669
44	1	0	-4.002884	-0.845478	-0.785307
45	1	0	-0.213966	3.045940	-1.621373
46	1	0	-1.892290	2.875971	-2.227773
47	1	0	-1.831620	-2.906007	3.734690

48	1	0	-2.743705	-1.879920	2.581643
49	1	0	-0.959664	1.038545	4.508900
50	1	0	-0.699377	1.584127	2.831146
51	1	0	3.761943	0.413268	1.346356
52	1	0	4.111543	-0.834010	0.110284
53	1	0	1.208239	-1.366617	-3.263600
54	1	0	2.793685	-0.616490	-2.898892

Table S05. PZ-T3 Structure 06 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.998432	2.836668	-1.503586
2	9	0	5.293894	2.977647	-1.132328
3	6	0	3.550005	1.418612	-1.187511
4	8	0	2.182809	1.300602	-1.587990
5	15	0	1.318271	0.001318	-1.206298
6	8	0	2.189009	-1.123528	-1.969718
7	6	0	1.736318	-2.474144	-2.030352
8	6	0	2.850740	-3.306678	-2.644794
9	9	0	2.453533	-4.599785	-2.700561
10	7	0	1.367553	-0.298638	0.375975
11	15	0	0.064948	-0.114834	1.285268
12	8	0	-0.162498	-1.426051	2.211017
13	6	0	0.925870	-1.975957	2.956775
14	6	0	0.374861	-3.124875	3.786214
15	9	0	-0.569826	-2.709327	4.657933
16	7	0	-1.335698	0.195883	0.579832
17	15	0	-1.470450	0.208034	-1.025182
18	8	0	-2.397061	1.457925	-1.458940
19	6	0	-1.915411	2.793936	-1.336463
20	6	0	-3.065238	3.731932	-1.669656
21	9	0	-2.633019	5.010662	-1.563162
22	7	0	-0.120713	0.170633	-1.878651
23	8	0	-2.400675	-0.993682	-1.545308
24	6	0	-3.710633	-1.195304	-1.010528
25	6	0	-4.216279	-2.532199	-1.529315
26	9	0	-4.303524	-2.559401	-2.873972
27	8	0	0.413941	1.036005	2.374050
28	6	0	-0.565058	1.431916	3.337030
29	6	0	0.132843	2.307491	4.365712
30	9	0	1.112809	1.638619	5.013222
31	9	0	3.274240	3.759566	-0.836018
32	9	0	3.911196	3.119406	-2.818316
33	9	0	3.154516	-2.909449	-3.895625
34	9	0	3.983247	-3.253946	-1.910260
35	9	0	-0.771906	2.711292	5.288124
36	9	0	0.681715	3.407015	3.813587
37	9	0	-3.526603	3.551808	-2.922102
38	9	0	-4.105500	3.575756	-0.822076
39	9	0	-0.169052	-4.091631	3.021080
40	9	0	1.383977	-3.676630	4.500233
41	9	0	-3.425949	-3.557577	-1.148245
42	9	0	-5.455404	-2.753977	-1.027873
43	1	0	4.177676	0.719620	-1.746841
44	1	0	3.659607	1.251219	-0.112060

45	1	0	1.528184	-2.868435	-1.030745
46	1	0	0.846368	-2.555749	-2.661060
47	1	0	-1.364148	2.008832	2.863483
48	1	0	-0.994009	0.568702	3.855407
49	1	0	1.360893	-1.236469	3.636351
50	1	0	1.700707	-2.360885	2.288199
51	1	0	-3.686531	-1.233013	0.082478
52	1	0	-4.390345	-0.408674	-1.349145
53	1	0	-1.589634	3.007146	-0.313456
54	1	0	-1.096312	2.975781	-2.038372

Table S06. PZ-T3 Structure 07 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.780382	-2.142938	-2.848057
2	9	0	3.829552	-2.749584	-4.057302
3	6	0	2.399275	-1.538461	-2.652511
4	8	0	2.375790	-0.926895	-1.360850
5	15	0	1.204737	0.129357	-0.983718
6	8	0	1.525601	1.397476	-1.936999
7	6	0	2.653257	2.238847	-1.676553
8	6	0	2.315792	3.628116	-2.194357
9	9	0	3.371891	4.447830	-1.985726
10	7	0	-0.219819	-0.426644	-1.456370
11	15	0	-1.386727	-0.616919	-0.378979
12	8	0	-2.664530	0.312296	-0.748587
13	6	0	-3.115042	0.414254	-2.101675
14	6	0	-4.339855	1.314746	-2.103632
15	9	0	-5.345304	0.799759	-1.362859
16	7	0	-1.079248	-0.349401	1.164916
17	15	0	0.314771	0.262622	1.683641
18	8	0	0.931660	-0.603244	2.886929
19	6	0	1.666630	-1.795301	2.624498
20	6	0	2.440372	-2.151380	3.885492
21	9	0	3.116366	-3.306144	3.665108
22	7	0	1.429761	0.510105	0.550193
23	8	0	0.054958	1.583376	2.557129
24	6	0	-0.810352	2.610568	2.077372
25	6	0	-1.016966	3.604676	3.210341
26	9	0	-1.592771	3.037057	4.287966
27	8	0	-1.947320	-2.119251	-0.592622
28	6	0	-2.976391	-2.626532	0.261077
29	6	0	-3.287651	-4.042460	-0.195954
30	9	0	-3.730442	-4.077365	-1.471277
31	9	0	4.074068	-3.063617	-1.909080
32	9	0	4.750028	-1.201602	-2.818562
33	9	0	2.044509	3.629565	-3.515648
34	9	0	1.247646	4.156697	-1.557289
35	9	0	-4.257966	-4.557580	0.594515
36	9	0	-2.211858	-4.851692	-0.113011
37	9	0	3.337129	-1.203463	4.218960
38	9	0	1.628654	-2.344884	4.943835
39	9	0	-4.067349	2.545545	-1.626243
40	9	0	-4.788050	1.449242	-3.373923

41	9	0	0.139192	4.171475	3.608780
42	9	0	-1.834320	4.593922	2.773586
43	1	0	2.231324	-0.808114	-3.450041
44	1	0	1.649492	-2.331455	-2.715696
45	1	0	2.858443	2.308402	-0.604662
46	1	0	3.537028	1.870144	-2.205179
47	1	0	-2.639940	-2.655470	1.301108
48	1	0	-3.889348	-2.027936	0.185433
49	1	0	-3.404534	-0.562361	-2.502531
50	1	0	-2.343231	0.860122	-2.734852
51	1	0	-0.358895	3.143374	1.234355
52	1	0	-1.784274	2.203520	1.790188
53	1	0	0.990711	-2.625001	2.394597
54	1	0	2.381893	-1.650842	1.809245

Table S07. PZ-T4 Structure 01 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.708195	-2.026320	0.027342
2	7	0	1.750360	-0.851190	-0.017270
3	15	0	2.012749	0.697579	-0.046023
4	7	0	0.872025	1.782026	-0.020114
5	15	0	-0.687952	1.991406	0.017272
6	7	0	-1.730362	0.815828	0.014056
7	15	0	-1.993717	-0.732812	-0.003530
8	7	0	-0.852172	-1.817255	0.007598
9	8	0	3.032248	0.950419	1.191175
10	8	0	2.893223	1.082837	-1.353523
11	8	0	-0.929928	2.935260	1.314672
12	8	0	-1.144056	2.927780	-1.227990
13	8	0	-2.897643	-1.125533	-1.292655
14	8	0	-2.990236	-0.979438	1.253336
15	8	0	0.971495	-2.945042	1.339521
16	8	0	1.143768	-2.989331	-1.204680
17	6	0	3.404430	2.279261	1.558409
18	6	0	-2.256550	3.263444	1.728719
19	6	0	-0.345759	4.043847	-1.623558
20	6	0	-3.357577	-2.306243	1.632146
21	6	0	2.304240	-3.248849	1.751136
22	6	0	-3.980000	-0.286725	-1.697782
23	6	0	0.342348	-4.113965	-1.566077
24	6	0	3.970304	0.243292	-1.771109
25	6	0	4.461783	2.171065	2.645392
26	1	0	3.837416	2.823475	0.713113
27	1	0	2.544929	2.827904	1.952919
28	6	0	-2.142638	4.254108	2.876211
29	1	0	-2.823020	3.738855	0.921725
30	1	0	-2.784972	2.372960	2.079961
31	6	0	-4.390794	-2.192715	2.741569
32	1	0	-3.810399	-2.851588	0.798005
33	1	0	-2.491061	-2.856088	2.009330
34	6	0	2.209161	-4.172371	2.954870
35	1	0	2.858162	-3.769708	0.963557
36	1	0	2.838678	-2.340503	2.042349
37	6	0	-4.703023	-0.994418	-2.832499
38	1	0	-4.694138	-0.130092	-0.883103
39	1	0	-3.610694	0.676841	-2.059315
40	6	0	-1.128839	4.810129	-2.677424
41	1	0	-0.153425	4.719165	-0.783919
42	1	0	0.600936	3.710053	-2.056723
43	6	0	4.674405	0.946123	-2.920611

44	1	0	4.697304	0.091569	-0.966915
45	1	0	3.596480	-0.722530	-2.121853
46	6	0	0.983040	-4.755409	-2.786463
47	1	0	0.313865	-4.857522	-0.763206
48	1	0	-0.674311	-3.804261	-1.823399
49	9	0	-5.734691	-0.222266	-3.247383
50	9	0	-3.899703	-1.218054	-3.890874
51	9	0	-5.209859	-2.185696	-2.443425
52	9	0	3.458989	-4.483858	3.371531
53	9	0	1.556555	-3.602567	3.986967
54	9	0	1.574673	-5.328006	2.655565
55	9	0	-3.385562	4.587191	3.296440
56	9	0	-1.471061	3.744419	3.927779
57	9	0	-1.515519	5.391246	2.501243
58	9	0	-4.758073	-3.436084	3.131050
59	9	0	-3.913118	-1.543289	3.821693
60	9	0	-5.503213	-1.543680	2.331419
61	9	0	4.833652	3.416064	3.024689
62	9	0	4.009611	1.521957	3.736657
63	9	0	5.567073	1.524576	2.212320
64	9	0	-0.398987	5.875354	-3.083214
65	9	0	-1.402271	4.056794	-3.761142
66	9	0	-2.303247	5.274169	-2.194690
67	9	0	0.249028	-5.831592	-3.155388
68	9	0	1.042621	-3.912104	-3.835696
69	9	0	2.240306	-5.181635	-2.532281
70	9	0	5.698736	0.172353	-3.350018
71	9	0	3.852926	1.165569	-3.966245
72	9	0	5.187578	2.139003	-2.545302

Table S08. PZ-T4 Structure 02 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.429991	1.958851	-0.278390
2	7	0	1.118671	1.673157	-0.372555
3	15	0	2.088161	0.425488	-0.417502
4	7	0	1.646153	-1.006239	-0.909461
5	15	0	0.581431	-2.116502	-0.541240
6	7	0	-0.793150	-1.707300	0.162006
7	15	0	-1.880771	-0.593753	-0.160835
8	7	0	-1.521206	0.868013	-0.638894
9	8	0	3.308380	0.924947	-1.348360
10	8	0	2.763886	0.206445	1.052857
11	8	0	0.380713	-2.934555	-1.912988
12	8	0	1.214236	-3.283373	0.385393
13	8	0	-2.787096	-0.425343	1.173310
14	8	0	-2.864643	-1.247691	-1.277089
15	8	0	-0.810134	3.186657	-1.255881
16	8	0	-0.642756	2.552519	1.222131
17	6	0	4.322438	0.008641	-1.763766
18	6	0	-0.496210	-4.058585	-1.974310
19	6	0	1.437877	-3.078370	1.780089
20	6	0	-3.670417	-0.490268	-2.179925
21	6	0	0.075747	4.297376	-1.407275
22	6	0	-3.307252	-1.543516	1.890450
23	6	0	-1.936660	2.972458	1.665836
24	6	0	3.161881	1.330586	1.841386
25	6	0	5.315956	0.786340	-2.611821
26	1	0	4.857948	-0.410868	-0.906451
27	1	0	3.893319	-0.796911	-2.364957
28	6	0	-0.870996	-4.273940	-3.432377
29	1	0	0.008027	-4.955763	-1.604944
30	1	0	-1.415670	-3.881497	-1.409295

31	6	0	-5.136878	-0.577413	-1.781083
32	1	0	-3.364355	0.558740	-2.204887
33	1	0	-3.558551	-0.935556	-3.170879
34	6	0	-0.502414	5.192807	-2.491688
35	1	0	0.144226	4.877232	-0.481709
36	1	0	1.070302	3.964310	-1.715337
37	6	0	-3.156515	-1.262501	3.378063
38	1	0	-4.369580	-1.663212	1.661862
39	1	0	-2.762365	-2.462960	1.661223
40	6	0	1.866295	-4.410486	2.373562
41	1	0	2.234920	-2.347903	1.947180
42	1	0	0.521247	-2.752598	2.280376
43	6	0	3.924547	0.791018	3.039946
44	1	0	3.826306	1.997327	1.283181
45	1	0	2.289295	1.886658	2.194385
46	6	0	-1.732837	4.093715	2.671886
47	1	0	-2.545239	3.360492	0.843997
48	1	0	-2.456877	2.143516	2.151813
49	9	0	-3.726877	-2.265714	4.083566
50	9	0	-1.858657	-1.181554	3.749085
51	9	0	-3.753786	-0.107425	3.741663
52	9	0	0.299097	6.274150	-2.642354
53	9	0	-0.581673	4.566101	-3.682865
54	9	0	-1.738716	5.636381	-2.178843
55	9	0	-1.684925	-5.353758	-3.520278
56	9	0	-1.535888	-3.215497	-3.948373
57	9	0	0.203444	-4.500615	-4.211846
58	9	0	-5.888952	0.093175	-2.682108
59	9	0	-5.578744	-1.853698	-1.738610
60	9	0	-5.367862	-0.034505	-0.561852
61	9	0	6.291471	-0.055448	-3.028494
62	9	0	4.742269	1.329695	-3.703488
63	9	0	5.902924	1.785745	-1.916871
64	9	0	2.069391	-4.258304	3.702620
65	9	0	0.924895	-5.365943	2.205671
66	9	0	3.012587	-4.867765	1.828855
67	9	0	-2.934583	4.506308	3.134475
68	9	0	-0.990452	3.705630	3.728349
69	9	0	-1.116149	5.162811	2.113286
70	9	0	4.300691	1.819858	3.832449
71	9	0	3.173310	-0.052522	3.781344
72	9	0	5.039767	0.122926	2.671004

Table S09. PZ-T4 Structure 03 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.741316	-1.144588	-0.446068
2	7	0	0.387507	-1.918503	-0.734100
3	15	0	-1.150110	-1.741144	-0.371403
4	7	0	-1.916525	-0.393212	-0.700933
5	15	0	-1.768306	1.150176	-0.349185
6	7	0	-0.425096	1.935293	-0.656848
7	15	0	1.122101	1.744673	-0.341562
8	7	0	1.877797	0.411015	-0.745127
9	8	0	2.173554	-1.530322	1.060151
10	8	0	2.923442	-1.863519	-1.281900
11	8	0	1.481674	2.027502	1.207217
12	8	0	1.874751	2.988716	-1.046902
13	8	0	-2.149010	1.477892	1.184742
14	8	0	-2.979263	1.899277	-1.114398
15	8	0	-1.470128	-2.087308	1.173384
16	8	0	-1.922492	-2.955304	-1.107123
17	6	0	3.156938	-1.558261	-2.650675

18	6	0	3.376429	-1.017472	1.646960
19	6	0	1.588141	3.370409	-2.386225
20	6	0	0.968766	3.176649	1.892992
21	6	0	-3.325343	0.930858	1.794097
22	6	0	-3.237207	1.668467	-2.493290
23	6	0	-0.940056	-3.263744	1.797236
24	6	0	-1.683840	-3.263366	-2.474611
25	6	0	-1.550115	-3.352499	3.186954
26	1	0	-1.220525	-4.161099	1.239212
27	1	0	0.146425	-3.195706	1.891919
28	6	0	3.647388	-1.827058	2.905188
29	1	0	4.227783	-1.137305	0.971719
30	1	0	3.250778	0.032671	1.920968
31	6	0	1.664855	3.244415	3.242918
32	1	0	1.193361	4.093952	1.342278
33	1	0	-0.107620	3.081118	2.054424
34	6	0	-3.493861	1.611945	3.142915
35	1	0	-4.212838	1.138068	1.190260
36	1	0	-3.212326	-0.144387	1.952044
37	6	0	-4.571277	2.315148	-2.833534
38	1	0	-2.465620	2.127071	-3.119968
39	1	0	-3.308644	0.597186	-2.702970
40	6	0	2.322053	4.673584	-2.663657
41	1	0	1.945686	2.618022	-3.096501
42	1	0	0.516001	3.539920	-2.521686
43	6	0	-2.473649	-4.518447	-2.813095
44	1	0	-2.029990	-2.456704	-3.128772
45	1	0	-0.622335	-3.461977	-2.648887
46	6	0	4.503084	-2.150785	-3.038623
47	1	0	2.389506	-2.007457	-3.289172
48	1	0	3.196096	-0.476571	-2.808538
49	9	0	-4.836189	2.101226	-4.145715
50	9	0	-5.585920	1.792171	-2.115147
51	9	0	-4.562495	3.646615	-2.625921
52	9	0	2.056715	5.061836	-3.935076
53	9	0	1.925070	5.662623	-1.836714
54	9	0	3.657715	4.545011	-2.541339
55	9	0	-2.253038	-4.834046	-4.112926
56	9	0	-2.097179	-5.572781	-2.060913
57	9	0	-3.800224	-4.347462	-2.649355
58	9	0	4.739890	-1.874459	-4.344535
59	9	0	5.514341	-1.628628	-2.314402
60	9	0	4.536075	-3.489227	-2.887105
61	9	0	4.758788	-1.344106	3.507352
62	9	0	2.629765	-1.754150	3.786982
63	9	0	3.858088	-3.132884	2.632553
64	9	0	1.185157	4.305229	3.932140
65	9	0	1.453707	2.135873	3.980759
66	9	0	3.000748	3.401940	3.117137
67	9	0	-4.582638	1.098620	3.760932
68	9	0	-2.428330	1.421249	3.946817
69	9	0	-3.677876	2.944368	3.018909
70	9	0	-1.059512	-4.447344	3.812449
71	9	0	-1.259296	-2.274120	3.941455
72	9	0	-2.895646	-3.468691	3.142921

Table S10. PZ-T4 Structure 05 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.818226	0.833651	0.229830
2	7	0	-0.700029	1.672302	-0.529326
3	15	0	0.863403	1.799157	-0.269578

4	7	0	1.668171	0.724559	0.583088
5	15	0	1.803181	-0.849809	0.404446
6	7	0	0.760462	-1.695741	-0.448867
7	15	0	-0.818411	-1.825746	-0.298506
8	7	0	-1.685353	-0.733466	0.467077
9	8	0	-1.450480	-1.980437	-1.782075
10	8	0	-1.087339	-3.247967	0.422351
11	8	0	-2.043312	1.538295	1.671107
12	8	0	-3.209459	1.055182	-0.565267
13	8	0	3.270775	-1.109682	-0.221342
14	8	0	1.863591	-1.516192	1.881746
15	8	0	1.602516	1.915466	-1.707889
16	8	0	1.090213	3.240217	0.427709
17	6	0	2.401880	3.686477	0.773016
18	6	0	-2.834313	0.935187	2.695509
19	6	0	1.023607	2.625582	-2.802649
20	6	0	3.714917	-2.435494	-0.510875
21	6	0	-0.787384	-2.691283	-2.827340
22	6	0	2.536465	-0.881936	2.969194
23	6	0	-3.643000	2.362075	-0.942365
24	6	0	-2.413465	-3.689424	0.712478
25	6	0	-2.510113	-5.164350	0.351945
26	1	0	-2.610388	-3.577311	1.781619
27	1	0	-3.168871	-3.145048	0.139751
28	6	0	-1.409255	-2.249957	-4.142932
29	1	0	0.278709	-2.450610	-2.845877
30	1	0	-0.932594	-3.769897	-2.717011
31	6	0	1.767869	2.209287	-4.061453
32	1	0	-0.031938	2.366730	-2.919536
33	1	0	1.136838	3.705832	-2.671184
34	6	0	2.476802	5.179952	0.493977
35	1	0	2.581968	3.518828	1.837836
36	1	0	3.177706	3.189370	0.184499
37	6	0	5.219353	-2.478467	-0.291796
38	1	0	3.254687	-3.177920	0.147102
39	1	0	3.501665	-2.683565	-1.553651
40	6	0	-2.497202	1.631686	4.004230
41	1	0	-3.900839	1.070768	2.493922
42	1	0	-2.598312	-0.127507	2.794731
43	6	0	-5.135327	2.464748	-0.664642
44	1	0	-3.133084	3.149142	-0.380598
45	1	0	-3.477154	2.507808	-2.012720
46	6	0	2.063885	-1.550313	4.250446
47	1	0	3.619964	-1.011289	2.886915
48	1	0	2.285182	0.180857	3.015383
49	9	0	-3.235747	1.079188	4.997332
50	9	0	-1.195221	1.496554	4.332658
51	9	0	-2.774995	2.951200	3.968897
52	9	0	2.681080	-0.965908	5.305608
53	9	0	0.732369	-1.424371	4.427957
54	9	0	2.357733	-2.867205	4.278899
55	9	0	5.675247	-3.720395	-0.579561
56	9	0	5.879450	-1.602998	-1.073575
57	9	0	5.546354	-2.206495	0.993613
58	9	0	-0.796041	-2.901389	-5.160665
59	9	0	-2.726850	-2.533561	-4.206602
60	9	0	-1.265958	-0.924792	-4.353739
61	9	0	1.235420	2.862678	-5.122657
62	9	0	3.080856	2.515348	-4.005102
63	9	0	1.666330	0.884942	-4.297537

64	9	0	3.707112	5.635202	0.827556
65	9	0	2.275866	5.456973	-0.816496
66	9	0	1.569608	5.880937	1.200850
67	9	0	-3.755649	-5.613290	0.632754
68	9	0	-2.283036	-5.375758	-0.966570
69	9	0	-1.632290	-5.919393	1.040505
70	9	0	-5.574373	3.692158	-1.028751
71	9	0	-5.848587	1.549471	-1.348957
72	9	0	-5.415995	2.299768	0.650355

Table S11. PZ-T4 Structure 07 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.820151	-0.593128	-0.088536
2	7	0	0.684254	-1.469340	0.593757
3	15	0	-0.854383	-1.669165	0.253877
4	7	0	-1.856561	-0.439033	0.126957
5	15	0	-1.735957	1.060217	0.638615
6	7	0	-0.511562	1.994481	0.236990
7	15	0	0.539933	1.858436	-0.949181
8	7	0	1.481003	0.588186	-1.098842
9	8	0	-0.275234	2.043425	-2.342814
10	8	0	1.517101	3.142664	-0.876683
11	8	0	2.745105	0.033414	1.086841
12	8	0	2.784936	-1.632336	-0.861657
13	8	0	-3.072085	1.837818	0.169429
14	8	0	-1.825987	1.036900	2.259893
15	8	0	-0.939816	-2.523678	-1.121785
16	8	0	-1.485894	-2.643335	1.377307
17	6	0	-0.825244	-3.856558	1.743113
18	6	0	3.077787	-0.715968	2.257073
19	6	0	-2.187874	-2.742169	-1.781665
20	6	0	-4.356785	1.239640	0.339000
21	6	0	0.252796	1.649074	-3.606632
22	6	0	-1.408897	2.129239	3.075251
23	6	0	3.939467	-1.171395	-1.567737
24	6	0	0.986937	4.456808	-0.705921
25	6	0	2.132211	5.367624	-0.292938
26	1	0	0.565788	4.833100	-1.643145
27	1	0	0.224175	4.473994	0.077043
28	6	0	-0.915148	1.245246	-4.493353
29	1	0	0.775489	2.484072	-4.083159
30	1	0	0.924795	0.792930	-3.505812
31	6	0	-2.089459	-4.061618	-2.531326
32	1	0	-3.018757	-2.816711	-1.074513
33	1	0	-2.380246	-1.938803	-2.496985
34	6	0	-1.500957	-4.388420	2.996631
35	1	0	-0.919485	-4.606415	0.952129
36	1	0	0.230078	-3.675128	1.963021
37	6	0	-5.398155	2.266033	-0.077457
38	1	0	-4.458506	0.354754	-0.294391
39	1	0	-4.538942	0.970334	1.384010
40	6	0	4.478898	-0.309379	2.686462
41	1	0	2.377277	-0.480773	3.062079
42	1	0	3.078095	-1.793164	2.070648
43	6	0	4.369375	-2.274975	-2.520685
44	1	0	3.712561	-0.275902	-2.152703
45	1	0	4.760461	-0.967713	-0.874663
46	6	0	-0.851423	1.558173	4.370081
47	1	0	-0.621895	2.709317	2.586836
48	1	0	-2.259768	2.773227	3.316647

49	9	0	4.813934	-0.983114	3.811653
50	9	0	5.400212	-0.608737	1.738471
51	9	0	4.576281	1.007690	2.945871
52	9	0	-0.449499	2.576486	5.166875
53	9	0	-1.762760	0.835695	5.049667
54	9	0	0.219855	0.760599	4.148876
55	9	0	-6.631868	1.725481	0.072935
56	9	0	-5.342391	3.381393	0.682946
57	9	0	-5.263884	2.639253	-1.364717
58	9	0	-0.446285	0.902929	-5.716081
59	9	0	-1.583092	0.178634	-3.994589
60	9	0	-1.806640	2.242544	-4.656006
61	9	0	-3.254601	-4.289984	-3.182609
62	9	0	-1.097563	-4.065647	-3.440810
63	9	0	-1.878636	-5.101353	-1.689237
64	9	0	-0.901783	-5.549876	3.356513
65	9	0	-1.401226	-3.533294	4.033963
66	9	0	-2.811264	-4.644821	2.799262
67	9	0	1.657214	6.629459	-0.149472
68	9	0	2.681601	4.996769	0.880429
69	9	0	3.114970	5.400452	-1.216841
70	9	0	5.479638	-1.870210	-3.185107
71	9	0	4.669509	-3.420425	-1.875233
72	9	0	3.420123	-2.555441	-3.437241

Table S12. PZ-T4 Structure 08 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.311140	1.303110	-0.476235
2	15	0	2.079503	-0.000869	-0.000123
3	7	0	1.310454	-1.304517	0.475784
4	15	0	-0.000843	-2.051658	0.000039
5	15	0	0.000841	2.051641	0.000038
6	7	0	-1.310463	1.304504	0.475769
7	15	0	-2.079506	0.000847	-0.000123
8	7	0	-1.311141	-1.303129	-0.476241
9	8	0	-3.072218	0.287951	-1.247464
10	8	0	-3.072041	-0.285760	1.247482
11	8	0	-0.452113	3.047418	-1.198952
12	8	0	0.455030	3.046080	1.199683
13	8	0	0.452121	-3.047428	-1.198953
14	8	0	-0.455037	-3.046103	1.199676
15	8	0	3.072196	-0.287984	-1.247476
16	8	0	3.072054	0.285735	1.247468
17	6	0	3.894217	-1.456997	-1.263145
18	6	0	3.895472	1.453755	1.262918
19	6	0	-0.515868	3.774819	1.953860
20	6	0	0.519669	3.775592	-1.952527
21	6	0	-3.895478	-1.453767	1.262928
22	6	0	-3.894217	1.456980	-1.263144
23	6	0	0.515857	-3.774839	1.953861
24	6	0	-0.519653	-3.775598	-1.952543
25	6	0	-5.021535	-1.202692	2.253810
26	1	0	-4.342623	-1.649941	0.283789
27	1	0	-3.320208	-2.322624	1.593438
28	6	0	0.237458	-4.690224	-2.901491
29	1	0	-1.145016	-4.396661	-1.303886
30	1	0	-1.146764	-3.094517	-2.533486
31	6	0	-0.242364	-4.688739	2.902620
32	1	0	1.141071	-4.396492	1.305626
33	1	0	1.143213	-3.094112	2.534950
34	6	0	-5.019789	1.207640	-2.255009
35	1	0	-4.341885	1.653342	-0.284282

36	1	0	-3.317641	2.325264	-1.592884
37	6	0	-0.237434	4.690231	-2.901471
38	1	0	1.145029	4.396648	-1.303860
39	1	0	1.146781	3.094516	-2.533473
40	6	0	0.242349	4.688739	2.902602
41	1	0	-1.141090	4.396457	1.305619
42	1	0	-1.143216	3.094096	2.534961
43	6	0	5.019808	-1.207629	-2.254982
44	1	0	4.341866	-1.653358	-0.284274
45	1	0	3.317664	-2.325288	-1.592904
46	6	0	5.021512	1.202710	2.253828
47	1	0	4.342634	1.649925	0.283786
48	1	0	3.320181	2.322607	1.593406
49	9	0	-0.649167	-5.392434	-3.643954
50	9	0	1.034734	-4.002933	-3.744935
51	9	0	1.013874	-5.575582	-2.237348
52	9	0	5.818705	-2.299569	-2.300590
53	9	0	4.563828	-0.974304	-3.501072
54	9	0	5.783132	-0.151466	-1.893759
55	9	0	0.643380	-5.391114	3.645963
56	9	0	-1.039904	-4.000735	3.745265
57	9	0	-1.018763	-5.573944	2.238262
58	9	0	5.821738	2.293669	2.299286
59	9	0	4.566188	0.969403	3.500160
60	9	0	5.783323	0.145774	1.891600
61	9	0	-0.643397	5.391117	3.645940
62	9	0	1.039900	4.000755	3.745253
63	9	0	1.018736	5.573943	2.238229
64	9	0	0.649198	5.392444	-3.643923
65	9	0	-1.034706	4.002950	-3.744928
66	9	0	-1.013852	5.575584	-2.237325
67	9	0	-5.821781	-2.293636	2.299264
68	9	0	-4.566234	-0.969377	3.500150
69	9	0	-5.783321	-0.145747	1.891553
70	9	0	-5.818661	2.299598	-2.300630
71	9	0	-4.563784	0.974311	-3.501089
72	9	0	-5.783144	0.151492	-1.893809

Table S13. PZ-T4 Structure 09 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.685053	0.959017	0.012845
2	7	0	-0.377167	1.722609	-0.440645
3	15	0	1.150403	1.683449	-0.012374
4	7	0	1.856100	0.347278	0.464698
5	15	0	1.798138	-1.165341	-0.001529
6	7	0	0.516445	-1.835969	-0.632477
7	15	0	-1.034756	-1.864706	-0.313402
8	7	0	-1.727119	-0.589733	0.361424
9	8	0	1.462518	2.698478	1.211508
10	8	0	1.887739	2.357712	-1.287057
11	8	0	3.018048	-1.362161	-1.051064
12	8	0	2.214100	-2.074031	1.280999
13	8	0	-1.706202	-2.298997	-1.705938
14	8	0	-1.457106	-3.128585	0.604659
15	8	0	-2.258422	1.762555	1.302586
16	8	0	-2.809127	1.195429	-1.135202
17	6	0	-1.203835	-3.157001	2.007350
18	6	0	-3.121838	-2.458812	-1.823609
19	6	0	-2.907183	2.447303	-1.819017

20	6	0	3.314856	2.411233	-1.352481
21	6	0	3.159141	-2.587141	-1.777107
22	6	0	3.278909	-1.673510	2.146409
23	6	0	-3.446046	1.326881	1.965274
24	6	0	0.863931	3.994849	1.241345
25	6	0	-4.137104	2.380889	-2.709735
26	1	0	-3.037487	3.277700	-1.118385
27	1	0	-2.022538	2.618344	-2.437399
28	6	0	3.677906	3.352276	-2.490427
29	1	0	3.746602	2.811836	-0.430171
30	1	0	3.730789	1.422058	-1.561748
31	6	0	1.570101	4.796090	2.323780
32	1	0	0.991043	4.521482	0.290337
33	1	0	-0.197912	3.923449	1.491299
34	6	0	-3.742100	2.323038	3.074692
35	1	0	-4.299590	1.308804	1.280695
36	1	0	-3.304439	0.337335	2.407040
37	6	0	3.364525	-2.704203	3.259799
38	1	0	4.235841	-1.654754	1.615692
39	1	0	3.075184	-0.691906	2.582748
40	6	0	4.461311	-2.501279	-2.555717
41	1	0	3.217315	-3.447095	-1.103115
42	1	0	2.328254	-2.719000	-2.474555
43	6	0	-1.967116	-4.337643	2.586363
44	1	0	-0.137873	-3.295496	2.210405
45	1	0	-1.563532	-2.243368	2.489615
46	6	0	-3.407280	-2.978188	-3.224342
47	1	0	-3.495497	-3.190616	-1.102242
48	1	0	-3.632974	-1.500684	-1.696694
49	9	0	1.013361	6.028337	2.393330
50	9	0	1.463465	4.222612	3.537743
51	9	0	2.886314	4.952232	2.057567
52	9	0	5.026073	3.426865	-2.589894
53	9	0	3.195755	2.934462	-3.676295
54	9	0	3.210187	4.602646	-2.274884
55	9	0	-4.868434	1.942491	3.720804
56	9	0	-2.745247	2.387941	3.980212
57	9	0	-3.940961	3.570571	2.594683
58	9	0	-4.263867	3.550838	-3.377375
59	9	0	-4.058270	1.388635	-3.617479
60	9	0	-5.268018	2.190040	-1.992151
61	9	0	4.342763	-2.349857	4.123510
62	9	0	2.208399	-2.792067	3.955363
63	9	0	3.651012	-3.937452	2.791603
64	9	0	4.634329	-3.643043	-3.259670
65	9	0	4.469544	-1.470415	-3.425312
66	9	0	5.528886	-2.353669	-1.738388
67	9	0	-1.756467	-4.387699	3.922477
68	9	0	-3.299197	-4.225973	2.382783
69	9	0	-1.569826	-5.511563	2.058262
70	9	0	-4.747170	-3.123472	-3.367705
71	9	0	-2.977402	-2.132913	-4.181548
72	9	0	-2.835612	-4.179056	-3.448418

Table S14. PZ-T4 Structure 10 conformation

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	15	0	-1.537279	0.119261	-1.463742
2	7	0	-2.159277	0.000573	-0.001015
3	15	0	-1.539138	-0.121937	1.462161
4	7	0	0.000267	-0.007429	1.690724
5	7	0	0.001916	-0.000371	-1.690714
6	15	0	1.540882	-0.120045	-1.462117
7	7	0	2.161519	0.000679	0.001034
8	15	0	1.538996	0.117569	1.463721
9	8	0	-2.001567	-1.514601	2.135852
10	8	0	-2.335927	0.907901	2.426712
11	8	0	1.999577	-1.513973	-2.136012
12	8	0	2.340370	0.907762	-2.426514
13	8	0	1.993300	1.512118	2.139448
14	8	0	2.340291	-0.909072	2.427822
15	8	0	-1.995529	1.512456	-2.139328
16	8	0	-2.335732	-0.909585	-2.427940
17	6	0	3.360133	1.921921	2.142589
18	6	0	-3.363580	1.918162	-2.142728
19	6	0	3.367741	-1.919297	-2.138538
20	6	0	-3.370879	-1.916014	2.138634
21	6	0	2.122484	-2.313938	2.324834
22	6	0	-2.116617	-2.314072	-2.322580
23	6	0	-2.114907	2.312099	2.321445
24	6	0	2.120372	2.312294	-2.323609
25	6	0	-3.099586	-3.005441	-3.253928
26	1	0	-1.100088	-2.571939	-2.635770
27	1	0	-2.300875	-2.674496	-1.305880
28	6	0	-3.097588	3.004793	3.252112
29	1	0	-1.098257	2.568685	2.635315
30	1	0	-2.298013	2.672665	1.304592
31	6	0	-3.400927	3.435201	-2.045767
32	1	0	-3.841759	1.611459	-3.076823
33	1	0	-3.909663	1.508531	-1.288153
34	6	0	3.103484	3.002644	-3.255556
35	1	0	1.103880	2.569054	-2.637826
36	1	0	2.303762	2.674452	-1.307378
37	6	0	3.405439	-3.436315	-2.041452
38	1	0	3.846453	-1.612539	-3.072343
39	1	0	3.913190	-1.509441	-1.283655
40	6	0	3.106043	-3.002755	3.257445
41	1	0	1.106174	-2.572184	2.638398
42	1	0	2.307079	-2.675918	1.308755
43	6	0	3.393014	3.439015	2.044935
44	1	0	3.839257	1.617062	3.076803
45	1	0	3.907392	1.513507	1.288183
46	6	0	-3.412824	-3.432966	2.042189
47	1	0	-3.848680	-1.607511	3.072332
48	1	0	-3.915209	-1.504996	1.283598
49	9	0	4.691002	-3.854222	-2.075047
50	9	0	2.858405	-3.879370	-0.882173
51	9	0	2.746029	-4.034494	-3.052167
52	9	0	2.913950	-4.340706	3.189043
53	9	0	4.389000	-2.751223	2.916376
54	9	0	2.943353	-2.624791	4.541360
55	9	0	-4.699570	-3.847235	2.076089
56	9	0	-2.867152	-3.878036	0.883071
57	9	0	-2.755034	-4.032532	3.053136
58	9	0	-2.906318	-4.343088	-3.183111

59	9	0	-4.382746	-2.754390	-2.913291
60	9	0	-2.937247	-2.629665	-4.538536
61	9	0	-2.902696	4.342196	3.181218
62	9	0	-4.380847	2.755217	2.910754
63	9	0	-2.936452	2.629010	4.536870
64	9	0	2.909503	4.340315	-3.187054
65	9	0	4.386598	2.752838	-2.913803
66	9	0	2.942037	2.624657	-4.539621
67	9	0	4.677200	3.861068	2.078990
68	9	0	2.845097	3.879868	0.885228
69	9	0	2.731178	4.035469	3.055102
70	9	0	-4.686365	3.853439	-2.080128
71	9	0	-2.854415	3.878195	-0.886245
72	9	0	-2.740802	4.033112	-3.056191

Table S15. PZ-T4 Structure 11 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.390551	1.591349	0.139532
2	7	0	-1.947795	0.177467	-0.285639
3	15	0	-1.598261	-1.366907	-0.235123
4	7	0	-0.179996	-1.894006	0.200156
5	7	0	0.158106	1.889482	0.242138
6	15	0	1.606540	1.367325	-0.086571
7	7	0	1.961267	-0.175826	-0.126992
8	15	0	1.371742	-1.595665	0.229636
9	8	0	-1.897406	-2.024035	-1.681626
10	8	0	-2.729786	-2.118703	0.646934
11	8	0	2.015630	2.042974	-1.497564
12	8	0	2.665560	2.108488	0.888997
13	8	0	1.957338	-1.970191	1.689064
14	8	0	2.132709	-2.713818	-0.659871
15	8	0	-2.091838	1.946572	1.552162
16	8	0	-2.076013	2.723240	-0.793299
17	6	0	1.646280	-3.218322	2.310729
18	6	0	-1.834805	3.188698	2.209300
19	6	0	3.294066	1.801621	-2.087635
20	6	0	-3.122639	-1.765125	-2.369008
21	6	0	1.706908	-3.034484	-1.982842
22	6	0	-1.531649	3.072416	-2.064599
23	6	0	-3.180850	-1.588393	1.891491
24	6	0	3.040626	1.558295	2.150183
25	6	0	3.091297	1.537268	-3.571434
26	1	0	3.923657	2.686861	-1.968405
27	1	0	3.786735	0.928700	-1.651511
28	6	0	2.213617	-4.432515	-2.300700
29	1	0	0.615716	-3.037714	-2.063771
30	1	0	2.137072	-2.335515	-2.706429
31	6	0	4.442049	2.053538	2.471091
32	1	0	2.361075	1.900829	2.936332
33	1	0	3.061299	0.465030	2.118224
34	6	0	-2.799174	-1.497249	-3.830600
35	1	0	-3.770520	-2.642798	-2.304289
36	1	0	-3.636320	-0.887607	-1.967665
37	6	0	-4.599537	-2.086131	2.118511
38	1	0	-2.549886	-1.944820	2.711176
39	1	0	-3.197665	-0.494746	1.875233
40	6	0	-1.656915	2.913393	3.694303
41	1	0	-0.921129	3.661951	1.840077
42	1	0	-2.687515	3.858201	2.071743
43	6	0	-2.024019	4.469859	-2.406228

44	1	0	-0.437960	3.090990	-2.040594
45	1	0	-1.880693	2.380683	-2.837153
46	6	0	1.340668	-2.955786	3.777064
47	1	0	0.769103	-3.690487	1.860480
48	1	0	2.509102	-3.885509	2.242462
49	9	0	-1.458326	4.083138	4.344780
50	9	0	-2.735616	2.313730	4.237911
51	9	0	-0.586439	2.120330	3.936219
52	9	0	-1.527181	4.833170	-3.611425
53	9	0	-3.369762	4.536148	-2.476477
54	9	0	-1.617934	5.384324	-1.497687
55	9	0	-3.949723	-1.300265	-4.514564
56	9	0	-2.033424	-0.390751	-3.983876
57	9	0	-2.143510	-2.525053	-4.407138
58	9	0	4.830636	1.546167	3.663790
59	9	0	5.341007	1.660952	1.540808
60	9	0	4.504354	3.398811	2.553970
61	9	0	4.294535	1.349610	-4.160965
62	9	0	2.347552	0.426680	-3.789598
63	9	0	2.478057	2.563283	-4.195879
64	9	0	1.831032	-4.769357	-3.554320
65	9	0	3.559184	-4.514190	-2.242993
66	9	0	1.712630	-5.356647	-1.451408
67	9	0	1.088344	-4.130991	4.398414
68	9	0	2.367844	-2.359969	4.416233
69	9	0	0.252487	-2.165105	3.932554
70	9	0	-5.056523	-1.604044	3.297380
71	9	0	-5.442129	-1.670951	1.146377
72	9	0	-4.668239	-3.432815	2.167693

Table S16. PZ-T4 Structure 13 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.979724	0.471221	-0.216704
2	7	0	-1.807454	-0.807997	0.710147
3	15	0	-0.702659	-1.955583	0.777861
4	7	0	0.820112	-1.592624	0.963382
5	15	0	1.947306	-0.649284	0.392202
6	7	0	1.748216	0.898534	0.120249
7	15	0	0.629200	1.805193	-0.561724
8	7	0	-0.770372	1.175117	-0.956451
9	8	0	-0.799455	-2.976861	-0.473344
10	8	0	-1.134394	-2.937015	1.984000
11	8	0	3.145836	-0.824105	1.459841
12	8	0	2.543263	-1.255851	-1.003713
13	8	0	0.371336	3.110605	0.337184
14	8	0	1.262164	2.497862	-1.881172
15	8	0	-2.760700	1.607089	0.630062
16	8	0	-3.042556	0.022575	-1.359908
17	6	0	1.862701	1.722714	-2.915215
18	6	0	1.451324	3.904500	0.828496
19	6	0	-3.881641	1.268163	1.447861
20	6	0	-1.022537	-2.507109	3.338238
21	6	0	-3.402263	0.925550	-2.407560
22	6	0	-2.049222	-3.468038	-0.963090
23	6	0	4.345887	-0.057298	1.360498
24	6	0	2.783143	-2.659261	-1.148084
25	6	0	0.881366	4.885077	1.841789

26	1	0	2.197481	3.283094	1.331193
27	1	0	1.914042	4.470719	0.015393
28	6	0	-4.448438	2.562531	2.010075
29	1	0	-4.665225	0.774025	0.865411
30	1	0	-3.575572	0.626108	2.277568
31	6	0	-4.726824	0.450267	-2.982753
32	1	0	-3.535732	1.945872	-2.036417
33	1	0	-2.646325	0.915264	-3.196611
34	6	0	2.845035	2.617620	-3.654404
35	1	0	2.413693	0.867274	-2.513083
36	1	0	1.104118	1.379260	-3.624824
37	6	0	-1.872074	-3.766560	-2.443703
38	1	0	-2.317220	-4.393697	-0.446492
39	1	0	-2.844801	-2.726424	-0.853205
40	6	0	-1.598592	-3.603947	4.219612
41	1	0	0.026152	-2.352316	3.608830
42	1	0	-1.595866	-1.591174	3.511500
43	6	0	4.054040	-2.832583	-1.963669
44	1	0	2.923074	-3.154826	-0.183739
45	1	0	1.950910	-3.126346	-1.680517
46	6	0	4.965075	0.013529	2.747601
47	1	0	5.055844	-0.541256	0.684100
48	1	0	4.138339	0.961260	1.022260
49	9	0	-1.489216	-3.227886	5.516064
50	9	0	-2.905677	-3.826762	3.963488
51	9	0	-0.946960	-4.774306	4.070558
52	9	0	4.297163	-4.149570	-2.146925
53	9	0	3.965818	-2.252928	-3.178426
54	9	0	5.130206	-2.297457	-1.336891
55	9	0	6.127106	0.706379	2.673836
56	9	0	4.162366	0.646367	3.629579
57	9	0	5.242379	-1.207228	3.248119
58	9	0	-3.023721	-4.270118	-2.940375
59	9	0	-1.562299	-2.656864	-3.150546
60	9	0	-0.893775	-4.671795	-2.666462
61	9	0	1.892231	5.655765	2.314333
62	9	0	-0.042265	5.702079	1.299717
63	9	0	0.314325	4.258287	2.892375
64	9	0	3.415502	1.914099	-4.660081
65	9	0	2.247136	3.699702	-4.193491
66	9	0	3.833449	3.058757	-2.844479
67	9	0	-5.093772	1.270410	-3.994185
68	9	0	-4.651474	-0.804361	-3.471270
69	9	0	-5.712569	0.468805	-2.056504
70	9	0	-5.514139	2.267195	2.794274
71	9	0	-3.552744	3.229096	2.762489
72	9	0	-4.871749	3.394940	1.035366

Table S17. PZ-T4 Structure 14 conformation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.982634	0.744773	-0.499656
2	7	0	1.581800	-0.747144	-0.825647
3	15	0	0.720606	-1.911842	-0.187073

4	7	0	-0.848819	-1.786539	-0.029841
5	15	0	-1.867058	-0.716971	0.536614
6	7	0	-1.486435	0.781519	0.847100
7	15	0	-0.543847	1.944885	0.345960
8	7	0	1.029245	1.763302	0.257968
9	8	0	1.286367	-2.356153	1.271939
10	8	0	1.026967	-3.160462	-1.165698
11	8	0	-3.131623	-0.640729	-0.486635
12	8	0	-2.492878	-1.367612	1.878530
13	8	0	-1.019339	2.534879	-1.092425
14	8	0	-0.842748	3.135499	1.397893
15	8	0	2.394953	1.463545	-1.893693
16	8	0	3.356750	0.656687	0.359314
17	6	0	-0.114350	4.360036	1.323352
18	6	0	-2.403035	2.766510	-1.376757
19	6	0	2.897985	0.762718	-3.029625
20	6	0	0.294680	-4.382898	-1.077167
21	6	0	3.997903	1.819693	0.876175
22	6	0	2.683142	-2.547452	1.513639
23	6	0	-3.673825	-1.828050	-1.066948
24	6	0	-3.359061	-0.606083	2.721243
25	6	0	-2.477853	3.422546	-2.745973
26	1	0	-2.959075	1.825844	-1.404246
27	1	0	-2.851440	3.446497	-0.646217
28	6	0	-3.627961	-1.433114	3.968034
29	1	0	-2.887539	0.335532	3.014961
30	1	0	-4.315345	-0.406063	2.227589
31	6	0	-0.231181	-4.736897	-2.460651
32	1	0	0.965906	-5.178024	-0.745500
33	1	0	-0.556371	-4.303286	-0.396358
34	6	0	-4.933673	-1.429094	-1.817706
35	1	0	-2.966042	-2.275381	-1.769431
36	1	0	-3.950032	-2.558547	-0.300015
37	6	0	4.361917	1.113486	-3.255547
38	1	0	2.799775	-0.319780	-2.913808
39	1	0	2.331207	1.094271	-3.902645
40	6	0	-1.012983	5.467506	1.852565
41	1	0	0.779753	4.305427	1.949789
42	1	0	0.166917	4.611553	0.296719
43	6	0	4.791279	1.404537	2.104782
44	1	0	4.689545	2.234813	0.137470
45	1	0	3.266055	2.573313	1.179142
46	6	0	2.876874	-3.891329	2.199524
47	1	0	3.271079	-2.539772	0.592478
48	1	0	3.044209	-1.760820	2.179738
49	9	0	-3.774304	3.661547	-3.051903
50	9	0	-1.821194	4.602814	-2.779412
51	9	0	-1.960424	2.640463	-3.716296
52	9	0	-0.339869	6.641271	1.811127
53	9	0	-2.132903	5.606467	1.106679
54	9	0	-1.395076	5.253561	3.126657
55	9	0	4.809033	0.481193	-4.364736
56	9	0	4.547950	2.439526	-3.431257
57	9	0	5.145244	0.733124	-2.218716
58	9	0	5.425423	2.487515	2.611751
59	9	0	3.993982	0.900803	3.074979
60	9	0	5.723681	0.471351	1.823749
61	9	0	4.192632	-4.080854	2.450208
62	9	0	2.214621	-3.972073	3.368731
63	9	0	2.455496	-4.921029	1.422462

64	9	0	-0.890879	-5.918054	-2.394971
65	9	0	-1.098150	-3.808695	-2.930477
66	9	0	0.756535	-4.863627	-3.368276
67	9	0	-5.461546	-2.521098	-2.416082
68	9	0	-5.873190	-0.915440	-0.992122
69	9	0	-4.686460	-0.509037	-2.773942
70	9	0	-4.447650	-0.733185	4.789645
71	9	0	-4.237423	-2.603983	3.680022
72	9	0	-2.500075	-1.714129	4.648642