

Supporting Information

Optical Waveguide from 4-Aryl-4H-1,2,4-triazole-based Supramolecular Structures

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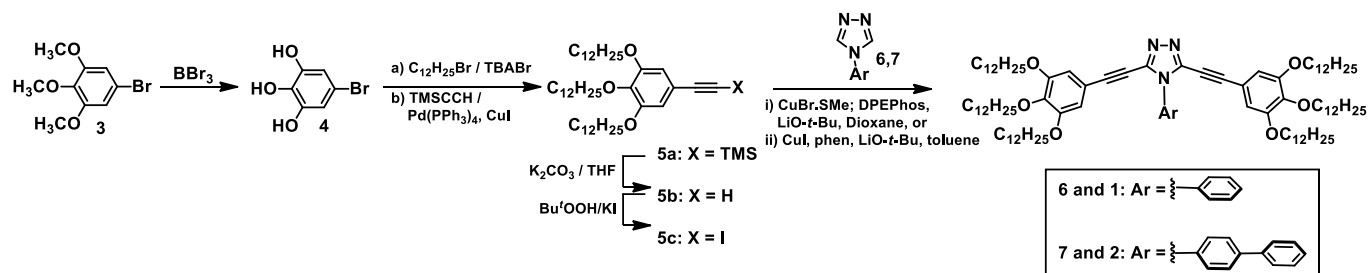
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Scheme S1. Synthesis of 4-aryl-4H-1,2,4-triazoles **1** and **2**.

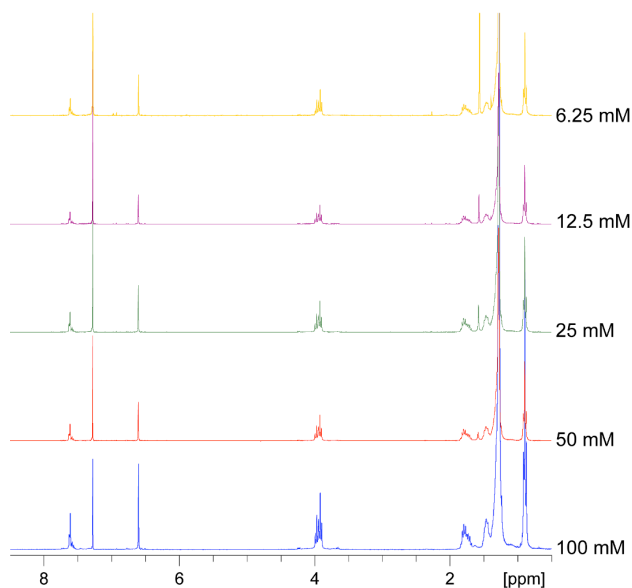


Figure S1. Partial concentration-dependent ^1H NMR spectra of **1** in CDCl_3 (300 MHz, 298 K).

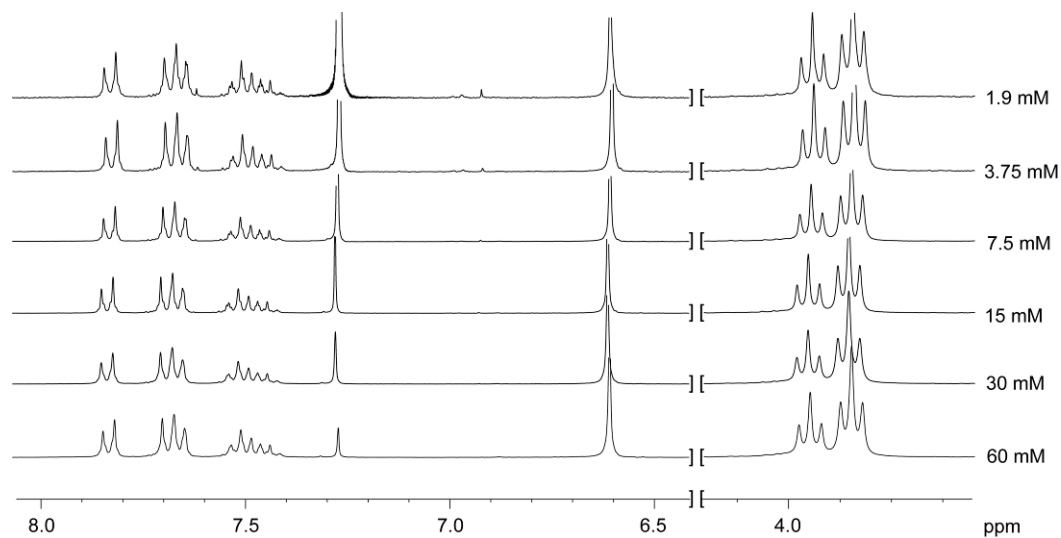


Figure S2. Partial concentration-dependent ^1H NMR spectra of **2** in CDCl_3 (300 MHz, 298 K).

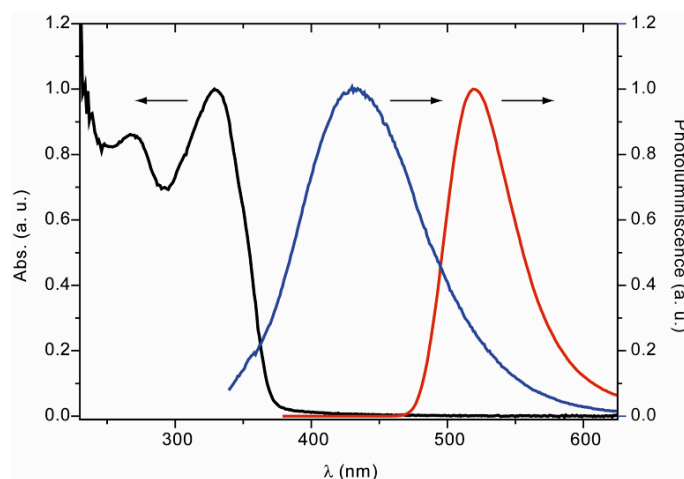


Figure S3. Normalized UV-Vis and PL spectra of the triazole **2** in solution (298 K, CHCl_3 , 1×10^{-4} M) (black and red lines, respectively) and PL the aggregates formed by **2** in acetonitrile (blue line).

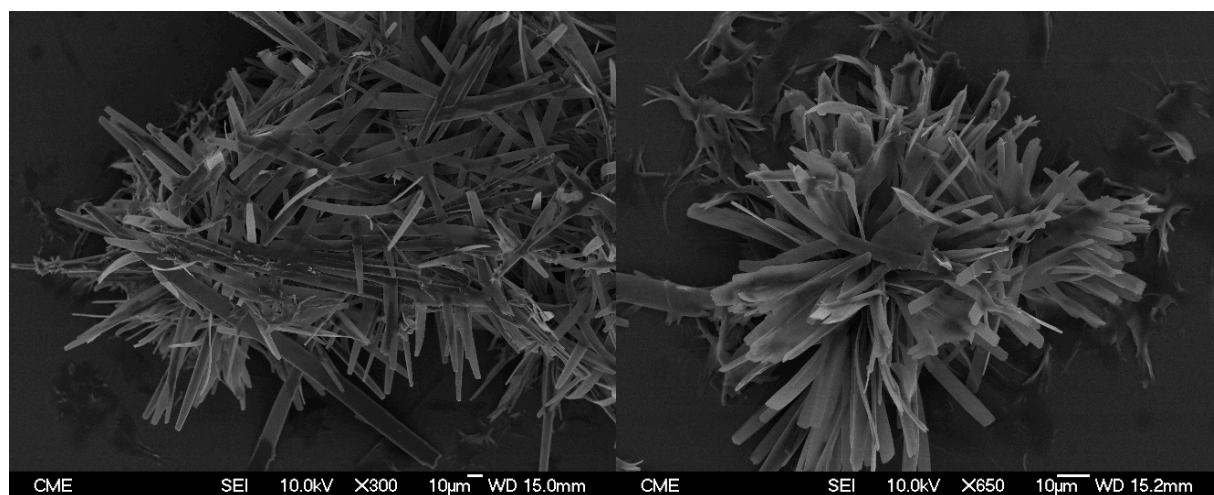


Figure S4. SEM images of the aggregated formed upon self-assembly of triazole **1** in acetonitrile (glass substrate, 298 K).

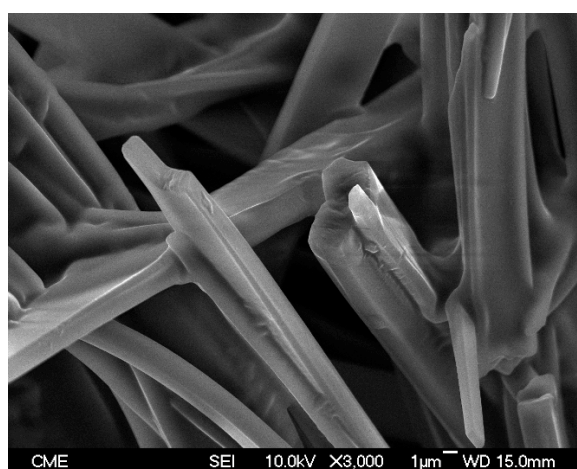


Figure S5. SEM image of the aggregated formed upon self-assembly of triazole **2** in acetonitrile (glass substrate, 298 K).

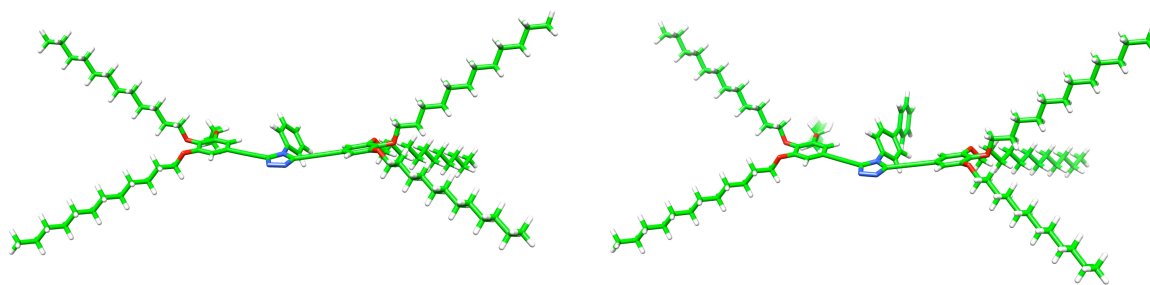


Figure S6. Side view of the calculated geometry of compounds **1** (left) and **2** (right).

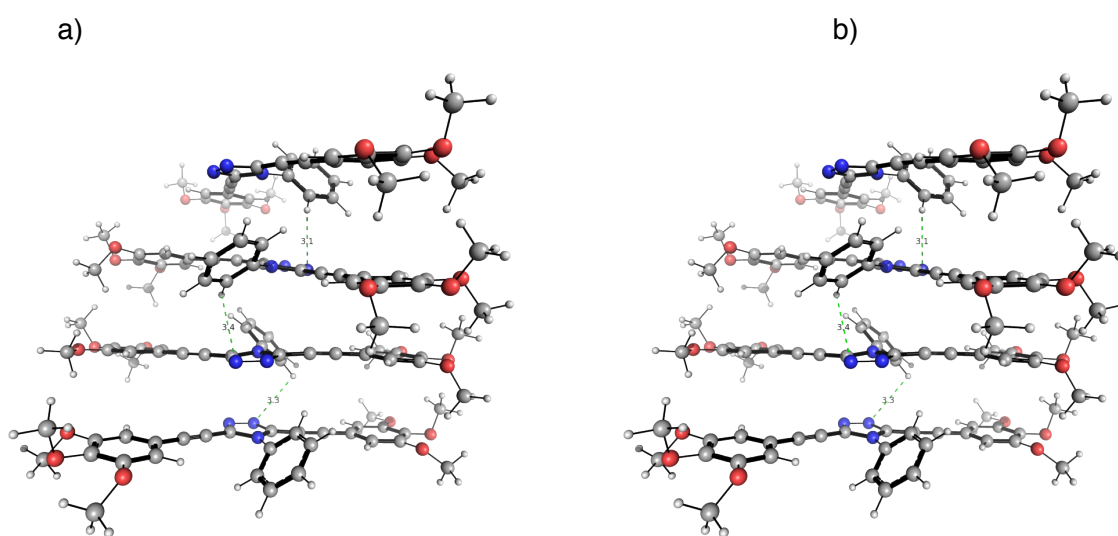


Figure S7. Two possible aggregation disposition of 4-phenyl-4*H*-1,2,4-triazol optimized at MPWB1K/6-31G** level of theory. a) Tetramer **A**, b) Tetramer **B**.

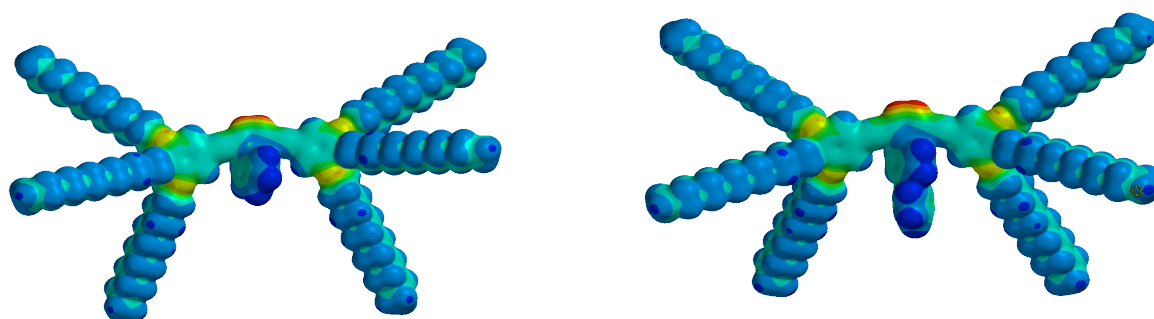


Figure S8. Molecular electrostatic potential calculated for compounds **1** (left) and **2** (right).

2. Computational Section.

All calculations included in this paper were carried out using the GAUSSIAN 09¹ series of programs. In order to include electron correlation at a reasonable computational cost, Density Functional Theory (DFT)² was used. Some of these calculations were carried out by means of the three-parameter functional developed by Becke,³ which is usually denoted as B3LYP, with the standard 6-31G* basis set.⁴ Other ones, were performed using the hybrid meta exchange-correlation MPWB1K density functional⁵ developed by Truhlar and the 6-31** basis set.⁶

Initially, the geometry of compounds **1** and **2** were optimized at B3LYP/6-31G* (Figure S6), and the corresponding electrostatic potential maps were computed (Figure S8). The presence of the aromatic units and the long peripheral paraffinic chains in compounds **1** and **2** should favor the formation of organized supramolecular structures by the operation of π - π stacking and van der Waals interactions. Moreover, the charge distribution showed in the electrostatic potential maps indicated that the triazole rings should be alternated in the supramolecular assembly, in order to avoid the electrostatic interaction. To modelized the supramolecular assembly, we chosed a simplified structure in order to minimized the computational cost. In the monomer **1** the pedant dodecyl chains were replaced for metoxy groups. The widely used Becke's three-parameters B3LYP funtional is not adecuate to calculate the formation of supramolecular aggregates because it fails in describing dispersion forces and does not properly account for stacking π - π interactions. For these reason is necessary the employment the MPWB1K funtional. Truhlar et al. have reported a very comprensive study on a large data base of non-covalent interacting systems using different funtionals and concluded that the MPW1BK gives good performance for π - π stacking interactions and intermolecular hydrogen bonds using moderate basis sets. Recently, some authors have been employed succesfully this funtional.⁷ The optimized monomer was used in a second step to generate the dimer. At this point it had performed an optimization of intermolecular distance and the rotation angle for two triazol rings. Single points calculations for diferents values were carried out. All the results are showed in Figure S9.

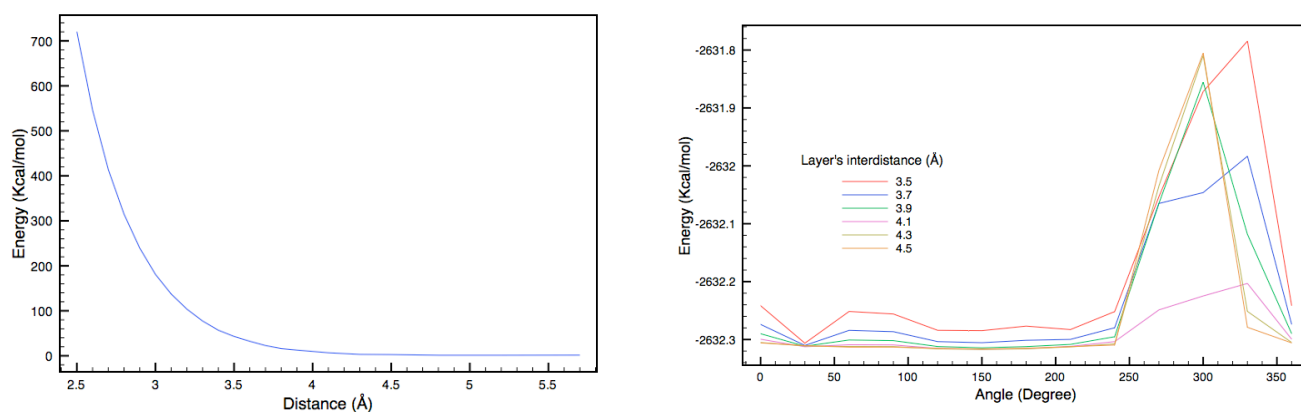


Figure S9. a) Intermolecular distance optimization. b) Torsion intermolecular angle optimization.

The optimal intermolecular distance between two monomers was 2.7 Å and the rotation angle was 150°. Taken in account these results, the trimer was generated in two different dispositions, trimer **A** and **B**. In trimer **A**, the triazol ring of the third unit was rotated 150° about the perpendicular axis to the molecular plane, possessing a similar disposition to unit **1**. On the contrary, in trimer **B** the third unit was rotated 150° in the same direction than that of the second unit, resulting in a helical organization. For the tetramer we considered again the same both dispositions. The geometries of all trimers and tetramers were fully relaxed. The optimized structures of both tetramers are shown in Figure S7. The obtained results indicated that the tetramer **A** is 9 kcal/mol more stable than tetramer **B**. A plausible explanation for this could be the existence of a threefold intermolecular hydrogen bonding between the N-1 and the *o*-H of the substituted phenyl at N-4. Moreover, the stabilization energy (in kcal/mol) per monomer unit for each supramolecular structure was computed. These energies are collected in Table S1.

Table S1

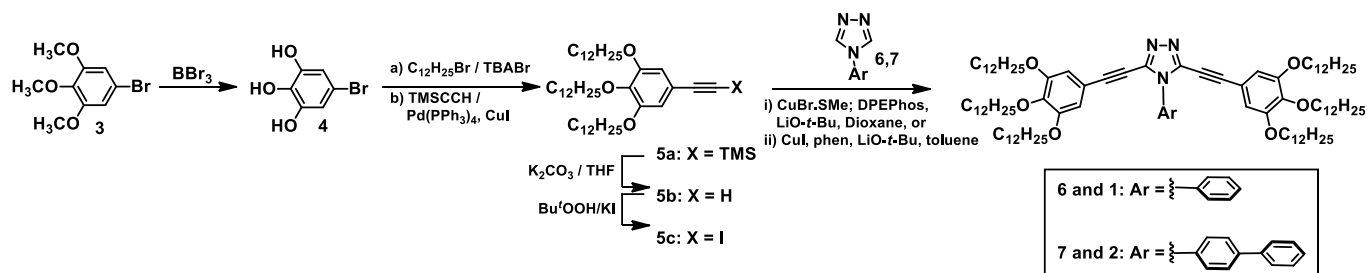
Structure	MPWB1K/6-31G**	MPWB1K/6-31G**// MPWB1K/cc-pVTZ
Monomer	0,00	0,00
Dimer	-12,12	-9,61
Trimer	-27,08	-20,44
Tetramer	-34,11	-25,02

These values possess a basis set superposition error (BSSE),⁸ which is always present in a supramolecular calculation of interacting molecular fragments. It has been recently shown that the best way of dealing with the BSSE is not to use CP corrections,⁹ which usually overcorrects for BSSE, but to make a computational effort by increasing the basis set. For this reason, the total energies for the aggregates were recalculated using MPWB1K/6-31G**// MPWB1K/cc-pVTZ. The employment of this more extended cc-pVTZ basis set¹⁰ led to a decrease of the BSSE near to 17-19%.

3. Experimental section

General. Commercially available reagents were used without further purification. Microwave irradiations were performed in a Discover® (CEM) focused microwave reactor. Yields refer to isolated and purified products. Reactions were monitored by thin-layer chromatography carried out on silica gel plates (60F-254) visualized under UV light. Column chromatography was performed on silica gel 60, (230-400 mesh). ¹H- and ¹³C-NMR spectra were recorded on a Varian Unity 500 or on a Bruker Avance 300 spectrometers at 298 K. Chemical shifts are reported in ppm (δ) using Me₄Si as the internal reference and coupling constants J are given in Hz. MALDI-TOF mass spectra were measured with a Bruker Autoflex II TOF/TOF spectrometer (Bremen, Germany) by using dithranol as the matrix. Samples co-crystallized with the matrix on the probe were ionized with a nitrogen laser pulse (337 nm) and accelerated under 20 kV with time-delayed extraction before entering the time-of-flight mass spectrometer. Matrix (10 mg/mL) and sample (1 mg/mL) were separately dissolved in methanol and mixed in a matrix/sample ratio ranging from 100:1 to 50:1. Typically, a 5 μL mixture of matrix and sample was applied to a MALDI-TOF MS probe and air-dried. MALDI-TOF MS in positive reflector mode was used for all samples. External calibration was performed by using Peptide Calibration Standard II (covered mass range: 700–3200 Da), Protein Calibration Standard I (covered mass range: 5000–17500 Da) and Protein Calibration Standard II (covered mass range: 20000–70000 Da) from Care (Bruker). The applied peak (m/z determination) detection method was the threshold centroid at 50% height of the peak maximum. SEM images were obtained from on a JEOL JSM 6335F microscope working at 10kV. Fluorescence images were recorded on a Leica TCE SP2 confocal microscope.

4. Synthetic details and characterization



5-bromo-1,2,3-trimethoxybenzene (**3**) was purchased from a commercial source. Compounds **4**, **5a-c** and **6** were prepared according to previously reported synthetic procedures¹¹ and showed identical spectroscopic properties to those reported therein.

4-phenyl-3,5-bis((3,4,5-tris(dodecyloxy)phenyl)ethynyl)-4H-1,2,4-triazole (**1**)

A flame dried tube under argon was charged with 4-phenyl-4H-1,2,4-triazole (0.019 g, 0.128 mmol), CuBr·SMe₂ (0.0078 g, 0.0384 mmol), DPEPhos (0.02 g, 0.0384 mmol) and Li^tBuO (0.043 g, 0.537 mmol). After that, a solution of 1,2,3-tris(dodecyloxy)-5-(iodoethynyl)benzene (0.4 g, 0.512 mmol) in dry dioxane (4 mL) was added to the mixture. The sealed tube with a Teflon cap containing the resulting mixture was irradiated at 130°C during 30 min at 300 W. The reaction mixture was diluted with EtOAc (2mL) and water was added (5 mL). This mixture was extracted with EtOAc (3 x 5 mL) and the combined organic layers were dried over MgSO₄. Solvents were removed under reduced pressure and the crude was purified by flash chromatography on silica gel using hexane/EtOAc (98/2) as a solvent mixture to afford compound **1** (0.116 g, 62 %). ¹H-RMN (CDCl₃, 500 MHz): 7.59-7.60 (m, 5H, H-Ph), 6.58 (s, 4H, 2 x o-H), 3.95 (t, 4H, *J* = 6.6 Hz, 2 x CH₂), 3.90 (t, 8H, *J* = 6.5 Hz, 4 x CH₂), 1.76-1.79 (m, 12H, 6 x CH₂), 1.43-1.45 (m, 12H, 6 x CH₂), 1.22-1.33 (m, 96H, CH₂), 0.87-0.89 (t, 18H, *J* = 6.7 Hz, 6 x CH₃). ¹³C-RMN (CDCl₃, 500 MHz): 14.09, 22.67, 26.05, 29.25, 29.35, 29.37, 29.55, 29.63, 29.65, 29.69, 29.73, 30.28, 31.92, 69.24, 73.62, 73.96, 97.97, 110.49, 114.76, 126.31, 129.21, 133.48, 139.27, 140.18, 140.63, 153.04. MS (electrospray) *m/z* (%) 1450,94 (92) 1451,94 (100) [M+]⁺, 1452,94 (40). HRMS (MALDI-TOF): calcd. for C₉₆H₁₆₀N₃O₃ [M+H]⁺, 1451.2307; found, 1451.2324.

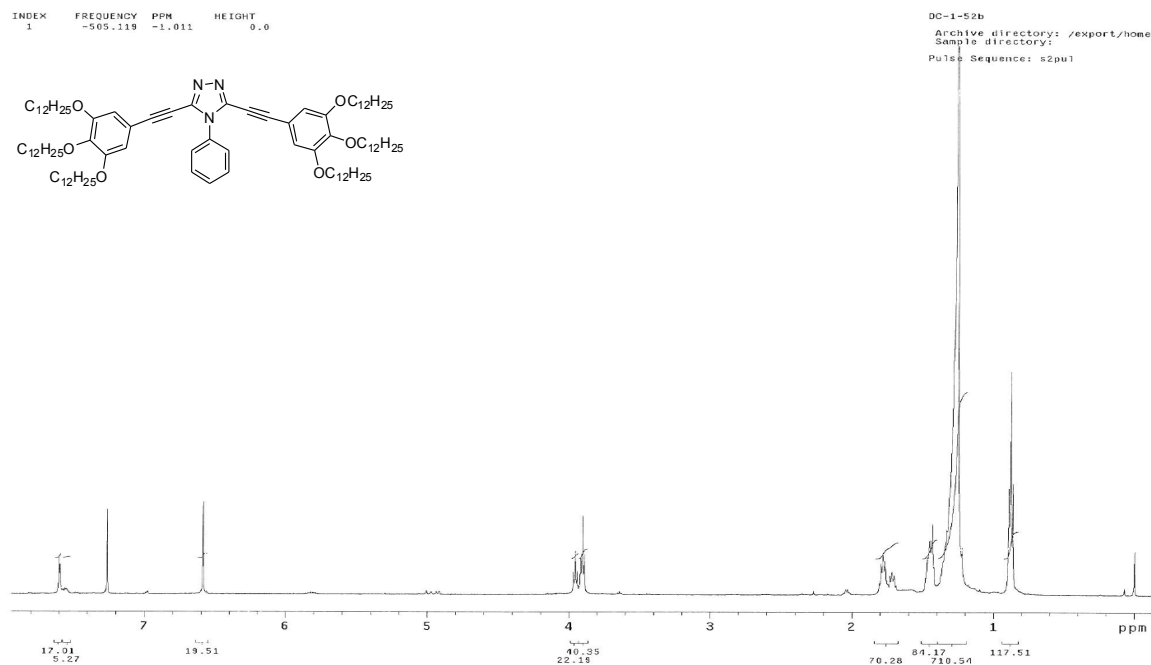
4-([1,1'-biphenyl]-4-yl)-3,5-bis((3,4,5-tris(dodecyloxy)phenyl)ethynyl)-4H-1,2,4-triazole (**2**)

A flame dried tube under argon was charged with 4-([1,1'-biphenyl]-4-yl)-4H-1,2,4-triazole (0.028 g, 0.128 mmol), CuBr·SMe₂ (0.0078 g, 0.0384 mmol), DPEPhos (0.02 g, 0.0384 mmol) and Li^tBuO (0.043 g, 0.537 mmol). After that, a solution of 1,2,3-tris(dodecyloxy)-5-(iodoethynyl)benzene (0.4 g, 0.512 mmol) in dry dioxane (4 mL) was added to the mixture. The sealed tube with a Teflon cap containing the resulting mixture was irradiated at 130°C during 30 min at 300 W. The reaction mixture was diluted with EtOAc (2mL) and water (4 mL) was added. This mixture was extracted with EtOAc (3 x 5mL) and the combined organic layers were dried over MgSO₄. Solvents were removed under reduced pressure and the crude was purified by flash chromatography on silica gel using hexane/EtOAc (98/2) as a solvent

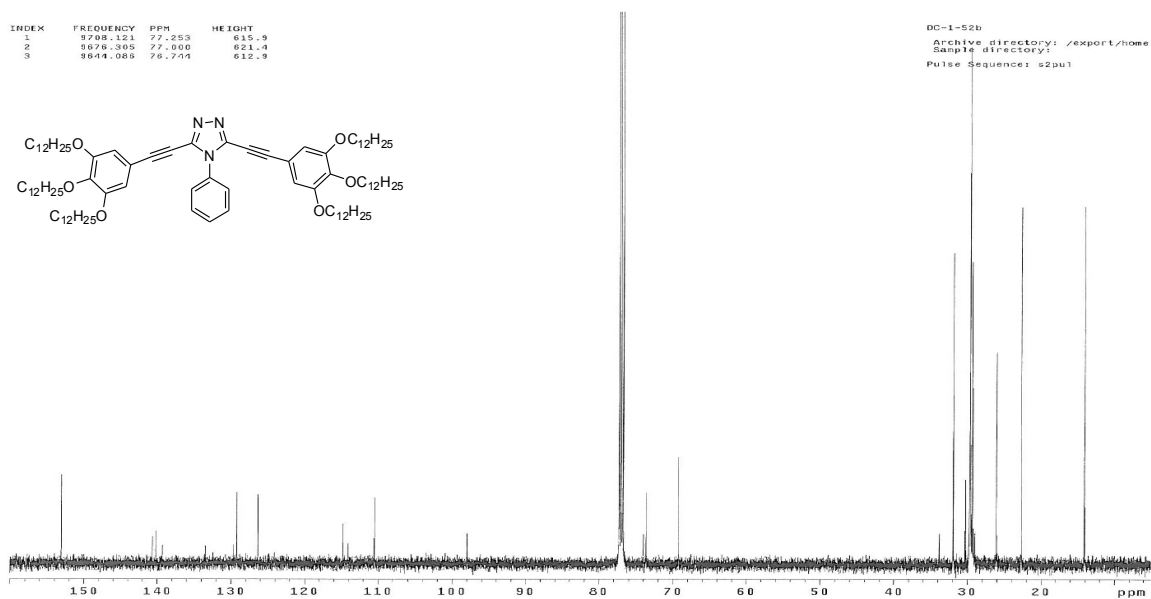
mixture to afford compound **2** (0.133 g, 68 %). ^1H -RMN (CDCl_3 , 500 MHz): 7.82 (d, 2H, $J = 8.4$ Hz, m' -H), 7.67 (d, 2H, $J = 8.4$ Hz, o' -H), 7.64 (d, 2H, $J = 7.3$ Hz, o'' -H), 7.49 (t, 2H, $J = 7.3$ Hz, m'' -H), 7.43 (t, 1H, $J = 7.3$ Hz, p'' -H), 6.60 (s, 4H, o -H), 3.94 (t, 4H, $J = 6.6$ Hz, 2 x O-CH₂), 3.86 (t, 8H, $J = 6.3$ Hz, 4 x O-CH₂), 1.73-1.69 (m, 12H, 6 x CH₂), 1.41-1.37 (m, 12H, 6 x CH₂), 1.29-1.23 (m, 96H, CH₂), 0.88 (t, 18H, $J = 6.6$ Hz, 6 x CH₃). ^{13}C -RMN (CDCl_3 , 125 MHz): 14.09, 22.67, 26.00, 26.02, 29.19, 29.35, 29.37, 29.53, 29.59, 29.61, 29.64, 29.66, 29.68, 29.69, 29.71, 30.26, 69.1, 73.6, 74.0, 98.21, 110.32, 114.73, 126.67, 127.0, 127.71, 128.27, 129.14, 132.48, 139.38, 140.19, 142.59, 153.03. HRMS (MALDI-TOF): calcd. for $\text{C}_{102}\text{H}_{164}\text{N}_3\text{O}_3$ [M+H]⁺, 1527.2620; found, 1527.2662.

5. Collection of spectra

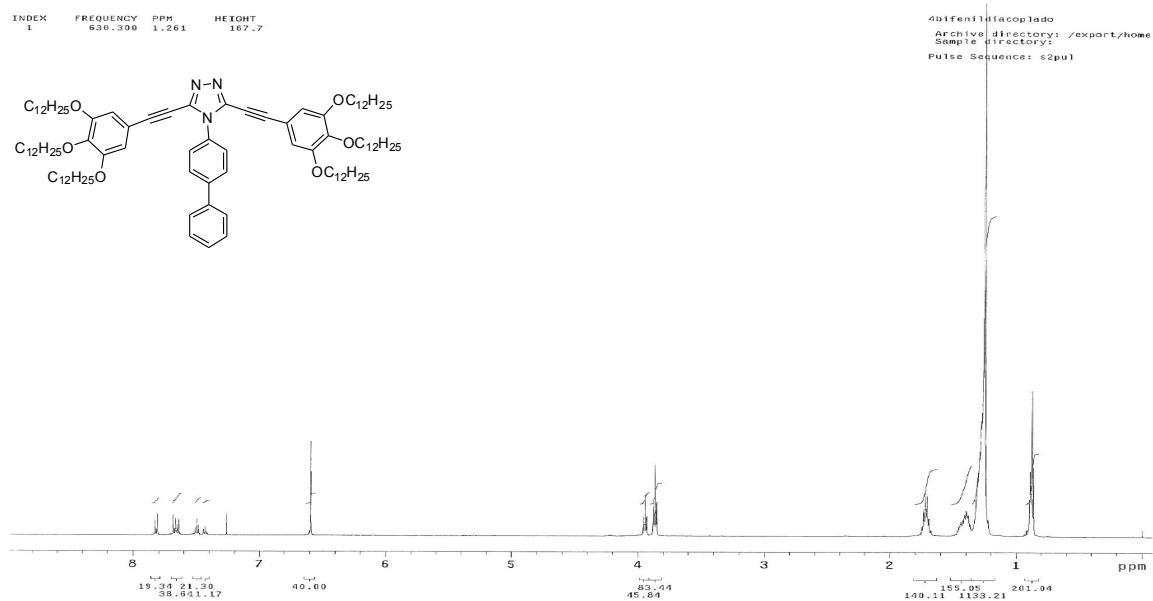
^1H NMR (CDCl_3 , 300 MHz, 298 K) of compound **1**.



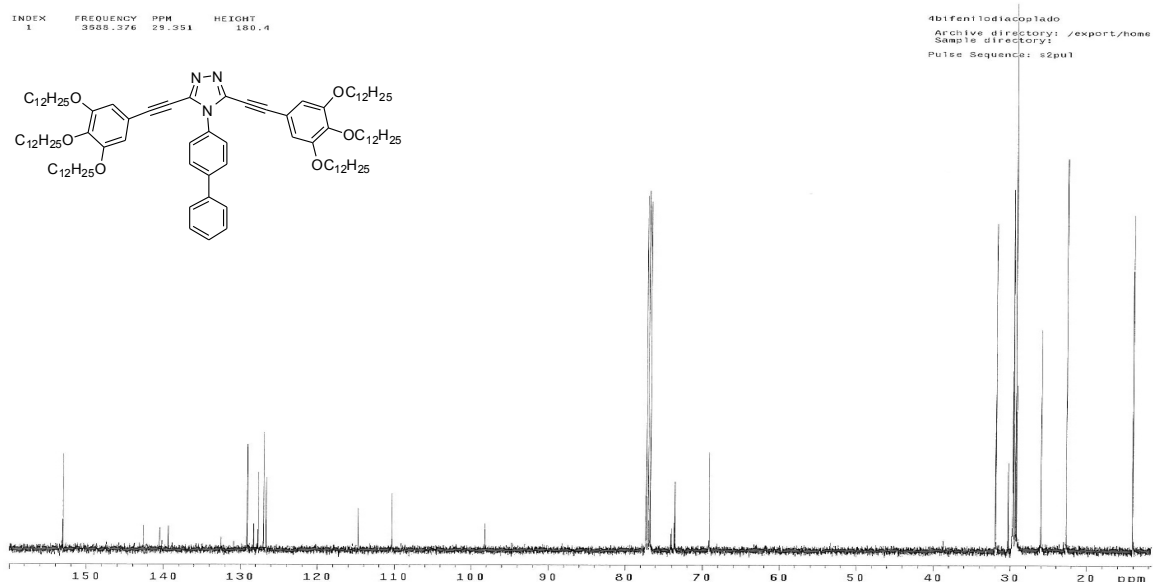
^{13}C NMR (CDCl_3 , 75 MHz, 298 K) of compound **1**.



^1H NMR (CDCl_3 , 300 MHz, 298 K) of compound **2**.



^{13}C NMR (CDCl_3 , 75 MHz, 298 K) of compound **2**.



6. Z-matrix coordinates of computed structures.

Compound 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.111969	-2.814262	-0.481132
2	6	0	1.071059	-2.801102	-0.543644
3	7	0	-0.021539	-1.967409	-0.375978
4	7	0	-0.697742	-4.058528	-0.702087
5	7	0	0.659831	-4.050961	-0.737153
6	6	0	-0.022830	-0.558171	-0.143636
7	6	0	-0.689378	-0.040127	0.970193
8	6	0	0.642239	0.289767	-1.033676
9	6	0	-0.693128	1.337440	1.187195
10	1	0	-1.192966	-0.711950	1.656925
11	6	0	0.643480	1.664460	-0.799568
12	1	0	1.145738	-0.127180	-1.899430
13	6	0	-0.025535	2.191202	0.306975
14	1	0	-1.211318	1.740722	2.052491
15	1	0	1.160669	2.324261	-1.490407
16	1	0	-0.026309	3.263152	0.482990
17	6	0	2.412686	-2.377025	-0.465530
18	6	0	3.577667	-2.038654	-0.387233
19	6	0	-2.453530	-2.395736	-0.379947
20	6	0	-3.616146	-2.056495	-0.274589
21	6	0	4.944640	-1.659284	-0.275147
22	6	0	5.317046	-0.303231	-0.326713
23	6	0	5.936015	-2.644015	-0.107475
24	6	0	6.654043	0.063516	-0.189251
25	1	0	4.569452	0.472858	-0.448095
26	6	0	7.271803	-2.276644	0.031149
27	1	0	5.670716	-3.694242	-0.059646
28	6	0	7.643755	-0.919923	-0.004683
29	8	0	6.976633	1.397619	-0.155992
30	8	0	8.205485	-3.249546	0.290331
31	8	0	8.960587	-0.554278	0.139417
32	6	0	7.717862	1.893009	-1.287629
33	6	0	9.125776	-3.546864	-0.778408
34	6	0	9.387874	-0.434117	1.514259
35	1	0	8.638216	1.311276	-1.409782
36	1	0	7.107990	1.772637	-2.195402
37	6	0	8.026774	3.360742	-1.032739
38	1	0	8.557048	-3.876818	-1.659946
39	1	0	9.685793	-2.643438	-1.046604
40	6	0	10.052134	-4.648265	-0.285196
41	1	0	8.777664	0.332361	2.010170
42	1	0	9.225643	-1.392666	2.022840
43	6	0	10.860129	-0.052926	1.525244
44	6	0	8.770975	4.019237	-2.201562
45	1	0	8.623509	3.437819	-0.114250
46	1	0	7.084650	3.890474	-0.839675

47	6	0	11.070262	-5.098245	-1.341109
48	1	0	9.439361	-5.501779	0.032817
49	1	0	10.575904	-4.288978	0.610631
50	6	0	11.414348	0.080890	2.949790
51	1	0	10.987577	0.891776	0.980282
52	1	0	11.425814	-0.814721	0.972590
53	6	0	9.106878	5.494547	-1.946626
54	1	0	9.699853	3.466262	-2.404882
55	1	0	8.163256	3.939021	-3.114918
56	6	0	11.999486	-6.207354	-0.830373
57	1	0	10.539806	-5.452643	-2.237035
58	1	0	11.674077	-4.237403	-1.664112
59	6	0	12.902221	0.454182	2.989679
60	1	0	10.835999	0.838322	3.498791
61	1	0	11.264850	-0.865870	3.489156
62	6	0	9.835886	6.167322	-3.116712
63	1	0	8.179300	6.045207	-1.731272
64	1	0	9.723642	5.573572	-1.039277
65	6	0	13.024639	-6.683650	-1.867471
66	1	0	12.528752	-5.850488	0.065512
67	1	0	11.391723	-7.063119	-0.501711
68	6	0	13.460730	0.570837	4.413527
69	1	0	13.479601	-0.298546	2.432901
70	1	0	13.052966	1.406022	2.459340
71	6	0	10.177834	7.640469	-2.858519
72	1	0	10.760547	5.612961	-3.336147
73	1	0	9.215703	6.091913	-4.022326
74	6	0	13.945956	-7.792101	-1.341746
75	1	0	12.496556	-7.043344	-2.763014
76	1	0	13.634291	-5.829216	-2.197252
77	6	0	14.949719	0.937769	4.461978
78	1	0	12.882943	1.323826	4.969837
79	1	0	13.304703	-0.381381	4.942045
80	6	0	10.899370	8.317544	-4.030999
81	1	0	10.802416	7.714947	-1.955844
82	1	0	9.253697	8.193377	-2.633179
83	6	0	14.974682	-8.280522	-2.369840
84	1	0	13.333923	-8.643615	-1.009069
85	1	0	14.472573	-7.430411	-0.445978
86	6	0	15.506855	1.042158	5.887487
87	1	0	15.106305	1.893312	3.939528
88	1	0	15.526688	0.187699	3.900764
89	6	0	11.244039	9.789719	-3.771011
90	1	0	11.822262	7.763352	-4.258318
91	1	0	10.273339	8.245179	-4.932867
92	6	0	15.892235	-9.387400	-1.834272
93	1	0	14.449208	-8.645214	-3.264971
94	1	0	15.587590	-7.430029	-2.703810
95	6	0	16.996598	1.405227	5.940742
96	1	0	14.930194	1.792495	6.448647
97	1	0	15.347667	0.086521	6.408987
98	6	0	11.962660	10.468253	-4.944445
99	1	0	10.321369	10.343368	-3.541418
100	1	0	11.871798	9.861698	-2.870305

101	6	0	16.922469	-9.882767	-2.857496
102	1	0	16.417210	-9.021317	-0.939321
103	1	0	15.278081	-10.236136	-1.498282
104	6	0	17.552418	1.502255	7.367282
105	1	0	17.572848	0.656609	5.376820
106	1	0	17.156181	2.362834	5.422921
107	1	0	12.884889	9.914057	-5.174632
108	1	0	11.334423	10.396953	-5.844916
109	6	0	12.308539	11.939943	-4.684369
110	1	0	16.398018	-10.251144	-3.751790
111	1	0	17.536686	-9.034473	-3.194748
112	6	0	17.838712	-10.987947	-2.316624
113	1	0	16.976371	2.251101	7.931158
114	1	0	17.391335	0.544601	7.884600
115	6	0	19.042426	1.862980	7.423632
116	6	0	13.027760	12.618554	-5.857320
117	1	0	12.936971	12.012278	-3.783989
118	1	0	11.386699	12.495261	-4.454778
119	6	0	18.868919	-11.487864	-3.337573
120	1	0	17.224633	-11.835747	-1.977617
121	1	0	18.364407	-10.619272	-1.423014
122	6	0	19.597872	1.956327	8.850496
123	1	0	19.204748	2.821869	6.908688
124	1	0	19.619317	1.115218	6.858958
125	6	0	13.369722	14.087736	-5.589245
126	1	0	12.399957	12.547095	-6.757018
127	1	0	13.949122	12.064063	-6.086094
128	6	0	19.779346	-12.590288	-2.786825
129	1	0	19.482828	-10.641217	-3.676694
130	1	0	18.343859	-11.858075	-4.229689
131	6	0	21.086517	2.315457	8.898666
132	1	0	19.435894	0.998282	9.364956
133	1	0	19.022495	2.704227	9.414630
134	1	0	14.023998	14.189233	-4.714487
135	1	0	12.464709	14.676261	-5.393895
136	1	0	13.884012	14.542209	-6.443838
137	1	0	19.196490	-13.464156	-2.470294
138	1	0	20.345066	-12.238342	-1.915227
139	1	0	20.502078	-12.926906	-3.538956
140	1	0	21.275944	3.287222	8.425991
141	1	0	21.691845	1.568415	8.370392
142	1	0	21.452279	2.370735	9.930424
143	6	0	-4.976302	-1.662710	-0.136623
144	6	0	-6.000648	-2.626711	-0.185874
145	6	0	-5.308262	-0.308596	0.054303
146	6	0	-7.329203	-2.244372	-0.021691
147	1	0	-5.768567	-3.675539	-0.333319
148	6	0	-6.637534	0.072749	0.224135
149	1	0	-4.535254	0.450856	0.095075
150	6	0	-7.660427	-0.893395	0.195617
151	8	0	-8.302172	-3.214026	0.003838
152	8	0	-6.917722	1.388829	0.494291
153	8	0	-8.969157	-0.513296	0.372353
154	6	0	-9.185808	-3.244175	-1.134944

155	6	0	-7.623270	2.105487	-0.537597
156	6	0	-9.463799	-0.710105	1.715634
157	1	0	-9.688531	-2.275508	-1.237169
158	1	0	-8.592484	-3.424429	-2.043089
159	6	0	-10.189566	-4.365092	-0.910318
160	1	0	-7.029910	2.075741	-1.463370
161	1	0	-8.587374	1.621737	-0.729408
162	6	0	-7.811733	3.538560	-0.062598
163	1	0	-9.361751	-1.769099	1.982657
164	1	0	-8.855061	-0.114941	2.409484
165	6	0	-10.920357	-0.274665	1.755492
166	6	0	-11.188107	-4.508398	-2.066447
167	1	0	-10.727568	-4.169911	0.026875
168	1	0	-9.641202	-5.305096	-0.766521
169	6	0	-8.534055	4.410253	-1.097995
170	1	0	-6.827126	3.965617	0.168887
171	1	0	-8.376980	3.524657	0.878649
172	6	0	-11.546309	-0.465648	3.143576
173	1	0	-11.481712	-0.851978	1.008923
174	1	0	-10.985528	0.778969	1.453589
175	6	0	-12.209124	-5.630871	-1.838729
176	1	0	-11.721094	-3.557144	-2.211490
177	1	0	-10.642989	-4.698234	-3.002662
178	6	0	-8.724721	5.861651	-0.638101
179	1	0	-7.969233	4.402155	-2.041924
180	1	0	-9.515804	3.970499	-1.327393
181	6	0	-13.021882	-0.049673	3.204610
182	1	0	-11.455722	-1.520219	3.442430
183	1	0	-10.975870	0.111186	3.886190
184	6	0	-13.224564	-5.778403	-2.979147
185	1	0	-11.675701	-6.582744	-1.700829
186	1	0	-12.746032	-5.445172	-0.896762
187	6	0	-9.441740	6.740031	-1.671281
188	1	0	-9.290755	5.872245	0.305002
189	1	0	-7.742551	6.299837	-0.407225
190	6	0	-13.655501	-0.256532	4.586387
191	1	0	-13.113937	1.007576	2.915336
192	1	0	-13.590144	-0.620145	2.455168
193	6	0	-14.245157	-6.899615	-2.744656
194	1	0	-13.756919	-4.825431	-3.116815
195	1	0	-12.688973	-5.965346	-3.921727
196	6	0	-9.623695	8.194642	-1.218665
197	1	0	-8.877881	6.722272	-2.615866
198	1	0	-10.426107	6.304187	-1.898230
199	6	0	-15.133605	0.149186	4.650166
200	1	0	-13.557037	-1.313546	4.875102
201	1	0	-13.088661	0.315932	5.335584
202	6	0	-15.269968	-7.045227	-3.877107
203	1	0	-14.774903	-6.715093	-1.798158
204	1	0	-13.712601	-7.853084	-2.612176
205	6	0	-10.335730	9.074076	-2.254649
206	1	0	-8.639031	8.628843	-0.989716
207	1	0	-10.189502	8.213709	-0.275283
208	6	0	-15.768969	-0.068898	6.029592

209	1	0	-15.698639	-0.419541	3.896641
210	1	0	-15.232646	1.207811	4.367399
211	6	0	-16.290470	-8.165570	-3.638137
212	1	0	-15.802188	-6.091434	-4.009640
213	1	0	-14.741482	-7.231044	-4.823989
214	6	0	-10.511460	10.530811	-1.806470
215	1	0	-9.771366	9.050889	-3.198844
216	1	0	-11.322000	8.642260	-2.481199
217	6	0	-17.248558	0.331263	6.093900
218	1	0	-15.666977	-1.127280	6.312207
219	1	0	-15.205370	0.501029	6.783250
220	6	0	-17.319922	-8.310046	-4.766501
221	1	0	-15.758226	-9.119631	-3.508230
222	1	0	-16.815997	-7.980906	-2.689305
223	6	0	-11.218454	11.411045	-2.845232
224	1	0	-11.078182	10.555012	-0.863730
225	1	0	-9.525091	10.961194	-1.577525
226	6	0	-17.884956	0.106945	7.471843
227	1	0	-17.350829	1.390537	5.814629
228	1	0	-17.811117	-0.236565	5.337823
229	1	0	-17.851754	-7.355692	-4.896779
230	1	0	-16.794951	-8.495794	-5.715421
231	6	0	-18.340767	-9.429405	-4.525434
232	1	0	-10.652301	11.384602	-3.788310
233	1	0	-12.205708	10.982063	-3.073091
234	6	0	-11.390728	12.868865	-2.399839
235	1	0	-17.781451	-0.952269	7.750959
236	1	0	-17.323076	0.675251	8.228084
237	6	0	-19.365066	0.504513	7.536423
238	6	0	-19.371352	-9.574696	-5.652585
239	1	0	-18.866145	-9.244250	-3.576441
240	1	0	-17.809718	-10.384326	-4.395520
241	6	0	-12.093355	13.750371	-3.440404
242	1	0	-10.403819	13.297769	-2.169746
243	1	0	-11.959439	12.896990	-1.458235
244	6	0	-20.002667	0.277513	8.913314
245	1	0	-19.927380	-0.062617	6.779428
246	1	0	-19.469603	1.564330	7.259414
247	6	0	-20.387355	-10.693913	-5.402613
248	1	0	-18.846825	-9.761388	-6.600551
249	1	0	-19.902111	-8.620726	-5.782643
250	6	0	-12.259882	15.204708	-2.988051
251	1	0	-13.079949	13.323030	-3.669897
252	1	0	-11.524822	13.722500	-4.380984
253	6	0	-21.480711	0.677060	8.968436
254	1	0	-19.441482	0.844476	9.669807
255	1	0	-19.899150	-0.781468	9.189667
256	1	0	-20.953292	-10.516540	-4.479671
257	1	0	-19.889231	-11.666178	-5.301999
258	1	0	-21.107798	-10.772574	-6.224872
259	1	0	-11.287573	15.669871	-2.783512
260	1	0	-12.855506	15.268399	-2.068960
261	1	0	-12.762845	15.807591	-3.752843
262	1	0	-22.074121	0.100681	8.247851

263	1	0	-21.613129	1.739543	8.729183
264	1	0	-21.906237	0.504389	9.963633

Compound 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.046534	-3.141618	-0.385472
2	6	0	1.135334	-3.081498	-0.464968
3	7	0	0.025485	-2.268057	-0.310387
4	7	0	-0.605962	-4.381639	-0.577294
5	7	0	0.750688	-4.344796	-0.623077
6	6	0	-0.005891	-0.855020	-0.113217
7	6	0	-0.684407	-0.317476	0.983496
8	6	0	0.641452	-0.009891	-1.018209
9	6	0	-0.717829	1.062082	1.165274
10	1	0	-1.186076	-0.976603	1.683841
11	6	0	0.613330	1.367115	-0.817462
12	1	0	1.166163	-0.431373	-1.869067
13	6	0	-0.068211	1.932533	0.273661
14	1	0	-1.270416	1.470501	2.006090
15	1	0	1.142030	2.013478	-1.511734
16	6	0	2.468054	-2.627284	-0.407622
17	6	0	3.627305	-2.266196	-0.347058
18	6	0	-2.396566	-2.750306	-0.288535
19	6	0	-3.566337	-2.434554	-0.189247
20	6	0	4.989400	-1.864806	-0.253970
21	6	0	5.341735	-0.503876	-0.317656
22	6	0	5.996535	-2.834454	-0.091914
23	6	0	6.674971	-0.117705	-0.197361
24	1	0	4.582050	0.261112	-0.434512
25	6	0	7.328415	-2.447591	0.029595
26	1	0	5.746611	-3.887964	-0.034574
27	6	0	7.680561	-1.086000	-0.018674
28	8	0	6.979765	1.220697	-0.174488
29	8	0	8.278014	-3.405758	0.285551
30	8	0	8.993610	-0.701066	0.109125
31	6	0	7.696736	1.720721	-1.319544
32	6	0	9.193903	-3.696477	-0.788743
33	6	0	9.431365	-0.563375	1.479032
34	1	0	8.622696	1.150468	-1.453521
35	1	0	7.074536	1.588271	-2.217210
36	6	0	7.990690	3.193455	-1.076083
37	1	0	8.622992	-4.039264	-1.663956
38	1	0	9.739623	-2.787195	-1.066378
39	6	0	10.138285	-4.782562	-0.295723
40	1	0	8.817749	0.201782	1.972770
41	1	0	9.282859	-1.518482	1.998196
42	6	0	10.900044	-0.168361	1.474991
43	6	0	8.712142	3.854032	-2.257947
44	1	0	8.598381	3.282424	-0.165887
45	1	0	7.044909	3.712916	-0.873640

46	6	0	11.154511	-5.227489	-1.355626
47	1	0	9.538642	-5.641495	0.032596
48	1	0	10.663889	-4.410669	0.593865
49	6	0	11.463062	-0.018756	2.894544
50	1	0	11.014947	0.773089	0.921753
51	1	0	11.468432	-0.929501	0.924203
52	6	0	9.035107	5.334304	-2.015314
53	1	0	9.644418	3.310273	-2.470444
54	1	0	8.093521	3.762140	-3.162850
55	6	0	12.098432	-6.323425	-0.843432
56	1	0	10.622355	-5.593197	-2.245979
57	1	0	11.747018	-4.362250	-1.687657
58	6	0	12.948770	0.364238	2.922516
59	1	0	10.883215	0.739302	3.441098
60	1	0	11.323248	-0.961976	3.442630
61	6	0	9.744276	6.007233	-3.197463
62	1	0	8.104329	5.876564	-1.792831
63	1	0	9.661183	5.425116	-1.115466
64	6	0	13.122715	-6.796523	-1.882896
65	1	0	12.629044	-5.955271	0.047072
66	1	0	11.501308	-7.183107	-0.505607
67	6	0	13.514338	0.493085	4.342523
68	1	0	13.527481	-0.388615	2.367285
69	1	0	13.090545	1.313512	2.385218
70	6	0	10.075493	7.484972	-2.951769
71	1	0	10.671569	5.460252	-3.424191
72	1	0	9.114620	5.920689	-4.095521
73	6	0	14.055974	-7.893680	-1.354575
74	1	0	12.593570	-7.166317	-2.773682
75	1	0	13.723289	-5.938815	-2.220709
76	6	0	15.001987	0.866632	4.381697
77	1	0	12.935958	1.247080	4.896857
78	1	0	13.365131	-0.456325	4.878008
79	6	0	10.779581	8.160702	-4.135591
80	1	0	10.708396	7.570586	-2.055894
81	1	0	9.148839	8.031200	-2.720657
82	6	0	15.084639	-8.380000	-2.383764
83	1	0	13.452567	-8.748226	-1.014012
84	1	0	14.583222	-7.522002	-0.463281
85	6	0	15.564824	0.980181	5.804256
86	1	0	15.152252	1.820147	3.853758
87	1	0	15.579440	0.116044	3.821673
88	6	0	11.115405	9.637074	-3.888084
89	1	0	11.704467	7.612372	-4.368918
90	1	0	10.145043	8.077878	-5.030597
91	6	0	16.012162	-9.476932	-1.844934
92	1	0	14.558755	-8.753763	-3.274899
93	1	0	15.690023	-7.526911	-2.724744
94	6	0	17.053735	1.347756	5.850127
95	1	0	14.988143	1.731587	6.363968
96	1	0	15.410520	0.026725	6.331181
97	6	0	11.818245	10.313245	-5.072400
98	1	0	10.190811	10.185362	-3.653475
99	1	0	11.750932	9.719468	-2.993733

100	6	0	17.042965	-9.970728	-2.868374
101	1	0	16.537161	-9.101898	-0.953715
102	1	0	15.405260	-10.328170	-1.502174
103	6	0	17.614346	1.451775	7.274288
104	1	0	17.629937	0.598452	5.287065
105	1	0	17.208751	2.303728	5.327946
106	1	0	12.741992	9.763822	-5.307846
107	1	0	11.182065	10.232102	-5.966445
108	6	0	12.156681	11.788800	-4.824691
109	1	0	16.518645	-10.347471	-3.759251
110	1	0	17.650600	-9.120189	-3.211823
111	6	0	17.967971	-11.066786	-2.323873
112	1	0	17.038617	2.201616	7.837170
113	1	0	17.456980	0.495839	7.795900
114	6	0	19.103813	1.815730	7.324409
115	6	0	12.861012	12.464510	-6.008306
116	1	0	12.792708	11.870934	-3.930499
117	1	0	11.233353	12.339624	-4.590332
118	6	0	18.999242	-11.565252	-3.344478
119	1	0	17.360348	-11.916832	-1.978921
120	1	0	18.493223	-10.689838	-1.433464
121	6	0	19.663605	1.914738	8.749183
122	1	0	19.262576	2.773243	6.805831
123	1	0	19.680337	1.067242	6.760320
124	6	0	13.196360	13.937388	-5.752390
125	1	0	12.225532	12.383641	-6.901797
126	1	0	13.783629	11.914196	-6.242003
127	6	0	19.918034	-12.658774	-2.789864
128	1	0	19.606897	-10.716410	-3.689323
129	1	0	18.474753	-11.943562	-4.233521
130	6	0	21.151806	2.276463	8.791589
131	1	0	19.504797	0.958093	9.267222
132	1	0	19.088732	2.663502	9.312684
133	1	0	13.858158	14.048252	-4.884449
134	1	0	12.289583	14.521524	-5.552094
135	1	0	13.699801	14.389786	-6.614514
136	1	0	19.341539	-13.534748	-2.467569
137	1	0	20.483159	-12.298528	-1.921280
138	1	0	20.641444	-12.994583	-3.541704
139	1	0	21.338208	3.247078	8.315365
140	1	0	21.756702	1.528782	8.263720
141	1	0	21.520698	2.335501	9.822026
142	6	0	-4.934768	-2.065611	-0.064464
143	6	0	-5.937568	-3.053219	-0.071757
144	6	0	-5.295744	-0.711323	0.066572
145	6	0	-7.275339	-2.694836	0.076099
146	1	0	-5.681471	-4.102037	-0.172043
147	6	0	-6.633645	-0.354118	0.213851
148	1	0	-4.539763	0.066166	0.072788
149	6	0	-7.634929	-1.342676	0.227998
150	8	0	-8.225906	-3.682874	0.144684
151	8	0	-6.954022	0.966431	0.415965
152	8	0	-8.954402	-0.990944	0.382888
153	6	0	-9.115476	-3.769825	-0.986215

154	6	0	-7.627237	1.613256	-0.682079
155	6	0	-9.386400	-0.935188	1.759784
156	1	0	-9.635893	-2.814586	-1.118936
157	1	0	-8.523968	-3.971322	-1.891274
158	6	0	-10.101384	-4.897789	-0.721293
159	1	0	-6.974940	1.585079	-1.567302
160	1	0	-8.551137	1.072792	-0.917531
161	6	0	-7.921538	3.048501	-0.272439
162	1	0	-9.216199	-1.914318	2.226079
163	1	0	-8.785473	-0.185778	2.291136
164	6	0	-10.862395	-0.569654	1.782556
165	6	0	-11.104769	-5.077540	-1.867965
166	1	0	-10.634581	-4.683771	0.214431
167	1	0	-9.541488	-5.827797	-0.558297
168	6	0	-8.638176	3.835507	-1.377518
169	1	0	-6.977447	3.542132	-0.007449
170	1	0	-8.535282	3.034302	0.637945
171	6	0	-11.418951	-0.486623	3.209975
172	1	0	-11.420372	-1.317916	1.204314
173	1	0	-10.997577	0.391367	1.268745
174	6	0	-12.114759	-6.205153	-1.617184
175	1	0	-11.647995	-4.134675	-2.029019
176	1	0	-10.562026	-5.279473	-2.803111
177	6	0	-8.940570	5.288768	-0.989050
178	1	0	-8.025454	3.826096	-2.291026
179	1	0	-9.578457	3.327228	-1.637116
180	6	0	-12.910078	-0.128010	3.259383
181	1	0	-11.261449	-1.448390	3.719807
182	1	0	-10.848121	0.258631	3.783010
183	6	0	-13.133943	-6.373120	-2.751338
184	1	0	-11.573594	-7.151187	-1.469741
185	1	0	-12.648277	-6.010645	-0.675099
186	6	0	-9.671572	6.071592	-2.087358
187	1	0	-9.544743	5.300805	-0.069919
188	1	0	-7.999583	5.801091	-0.740435
189	6	0	-13.469294	-0.048910	4.685533
190	1	0	-13.069314	0.834719	2.751535
191	1	0	-13.480970	-0.872418	2.685062
192	6	0	-14.147144	-7.498303	-2.503827
193	1	0	-13.673037	-5.425089	-2.896802
194	1	0	-12.600441	-6.565702	-3.694002
195	6	0	-9.970946	7.528047	-1.709400
196	1	0	-9.070008	6.052253	-3.008345
197	1	0	-10.614087	5.559025	-2.331039
198	6	0	-14.961170	0.304718	4.741636
199	1	0	-13.305350	-1.011388	5.192680
200	1	0	-12.897897	0.696325	5.258661
201	6	0	-15.174886	-7.655537	-3.632004
202	1	0	-14.674341	-7.309914	-1.556681
203	1	0	-13.609299	-8.448178	-2.367074
204	6	0	-10.711096	8.303883	-2.806762
205	1	0	-9.028085	8.043208	-1.472751
206	1	0	-10.567290	7.548523	-0.785042
207	6	0	-15.518236	0.380972	6.168967

208	1	0	-15.532514	-0.440243	4.168030
209	1	0	-15.125776	1.267752	4.235583
210	6	0	-16.190087	-8.779095	-3.385433
211	1	0	-15.711777	-6.704835	-3.767930
212	1	0	-14.648237	-7.843605	-4.579483
213	6	0	-11.009104	9.762251	-2.435195
214	1	0	-10.116398	8.279601	-3.732120
215	1	0	-11.654879	7.788996	-3.040548
216	6	0	-17.010504	0.732331	6.228363
217	1	0	-15.351794	-0.581848	6.674786
218	1	0	-14.946958	1.126354	6.742126
219	6	0	-17.221960	-8.930679	-4.510608
220	1	0	-15.653937	-9.730734	-3.253888
221	1	0	-16.713601	-8.593076	-2.435760
222	6	0	-11.754455	10.533295	-3.532411
223	1	0	-11.600973	9.787258	-1.508048
224	1	0	-10.065222	10.278774	-2.205488
225	6	0	-17.565946	0.807554	7.656381
226	1	0	-17.177322	1.695328	5.722910
227	1	0	-17.581866	-0.013077	5.655307
228	1	0	-17.757362	-7.978490	-4.642139
229	1	0	-16.698655	-9.117061	-5.460332
230	6	0	-18.238574	-10.052827	-4.264518
231	1	0	-11.163464	10.506217	-4.460108
232	1	0	-12.698803	10.016828	-3.760532
233	6	0	-12.052113	11.992576	-3.164860
234	1	0	-17.398369	-0.155374	8.161734
235	1	0	-16.994488	1.553118	8.229217
236	6	0	-19.058167	1.158005	7.717804
237	6	0	-19.271375	-10.203359	-5.388918
238	1	0	-18.762208	-9.867420	-3.314612
239	1	0	-17.704275	-11.005858	-4.134079
240	6	0	-12.800673	12.761266	-4.261482
241	1	0	-11.108090	12.511034	-2.939374
242	1	0	-12.641770	12.021006	-2.236225
243	6	0	-19.613121	1.233306	9.145935
244	1	0	-19.630758	0.412490	7.145838
245	1	0	-19.226942	2.121122	7.212870
246	6	0	-20.283410	-11.325218	-5.134671
247	1	0	-18.748498	-10.390089	-6.337790
248	1	0	-19.805335	-9.251236	-5.519392
249	6	0	-13.093833	14.217773	-3.887445
250	1	0	-13.744310	12.243712	-4.485795
251	1	0	-12.211697	12.733018	-5.189385
252	6	0	-21.103770	1.583324	9.198649
253	1	0	-19.041754	1.978770	9.717331
254	1	0	-19.445271	0.271039	9.650545
255	1	0	-20.847713	-11.147995	-4.210696
256	1	0	-19.782151	-12.295826	-5.033593
257	1	0	-21.005562	-11.407455	-5.955088
258	1	0	-12.166932	14.771442	-3.692797
259	1	0	-13.710112	14.278291	-2.981844
260	1	0	-13.629677	14.737827	-4.689806
261	1	0	-21.705210	0.838008	8.663552

262	1	0	-21.299020	2.558533	8.735520
263	1	0	-21.469070	1.626487	10.231145
264	6	0	-0.100521	3.402934	0.478009
265	6	0	-0.021855	3.953833	1.768225
266	6	0	-0.209891	4.280739	-0.613784
267	6	0	-0.051693	5.334155	1.960240
268	1	0	0.091251	3.295143	2.624765
269	6	0	-0.239696	5.661116	-0.422034
270	1	0	-0.299094	3.876063	-1.618194
271	6	0	-0.160751	6.194065	0.865885
272	1	0	0.019389	5.738319	2.966550
273	1	0	-0.333267	6.321143	-1.280423
274	1	0	-0.183842	7.270062	1.015349

Monomer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.079475	-1.808822	-0.079527
2	6	0	-1.082065	-1.806965	-0.088491
3	7	0	-0.000785	-0.963225	-0.082209
4	7	0	-0.673393	-3.061277	-0.095829
5	6	0	2.417753	-1.380851	-0.034559
6	6	0	-2.421551	-1.380899	-0.108821
7	6	0	3.577209	-1.035324	0.008877
8	6	0	-3.577003	-1.019410	-0.115542
9	6	0	4.936571	-0.633971	0.053088
10	6	0	5.273604	0.722820	0.010211
11	6	0	5.945746	-1.599532	0.125018
12	6	0	6.602913	1.103821	0.052471
13	1	0	4.508161	1.484617	-0.044950
14	6	0	7.274601	-1.213914	0.175941
15	1	0	5.703921	-2.652301	0.165357
16	6	0	7.614044	0.141859	0.141964
17	6	0	-4.938500	-0.622592	-0.098644
18	6	0	-5.943015	-1.594979	-0.103209
19	6	0	-5.283882	0.731458	-0.054587
20	6	0	-7.275893	-1.220134	-0.091339
21	1	0	-5.695930	-2.646551	-0.137938
22	6	0	-6.616506	1.102778	-0.029707
23	1	0	-4.524714	1.500707	-0.044385
24	6	0	-7.624319	0.133784	-0.062716
25	8	0	8.924587	0.510075	0.197952
26	8	0	-8.939791	0.487307	-0.061146
27	6	0	9.308722	1.041012	1.460385
28	1	0	9.194947	0.286492	2.241432
29	1	0	10.357406	1.316344	1.372484
30	1	0	8.714238	1.923044	1.704641
31	6	0	-9.380288	1.062903	-1.285000
32	1	0	-9.277194	0.346090	-2.101748

33	1	0	-10.431278	1.306740	-1.148416
34	1	0	-8.816385	1.968394	-1.512472
35	7	0	0.668704	-3.062240	-0.086614
36	6	0	0.004941	0.453001	-0.076630
37	6	0	-0.793137	1.138940	0.830480
38	6	0	0.812247	1.138049	-0.975879
39	6	0	-0.783186	2.524996	0.830312
40	1	0	-1.408821	0.585007	1.525777
41	6	0	0.824757	2.523907	-0.955910
42	1	0	1.417598	0.584558	-1.681696
43	6	0	0.027318	3.219447	-0.056687
44	1	0	-1.403038	3.062395	1.536753
45	1	0	1.452495	3.060796	-1.654901
46	1	0	0.036860	4.301591	-0.047739
47	8	0	-6.935135	2.429576	-0.033528
48	8	0	-8.231394	-2.182079	-0.181374
49	8	0	6.915936	2.431882	0.071105
50	8	0	8.236300	-2.162793	0.334315
51	6	0	9.105787	-2.327221	-0.775020
52	1	0	9.627091	-1.400187	-1.012653
53	1	0	9.828308	-3.087648	-0.486469
54	1	0	8.550869	-2.673502	-1.650825
55	6	0	7.562457	2.899433	-1.102702
56	1	0	6.916121	2.773131	-1.975670
57	1	0	7.750796	3.959808	-0.947328
58	1	0	8.506160	2.378610	-1.269276
59	6	0	-9.058040	-2.321926	0.962439
60	1	0	-9.612840	-1.405546	1.167057
61	1	0	-9.753933	-3.127409	0.737807
62	1	0	-8.463634	-2.596461	1.838491
63	6	0	-7.553735	2.889882	1.158296
64	1	0	-6.884534	2.762160	2.013396
65	1	0	-7.749790	3.950063	1.011858
66	1	0	-8.490748	2.365214	1.348331

Dimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.106080	-0.263228	-1.637556
2	6	0	-2.029982	-0.506694	-1.447213
3	7	0	-0.852309	-1.197920	-1.350007
4	7	0	-1.791756	0.747243	-1.784763
5	6	0	1.487683	-0.525519	-1.674461
6	6	0	-3.285604	-1.054808	-1.130025
7	6	0	2.679674	-0.735520	-1.716322
8	6	0	-4.361594	-1.511718	-0.816791
9	6	0	4.073048	-0.994322	-1.793924
10	6	0	4.619499	-2.099189	-1.133637
11	6	0	4.901828	-0.144095	-2.529070
12	6	0	5.976156	-2.346786	-1.227147
13	1	0	3.996038	-2.773509	-0.564312
14	6	0	6.263109	-0.396490	-2.624393

15	1	0	4.495335	0.708952	-3.053843
16	6	0	6.808212	-1.504282	-1.970751
17	6	0	-5.603843	-2.061753	-0.409082
18	6	0	-6.790873	-1.347579	-0.594574
19	6	0	-5.642016	-3.324166	0.192201
20	6	0	-7.993265	-1.872261	-0.149600
21	1	0	-6.786459	-0.372340	-1.060231
22	6	0	-6.846744	-3.850834	0.620202
23	1	0	-4.734675	-3.894247	0.341034
24	6	0	-8.030830	-3.121891	0.473308
25	8	0	8.141139	-1.786121	-2.075928
26	8	0	-9.218804	-3.612416	0.928630
27	6	0	8.422860	-2.762629	-3.069600
28	1	0	8.127494	-2.402335	-4.057268
29	1	0	9.497726	-2.924478	-3.047429
30	1	0	7.907594	-3.697917	-2.845386
31	6	0	-9.328501	-3.609451	2.346150
32	1	0	-9.295889	-2.587427	2.729698
33	1	0	-10.293481	-4.052701	2.580909
34	1	0	-8.529706	-4.199219	2.797811
35	7	0	-0.463347	0.898876	-1.903773
36	6	0	-0.678999	-2.579295	-1.072523
37	6	0	-1.383278	-3.511720	-1.824135
38	6	0	0.186830	-2.976549	-0.064190
39	6	0	-1.215760	-4.861328	-1.557823
40	1	0	-2.048956	-3.174072	-2.607290
41	6	0	0.353191	-4.330331	0.183414
42	1	0	0.696112	-2.234270	0.534095
43	6	0	-0.344392	-5.272946	-0.558624
44	1	0	-1.760937	-5.592136	-2.140899
45	1	0	1.019845	-4.645390	0.975304
46	1	0	-0.212727	-6.328417	-0.356246
47	7	0	0.376037	1.375064	1.640141
48	6	0	1.254090	0.400355	2.028944
49	6	0	-0.858486	0.821726	1.866567
50	6	0	0.674495	2.669153	1.139707
51	6	0	2.653609	0.529418	1.997180
52	7	0	0.591666	-0.653466	2.469666
53	7	0	-0.723269	-0.392497	2.366241
54	6	0	-2.064548	1.442199	1.500236
55	6	0	0.052188	3.777395	1.700224
56	6	0	1.590033	2.809452	0.105217
57	6	0	3.860008	0.625615	1.972217
58	6	0	-3.077725	1.967993	1.097374
59	6	0	0.347863	5.039097	1.209877
60	1	0	-0.652305	3.651721	2.510891
61	6	0	1.890117	4.078699	-0.364035
62	1	0	2.043829	1.931584	-0.332187
63	6	0	5.270730	0.742697	1.888023
64	6	0	-4.226139	2.601935	0.558783
65	6	0	1.269077	5.193642	0.183064
66	1	0	-0.137726	5.903956	1.639056
67	1	0	2.594468	4.191657	-1.176594
68	6	0	5.829758	1.724729	1.074364

69	6	0	6.094534	-0.137418	2.602151
70	6	0	-5.506658	2.248270	1.005509
71	6	0	-4.061547	3.553662	-0.442433
72	1	0	1.498153	6.181482	-0.196403
73	6	0	7.208580	1.802289	0.934246
74	1	0	5.207449	2.422517	0.533429
75	6	0	7.469772	-0.053495	2.458799
76	1	0	5.639312	-0.876531	3.244883
77	6	0	-6.611428	2.874153	0.454507
78	1	0	-5.610830	1.490942	1.765581
79	6	0	-5.175061	4.184522	-0.984622
80	1	0	-3.079482	3.795634	-0.820344
81	6	0	8.038080	0.892415	1.588288
82	6	0	-6.451730	3.862902	-0.530671
83	8	0	9.384392	0.968023	1.413242
84	8	0	-7.538307	4.486942	-1.065647
85	6	0	9.955840	-0.130878	0.717155
86	6	0	-8.143085	5.433651	-0.201803
87	1	0	9.422754	-0.324278	-0.216522
88	1	0	10.984515	0.149386	0.497562
89	1	0	9.948203	-1.030346	1.331900
90	1	0	-7.432816	6.218230	0.073876
91	1	0	-8.970113	5.874201	-0.755401
92	1	0	-8.526108	4.950776	0.697299
93	8	0	-6.859037	-5.058711	1.253599
94	8	0	-9.121022	-1.116829	-0.256877
95	8	0	-7.892671	2.624352	0.808042
96	8	0	-4.954739	5.132482	-1.926149
97	8	0	8.354485	-0.860260	3.089748
98	8	0	7.690748	2.754849	0.097550
99	8	0	6.490817	-3.474208	-0.657828
100	8	0	6.996298	0.396367	-3.444958
101	6	0	8.149337	1.028823	-2.907053
102	1	0	8.957744	0.317440	-2.744035
103	1	0	8.455693	1.762169	-3.649979
104	1	0	7.918309	1.544205	-1.972904
105	6	0	7.326362	-3.233753	0.461488
106	1	0	6.760995	-2.750317	1.261087
107	1	0	7.676468	-4.207010	0.800494
108	1	0	8.180135	-2.609925	0.191871
109	6	0	-10.110361	-1.635041	-1.130803
110	1	0	-10.504504	-2.583278	-0.764002
111	1	0	-10.906711	-0.894868	-1.165122
112	1	0	-9.704328	-1.769785	-2.136828
113	6	0	-8.116852	1.633802	1.782160
114	1	0	-7.672106	1.912534	2.742091
115	1	0	-9.195010	1.553861	1.890197
116	1	0	-7.720575	0.667680	1.464884
117	6	0	-5.748924	5.104972	-3.099547
118	1	0	-6.618257	5.755354	-3.012250
119	1	0	-5.109467	5.453682	-3.909444
120	1	0	-6.090442	4.092408	-3.318462
121	6	0	-7.533318	-6.089220	0.549310
122	1	0	-7.026892	-6.306059	-0.394687

123	1	0	-7.493887	-6.970482	1.186076
124	1	0	-8.572431	-5.821524	0.353906
125	6	0	7.852180	-1.720272	4.084259
126	1	0	7.181013	-2.475896	3.666651
127	1	0	8.716006	-2.214334	4.521280
128	1	0	7.321665	-1.163707	4.860855
129	6	0	8.800466	3.528814	0.527178
130	1	0	9.741678	3.100581	0.186973
131	1	0	8.665701	4.519841	0.095918
132	1	0	8.824561	3.607628	1.614378

Trimer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.743085	-0.071948	0.126641
2	6	0	1.296821	-0.290175	0.798976
3	7	0	0.003365	-0.293820	1.252901
4	7	0	1.317772	-0.075194	-0.503858
5	6	0	-2.146730	-0.017100	0.100249
6	6	0	2.405084	-0.566854	1.615338
7	6	0	-3.356233	0.016758	0.069037
8	6	0	3.332225	-0.815065	2.351253
9	6	0	-4.772002	0.045734	0.017069
10	6	0	-5.525333	-0.052772	1.187007
11	6	0	-5.405886	0.161098	-1.225846
12	6	0	-6.907159	-0.064118	1.097627
13	1	0	-5.045728	-0.134843	2.152309
14	6	0	-6.790190	0.175833	-1.301869
15	1	0	-4.797879	0.232899	-2.114422
16	6	0	-7.551874	0.052703	-0.131240
17	6	0	4.366039	-1.097177	3.277978
18	6	0	5.670853	-1.345890	2.858987
19	6	0	4.040958	-1.124861	4.640261
20	6	0	6.642140	-1.645927	3.802608
21	1	0	5.933619	-1.326713	1.810759
22	6	0	5.020564	-1.406063	5.577431
23	1	0	3.020958	-0.923276	4.931018
24	6	0	6.331625	-1.684190	5.160265
25	8	0	-8.907436	-0.016252	-0.219496
26	8	0	7.310565	-1.953948	6.064630
27	6	0	-9.595167	1.137007	0.239804
28	1	0	-9.326748	2.016302	-0.349425
29	1	0	-10.656159	0.928556	0.116369
30	1	0	-9.376108	1.325740	1.291215
31	6	0	7.200294	-3.224006	6.687016
32	1	0	7.256665	-4.023399	5.944435
33	1	0	8.043547	-3.305384	7.369512
34	1	0	6.268886	-3.305423	7.248697
35	7	0	0.048548	0.075162	-0.920022
36	6	0	-0.447396	-0.411261	2.596063
37	6	0	0.171514	0.345103	3.583130

38	6	0	-1.503878	-1.258446	2.901125
39	6	0	-0.276183	0.247506	4.891170
40	1	0	0.977081	1.019399	3.332856
41	6	0	-1.944334	-1.341620	4.212969
42	1	0	-1.959391	-1.856489	2.126722
43	6	0	-1.333618	-0.593196	5.209258
44	1	0	0.193402	0.855151	5.653772
45	1	0	-2.760318	-2.009915	4.455145
46	1	0	-1.684147	-0.662537	6.231219
47	7	0	0.064942	-3.795529	-0.662254
48	6	0	-0.997617	-3.905696	0.196232
49	6	0	1.163420	-3.944910	0.147275
50	6	0	0.038482	-3.691933	-2.077014
51	6	0	-2.342982	-3.839616	-0.208388
52	7	0	-0.563381	-4.123350	1.423316
53	7	0	0.781054	-4.141870	1.394482
54	6	0	2.479496	-3.788215	-0.322340
55	6	0	0.837071	-4.545376	-2.829248
56	6	0	-0.787002	-2.761870	-2.692952
57	6	0	-3.497458	-3.781959	-0.569626
58	6	0	3.582509	-3.581402	-0.775932
59	6	0	0.816051	-4.455103	-4.211701
60	1	0	1.467742	-5.268371	-2.330144
61	6	0	-0.809638	-2.692249	-4.077576
62	1	0	-1.387808	-2.095210	-2.092988
63	6	0	-4.835034	-3.697955	-1.034532
64	6	0	4.835098	-3.288169	-1.374233
65	6	0	-0.009206	-3.532298	-4.838813
66	1	0	1.441222	-5.115653	-4.798176
67	1	0	-1.445566	-1.961604	-4.560256
68	6	0	-5.072027	-3.347211	-2.360327
69	6	0	-5.904907	-4.031418	-0.193348
70	6	0	6.034231	-3.527906	-0.688192
71	6	0	4.848972	-2.735328	-2.651626
72	1	0	-0.025962	-3.465664	-5.918918
73	6	0	-6.372069	-3.297733	-2.847972
74	1	0	-4.254204	-3.119396	-3.029168
75	6	0	-7.196866	-4.004927	-0.691232
76	1	0	-5.702122	-4.330312	0.823935
77	6	0	7.239400	-3.226212	-1.303469
78	1	0	5.999996	-3.938831	0.309544
79	6	0	6.059456	-2.429070	-3.260603
80	1	0	3.928415	-2.529799	-3.178372
81	6	0	-7.447415	-3.615420	-2.018640
82	6	0	7.258378	-2.681262	-2.597990
83	8	0	-8.714394	-3.611019	-2.506414
84	8	0	8.445084	-2.383047	-3.198384
85	6	0	-9.531786	-2.552036	-2.017027
86	6	0	9.135891	-3.518637	-3.691173
87	1	0	-9.126573	-1.580716	-2.302429
88	1	0	-10.512151	-2.696684	-2.466956
89	1	0	-9.619794	-2.595649	-0.931410
90	1	0	8.538976	-4.041516	-4.443047
91	1	0	10.051100	-3.149243	-4.149855

92	1	0	9.388240	-4.203338	-2.880344
93	7	0	0.939430	3.954950	0.988741
94	6	0	0.120829	3.826827	2.078963
95	6	0	2.202366	3.814139	1.497626
96	6	0	0.559536	4.189758	-0.359277
97	6	0	-1.281657	3.841977	1.980961
98	7	0	0.846075	3.635422	3.164793
99	7	0	2.143212	3.626810	2.802754
100	6	0	3.351466	3.872905	0.691251
101	6	0	0.996438	3.331831	-1.359125
102	6	0	-0.253136	5.278447	-0.648029
103	6	0	-2.480565	3.866073	1.816145
104	6	0	4.282296	3.935485	-0.079403
105	6	0	0.613577	3.580031	-2.669186
106	1	0	1.606027	2.472517	-1.114326
107	6	0	-0.635000	5.509751	-1.960130
108	1	0	-0.578746	5.928459	0.153261
109	6	0	-3.877202	3.908232	1.570662
110	6	0	5.332307	4.010342	-1.029394
111	6	0	-0.199052	4.664180	-2.971369
112	1	0	0.939967	2.905759	-3.449663
113	1	0	-1.269156	6.355791	-2.191176
114	6	0	-4.332037	3.958320	0.256376
115	6	0	-4.795766	3.926230	2.624654
116	6	0	6.666750	3.865493	-0.627631
117	6	0	5.015933	4.227807	-2.365887
118	1	0	-0.497725	4.847330	-3.995622
119	6	0	-5.689608	4.062627	-0.035177
120	1	0	-3.635684	3.932437	-0.569540
121	6	0	-6.142373	4.017112	2.338952
122	1	0	-4.473457	3.885567	3.654762
123	6	0	7.666635	3.917860	-1.583088
124	1	0	6.887623	3.706551	0.416404
125	6	0	6.024034	4.279110	-3.323997
126	1	0	3.989089	4.348551	-2.680801
127	6	0	-6.609928	4.104795	1.018508
128	6	0	7.353462	4.106811	-2.940545
129	8	0	-7.955585	4.227628	0.799185
130	8	0	8.356735	4.133515	-3.863566
131	6	0	-8.462597	5.518748	1.101416
132	6	0	8.882883	2.853387	-4.169272
133	1	0	-8.042416	6.267535	0.425021
134	1	0	-9.540325	5.470061	0.958051
135	1	0	-8.240974	5.789701	2.133190
136	1	0	8.119594	2.220706	-4.632763
137	1	0	9.695929	3.013270	-4.874927
138	1	0	9.271461	2.364722	-3.273784
139	8	0	6.011904	-1.927878	-4.517912
140	8	0	8.456577	-3.436636	-0.758601
141	8	0	-7.031188	4.098791	3.370793
142	8	0	-5.968540	4.163204	-1.353365
143	8	0	-7.670843	-0.155066	2.229286
144	8	0	-7.494939	0.318273	-2.444423
145	8	0	-8.294844	-4.343904	0.025324

146	8	0	-6.520691	-2.905852	-4.138801
147	8	0	5.621313	4.453857	-4.603177
148	8	0	8.985333	3.774110	-1.320954
149	8	0	4.816559	-1.447053	6.912477
150	8	0	7.900257	-1.958282	3.376657
151	6	0	-7.441787	-3.602730	-4.963834
152	1	0	-8.429690	-3.144762	-4.938023
153	1	0	-7.037760	-3.555898	-5.975392
154	1	0	-7.530913	-4.645397	-4.655669
155	6	0	-8.090186	-5.030681	1.236745
156	1	0	-7.621302	-4.395140	1.992827
157	1	0	-9.075671	-5.330721	1.585608
158	1	0	-7.469273	-5.918085	1.085763
159	6	0	-6.763695	0.459066	-3.643121
160	1	0	-7.501939	0.623858	-4.424201
161	1	0	-6.090349	1.319575	-3.593131
162	1	0	-6.198695	-0.447212	-3.871459
163	6	0	-8.163623	-1.462259	2.464576
164	1	0	-7.354921	-2.121847	2.791800
165	1	0	-8.901585	-1.381782	3.259798
166	1	0	-8.632000	-1.876370	1.568142
167	6	0	-7.273431	3.983490	-1.859321
168	1	0	-7.929359	4.820136	-1.615255
169	1	0	-7.153773	3.929858	-2.940322
170	1	0	-7.720766	3.058325	-1.498786
171	6	0	-7.825096	2.936949	3.555565
172	1	0	-8.406981	3.105722	4.459244
173	1	0	-8.495479	2.780971	2.710062
174	1	0	-7.201755	2.050064	3.681052
175	6	0	6.422187	5.212213	-5.493556
176	1	0	7.145039	4.586908	-6.018341
177	1	0	5.732234	5.651895	-6.212628
178	1	0	6.959945	6.004037	-4.970294
179	6	0	9.360037	3.569574	0.019550
180	1	0	8.926025	2.649652	0.422062
181	1	0	10.443814	3.487427	0.021267
182	1	0	9.060293	4.411311	0.649889
183	6	0	8.897514	-1.010891	3.721010
184	1	0	8.993636	-0.919361	4.802485
185	1	0	9.830133	-1.380917	3.299511
186	1	0	8.668847	-0.033482	3.286780
187	6	0	3.513725	-1.183507	7.377965
188	1	0	2.797804	-1.919153	7.001313
189	1	0	3.562145	-1.248241	8.461772
190	1	0	3.181892	-0.182100	7.090736
191	6	0	6.823136	-0.807639	-4.821647
192	1	0	7.794027	-1.109755	-5.208378
193	1	0	6.283568	-0.236641	-5.576403
194	1	0	6.977165	-0.185884	-3.938939
195	6	0	8.506438	-3.990286	0.537956
196	1	0	8.014406	-4.966515	0.571967
197	1	0	9.561578	-4.115085	0.768174
198	1	0	8.055341	-3.326441	1.278744

Tetramer

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.833089	-2.048706	-0.080757
2	6	0	-1.241926	-2.132372	-0.668445
3	7	0	0.000617	-1.802433	-1.139350
4	7	0	-1.154998	-2.553014	0.580370
5	6	0	2.222108	-1.843143	-0.115284
6	6	0	-2.406924	-2.054819	-1.447602
7	6	0	3.418488	-1.671027	-0.177320
8	6	0	-3.379939	-1.984482	-2.162355
9	6	0	4.814069	-1.496055	-0.341150
10	6	0	5.324579	-1.243923	-1.618765
11	6	0	5.687372	-1.584697	0.742183
12	6	0	6.683053	-1.086958	-1.799116
13	1	0	4.662430	-1.154934	-2.468938
14	6	0	7.053049	-1.439696	0.554876
15	1	0	5.304920	-1.761137	1.738146
16	6	0	7.569094	-1.176024	-0.715998
17	6	0	-4.479915	-1.893417	-3.050059
18	6	0	-5.727456	-2.401045	-2.694182
19	6	0	-4.293363	-1.276465	-4.293931
20	6	0	-6.779326	-2.316298	-3.593220
21	1	0	-5.880691	-2.872641	-1.733478
22	6	0	-5.352768	-1.183841	-5.181241
23	1	0	-3.316878	-0.884704	-4.536981
24	6	0	-6.604285	-1.719998	-4.840429
25	8	0	8.888755	-1.040881	-0.988982
26	8	0	-7.659860	-1.627696	-5.692634
27	6	0	9.687606	-0.227670	-0.138636
28	1	0	10.084443	-0.799128	0.698723
29	1	0	10.507833	0.132658	-0.759206
30	1	0	9.122563	0.624646	0.241046
31	6	0	-7.566318	-2.468010	-6.832164
32	1	0	-7.529658	-3.518613	-6.535347
33	1	0	-8.465188	-2.289546	-7.416922
34	1	0	-6.687717	-2.220866	-7.430756
35	7	0	0.138096	-2.502184	0.945143
36	6	0	0.353004	-1.316176	-2.427571
37	6	0	-0.327725	-0.232970	-2.967286
38	6	0	1.384909	-1.934399	-3.120921
39	6	0	0.031663	0.225314	-4.226361
40	1	0	-1.110064	0.253626	-2.401940
41	6	0	1.735651	-1.463071	-4.375344
42	1	0	1.891992	-2.784445	-2.689659
43	6	0	1.059808	-0.386210	-4.931330
44	1	0	-0.485052	1.080171	-4.643141
45	1	0	2.528026	-1.955187	-4.924238
46	1	0	1.335721	-0.021977	-5.912778
47	7	0	0.538843	-5.808393	-1.029591
48	6	0	1.455555	-5.520918	-2.007268

49	6	0	-0.672027	-5.663301	-1.657408
50	6	0	0.790773	-6.229913	0.302096
51	6	0	2.847460	-5.544506	-1.809519
52	7	0	0.835612	-5.232081	-3.135641
53	7	0	-0.487851	-5.315459	-2.917419
54	6	0	-1.904767	-5.802443	-0.997476
55	6	0	0.156569	-7.365331	0.790374
56	6	0	1.676461	-5.512282	1.094318
57	6	0	4.038259	-5.543481	-1.589131
58	6	0	-2.939552	-5.885420	-0.375326
59	6	0	0.408565	-7.777925	2.089480
60	1	0	-0.523516	-7.915750	0.154872
61	6	0	1.930070	-5.942763	2.386775
62	1	0	2.144677	-4.619605	0.707624
63	6	0	5.416702	-5.536132	-1.260134
64	6	0	-4.116228	-5.974204	0.410960
65	6	0	1.297510	-7.071601	2.887909
66	1	0	-0.087375	-8.659719	2.473436
67	1	0	2.610623	-5.377092	3.009597
68	6	0	5.802302	-5.724309	0.066333
69	6	0	6.390985	-5.343257	-2.245833
70	6	0	-5.381372	-5.930738	-0.192185
71	6	0	-3.992414	-6.088634	1.792591
72	1	0	1.492210	-7.398018	3.901209
73	6	0	7.141456	-5.667811	0.412935
74	1	0	5.066345	-5.902530	0.837801
75	6	0	7.731831	-5.301198	-1.898254
76	1	0	6.084022	-5.242271	-3.276171
77	6	0	-6.513355	-6.030475	0.601212
78	1	0	-5.451364	-5.822878	-1.263939
79	6	0	-5.130890	-6.178906	2.583753
80	1	0	-3.020558	-6.099413	2.264294
81	6	0	8.119860	-5.408526	-0.552411
82	6	0	-6.392931	-6.167153	1.993823
83	8	0	9.407715	-5.353138	-0.139234
84	8	0	-7.509280	-6.275122	2.767629
85	6	0	10.247087	-4.322796	-0.645222
86	6	0	-8.105840	-7.560245	2.721010
87	1	0	9.690375	-3.395893	-0.794015
88	1	0	11.012700	-4.165733	0.113165
89	1	0	10.712083	-4.619626	-1.583171
90	1	0	-7.415565	-8.322864	3.091688
91	1	0	-8.980876	-7.519965	3.366960
92	1	0	-8.416826	-7.808317	1.704825
93	7	0	-0.547542	1.741478	1.240192
94	6	0	0.212572	2.209790	0.201270
95	6	0	-1.831393	1.784673	0.761485
96	6	0	-0.101520	1.261114	2.501038
97	7	0	-1.400507	5.698846	1.109244
98	6	0	1.611624	2.347141	0.240357
99	7	0	-0.562438	2.498732	-0.827955
100	7	0	-1.835794	2.238013	-0.479253
101	6	0	-2.947498	1.441381	1.541869
102	6	0	-0.554770	0.030721	2.958896

103	6	0	0.794534	2.017708	3.243483
104	6	0	-0.426473	5.484471	2.048325
105	6	0	-2.554799	5.302365	1.734357
106	6	0	-1.254543	6.287304	-0.174294
107	6	0	2.815385	2.467805	0.290891
108	6	0	-3.849318	1.133709	2.287726
109	6	0	-0.103144	-0.440720	4.181987
110	1	0	-1.229972	-0.562914	2.358782
111	6	0	1.245708	1.529019	4.459221
112	1	0	1.121549	2.978322	2.874493
113	6	0	0.936275	5.741429	1.823565
114	7	0	-0.963562	5.010981	3.156917
115	7	0	-2.287864	4.893589	2.960045
116	6	0	-3.799671	5.264484	1.083482
117	6	0	-2.084812	7.339777	-0.539624
118	6	0	-0.269814	5.825703	-1.037284
119	6	0	4.223799	2.595363	0.399858
120	6	0	-4.840725	0.745612	3.223733
121	6	0	0.797098	0.303353	4.931834
122	1	0	-0.442749	-1.406989	4.530622
123	1	0	1.939979	2.118848	5.043575
124	6	0	2.101374	5.950750	1.569873
125	6	0	-4.832121	5.245696	0.452908
126	6	0	-1.930350	7.926650	-1.786034
127	1	0	-2.837568	7.694759	0.150983
128	6	0	-0.116789	6.430493	-2.275085
129	1	0	0.352959	4.992468	-0.750540
130	6	0	4.841603	2.362439	1.629671
131	6	0	5.001292	2.928750	-0.711352
132	6	0	-6.182009	0.630602	2.843130
133	6	0	-4.442426	0.455534	4.528424
134	1	0	1.152585	-0.073655	5.882456
135	6	0	3.450158	6.208570	1.219806
136	6	0	-6.007451	5.243621	-0.339413
137	6	0	-0.944050	7.477915	-2.653658
138	1	0	-2.576591	8.746431	-2.071772
139	1	0	0.645414	6.065355	-2.951010
140	6	0	6.216278	2.485767	1.761119
141	1	0	4.258875	2.089951	2.498318
142	6	0	6.375334	3.034609	-0.585496
143	1	0	4.550596	3.101181	-1.678255
144	6	0	-7.121738	0.209907	3.772943
145	1	0	-6.457711	0.859652	1.825323
146	6	0	-5.390717	0.048655	5.455784
147	1	0	-3.398065	0.535051	4.794286
148	6	0	3.747243	6.659526	-0.066202
149	6	0	4.469865	6.018048	2.159475
150	6	0	-7.265342	5.026885	0.227731
151	6	0	-5.897254	5.484541	-1.712876
152	1	0	-0.822665	7.942921	-3.623528
153	6	0	6.999249	2.828039	0.652173
154	6	0	-6.731015	-0.075210	5.090105
155	6	0	5.062932	6.930652	-0.403285
156	1	0	2.964933	6.815493	-0.795570

157	6	0	5.784379	6.296878	1.816511
158	1	0	4.214913	5.661123	3.145562
159	6	0	-8.398230	5.018190	-0.570943
160	1	0	-7.372813	4.845069	1.287641
161	6	0	-7.030471	5.489347	-2.503874
162	1	0	-4.932957	5.659934	-2.169099
163	8	0	8.351680	2.932486	0.792034
164	8	0	-7.677050	-0.420795	5.999266
165	6	0	6.086161	6.754653	0.526245
166	6	0	-8.288374	5.237015	-1.947023
167	6	0	8.871928	4.248613	0.607408
168	6	0	-7.670339	-1.789900	6.353630
169	8	0	7.377879	7.033860	0.196666
170	8	0	-9.405419	5.210385	-2.728638
171	1	0	8.455867	4.931605	1.345962
172	1	0	9.949289	4.165396	0.737992
173	1	0	8.644952	4.624658	-0.390813
174	1	0	-6.712783	-2.076153	6.789664
175	1	0	-8.458610	-1.921495	7.092517
176	1	0	-7.883976	-2.418415	5.485583
177	6	0	7.665903	8.423795	0.177305
178	6	0	-9.478171	4.076229	-3.584433
179	1	0	7.527462	8.859502	1.169713
180	1	0	8.709749	8.520014	-0.114838
181	1	0	7.033053	8.940372	-0.546501
182	1	0	-9.539288	3.157782	-2.996596
183	1	0	-10.387674	4.192304	-4.170266
184	1	0	-8.613454	4.034132	-4.247993
185	8	0	5.353534	7.428571	-1.638030
186	8	0	6.836149	6.182879	2.655267
187	8	0	7.088172	3.411427	-1.685454
188	8	0	6.719731	2.338036	3.012144
189	8	0	7.163574	-0.778160	-3.037760
190	8	0	7.914126	-1.480690	1.614644
191	8	0	8.739590	-5.177185	-2.799100
192	8	0	7.472267	-5.822650	1.724874
193	8	0	-4.953051	-6.323091	3.918212
194	8	0	-7.781962	-6.034462	0.137986
195	8	0	-5.077920	-0.289883	6.735958
196	8	0	-8.437345	0.055594	3.517483
197	8	0	-5.283028	-0.604212	-6.400876
198	8	0	-7.983757	-2.865265	-3.262434
199	8	0	-9.596365	4.728526	0.004460
200	8	0	-6.905154	5.687489	-3.848605
201	6	0	6.589834	5.654889	3.940385
202	1	0	6.206402	4.634114	3.880849
203	1	0	7.551395	5.646306	4.447328
204	1	0	5.895044	6.285020	4.502375
205	6	0	7.923274	1.609959	3.199476
206	1	0	8.798060	2.250161	3.097377
207	1	0	7.874018	1.213640	4.212836
208	1	0	7.997921	0.778823	2.497693
209	6	0	8.043761	-2.741533	2.252098
210	1	0	8.597832	-3.444788	1.628398

211	1	0	8.590243	-2.564415	3.176000
212	1	0	7.072606	-3.179861	2.487200
213	6	0	6.007865	6.500320	-2.490591
214	1	0	5.356937	5.649536	-2.705100
215	1	0	6.225935	7.032620	-3.414472
216	1	0	6.931855	6.135615	-2.043404
217	6	0	8.074791	2.502684	-2.152654
218	1	0	8.414881	2.900265	-3.107496
219	1	0	8.920597	2.438569	-1.466270
220	1	0	7.655355	1.508136	-2.312425
221	6	0	7.836716	-1.844366	-3.679355
222	1	0	7.127378	-2.636707	-3.936650
223	1	0	8.266490	-1.437112	-4.592670
224	1	0	8.630079	-2.256912	-3.052697
225	6	0	8.446751	-5.466028	-4.146532
226	1	0	7.831224	-4.690305	-4.608325
227	1	0	9.403220	-5.509870	-4.662060
228	1	0	7.935474	-6.427678	-4.239496
229	6	0	8.290133	-6.942647	2.026138
230	1	0	9.301988	-6.811276	1.643808
231	1	0	8.311743	-7.018011	3.111618
232	1	0	7.859855	-7.858291	1.612704
233	6	0	-7.441079	6.918564	-4.304948
234	1	0	-6.919640	7.760223	-3.843496
235	1	0	-7.279166	6.943797	-5.379157
236	1	0	-8.508350	6.989897	-4.092236
237	6	0	-10.565947	5.761742	-0.053335
238	1	0	-10.891948	5.943756	-1.077216
239	1	0	-11.406941	5.420722	0.546894
240	1	0	-10.172928	6.688185	0.375406
241	6	0	-5.737778	-5.523103	4.786570
242	1	0	-6.643047	-6.041048	5.098388
243	1	0	-5.114713	-5.313413	5.655299
244	1	0	-6.018526	-4.583619	4.309083
245	6	0	-4.224032	0.594951	7.431777
246	1	0	-4.695283	1.573989	7.551457
247	1	0	-4.058845	0.150650	8.410353
248	1	0	-3.259301	0.725024	6.937489
249	6	0	-9.015668	-1.917286	-3.046345
250	1	0	-9.170137	-1.294905	-3.929352
251	1	0	-9.919064	-2.488026	-2.838901
252	1	0	-8.783131	-1.284813	-2.182775
253	6	0	-4.064738	0.009493	-6.754486
254	1	0	-3.247837	-0.712077	-6.801844
255	1	0	-4.218921	0.442903	-7.737918
256	1	0	-3.802259	0.798823	-6.047106
257	6	0	-7.972860	-5.924553	-1.254040
258	1	0	-7.466685	-6.731939	-1.790528
259	1	0	-9.044685	-6.004379	-1.416205
260	1	0	-7.627862	-4.961922	-1.638312
261	6	0	-8.890757	0.395484	2.231207
262	1	0	-8.435211	-0.237518	1.463774
263	1	0	-9.965436	0.232951	2.237983
264	1	0	-8.685490	1.443906	1.995908

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