Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Non-covalent Intermolecular Carbon-Carbon Interactions in Polyynes

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Supporting Information

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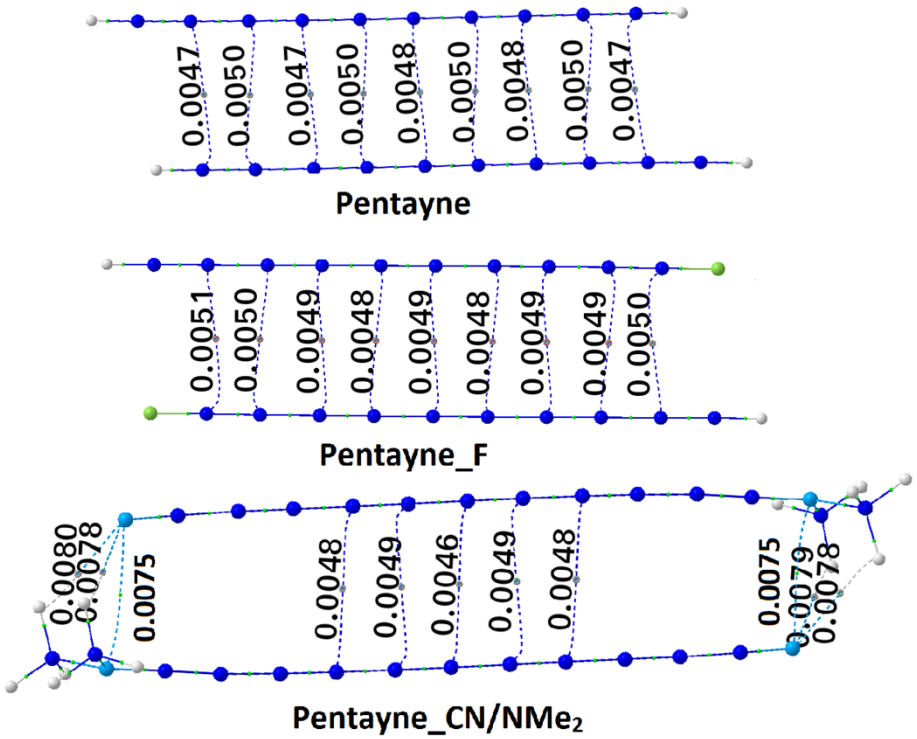

Figure S1. QTAIM plots of dimers of Pentayne, Pentayne_F and Pentayne_NMe_2

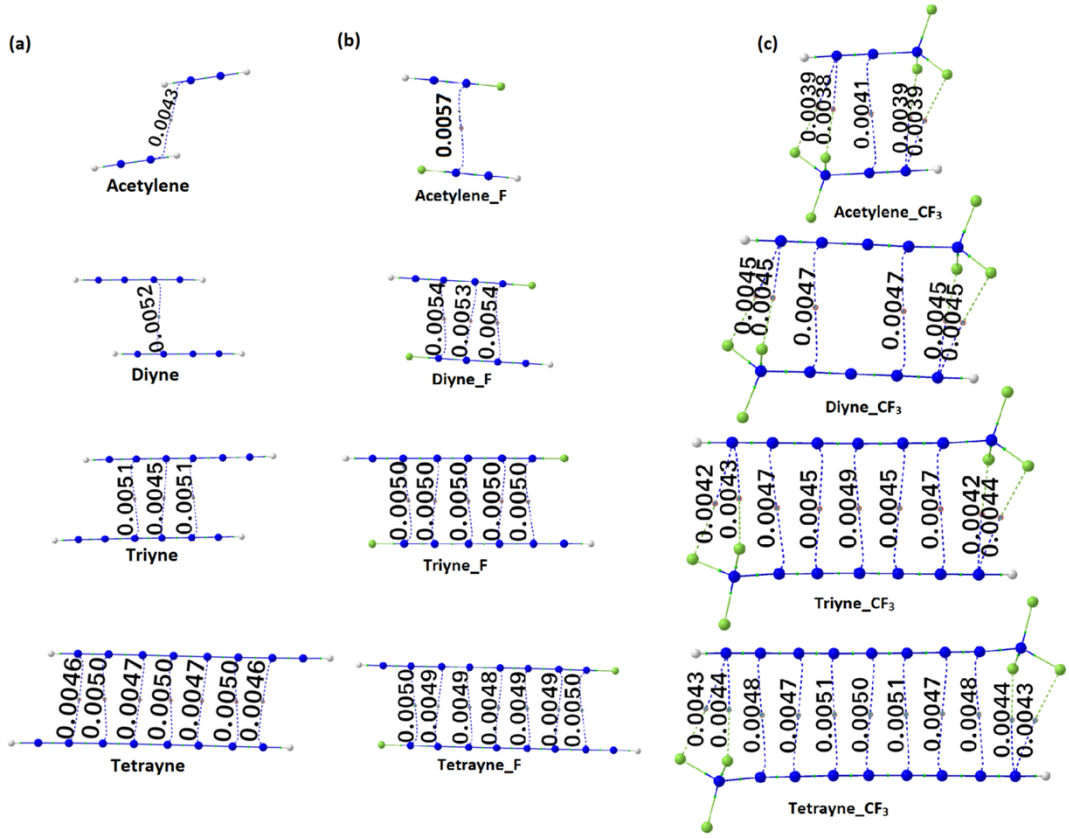

Figure S2. QTAIM plots of dimers of oligoynes that are (a) unsubstituted (b) substituted with F at one end and (c) substituted with CF_3 at one end and with 1 – 4 triple bonds along with the values of ρ (a u) at intermolecular BCPs.

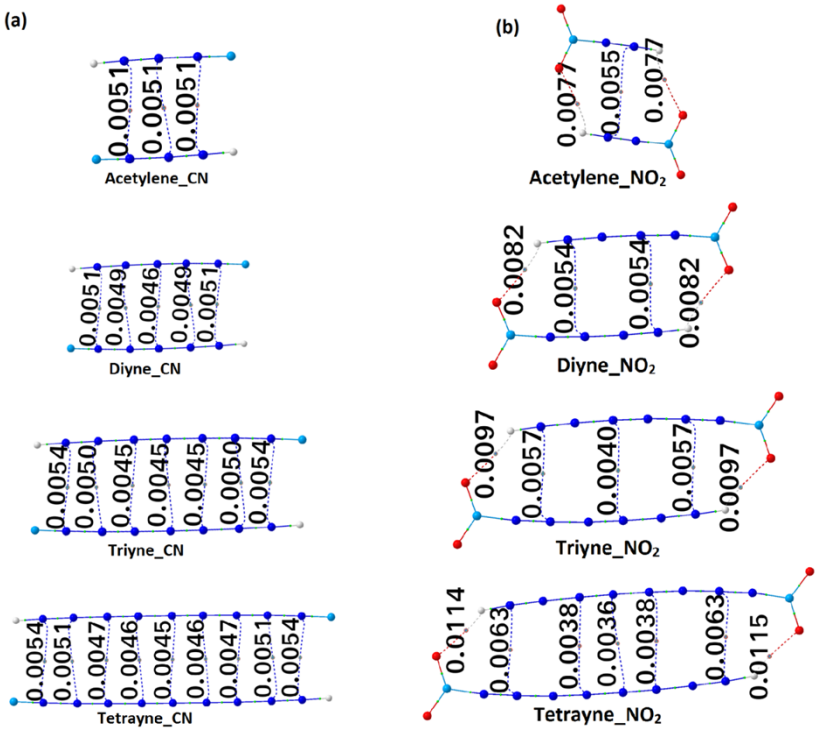

Figure S3. QTAIM plots of dimers of oligoynes that are substituted with (a) CN and (b) NO_2 at one end and with 1 – 4 triple bonds along with the values of ρ (a u) at intermolecular BCPs.

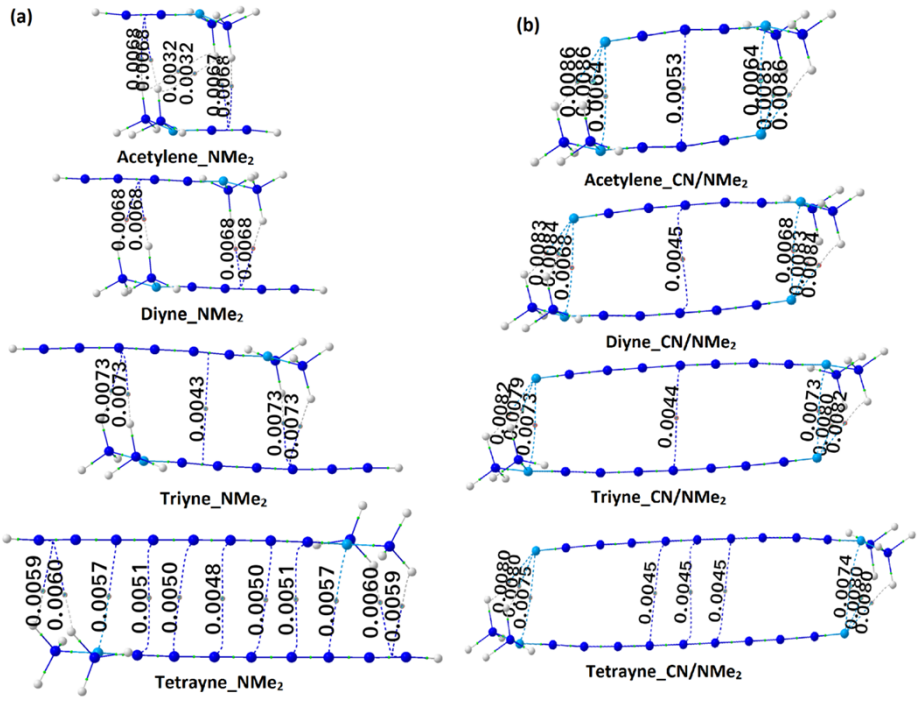

Figure S4. QTAIM plots of dimers of oligoynes that are substituted with (a) NMe_2 at one end and (b) NMe_2 at one end and CN at the other and with 1 – 4 triple bonds along with the values of ρ (a u) at intermolecular BCPs.

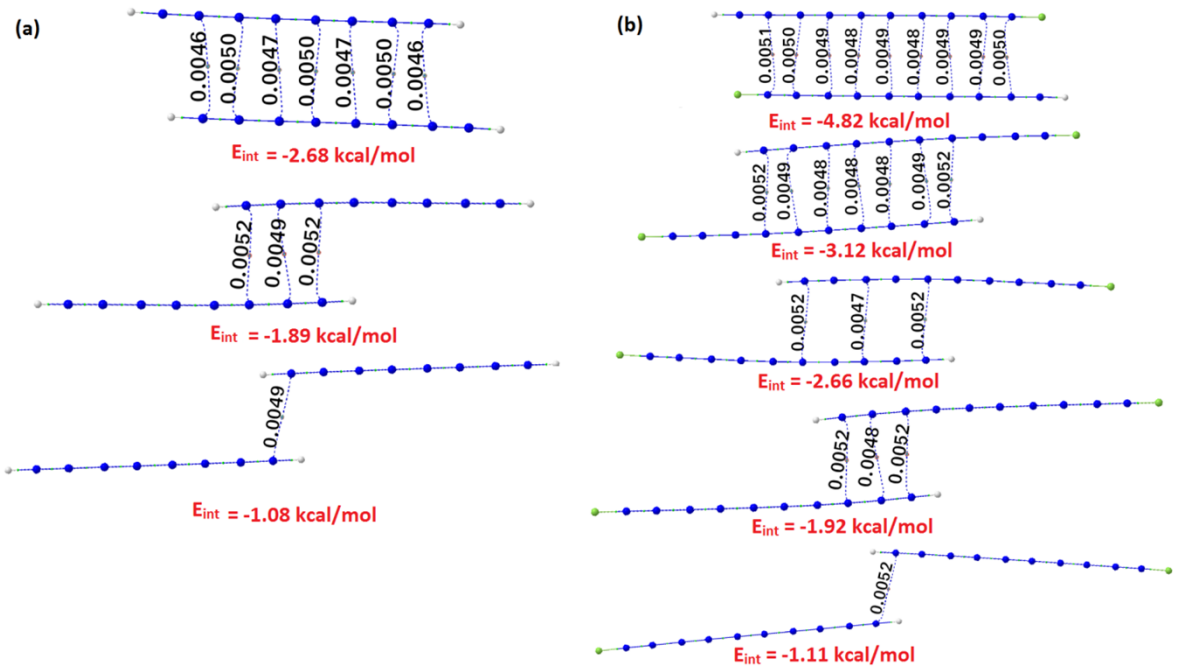

Figure S5. QTAIM plot of the different minima located by sliding one of the monomers of (a) tetrayne and (b) pentayne_F dimers over the other. The values of electron density (ρ) at intermolecular BCPs are given in au

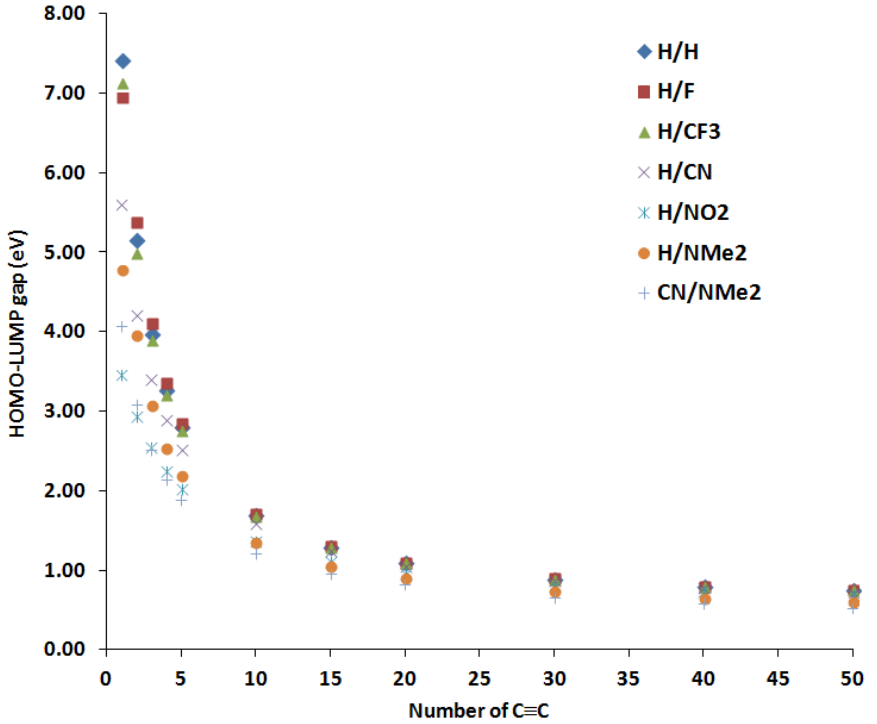

Figure S6. Variation of HOMO-LUMO gap of the polyyne molecules with different end groups and chain lengths

Table S1. SCF energy of all the polyynes dimers with different substitutions and chain lengths studied

# C atoms	H/H	H/F	H/CF3	H/CN	H/NO2	H/NMe2	NMe2/CN
2	-154.677176	-353.145994	-828.876862	-339.203049	-563.728707	-422.653775	-607.208384
4	-307.009592	-505.476262	-981.209933	-491.542609	-716.064188	-574.999026	-759.549879
6	-459.351117	-657.817858	-1133.551243	-643.886087	-868.407273	-727.345736	-911.894350
8	-611.695583	-810.162352	-1285.895758	-796.231580	-1020.752599	-879.691444	-1064.240433
10	-764.041555	-962.508263	-1438.241547	-948.577855	-1173.098806	-1032.039040	-1216.587172
20	-1525.775910	-1724.242407	-2199.974856	-1710.312006	-1934.833346	-1793.777508	-1978.322231
30	-2287.513480	-2485.980014	-2961.712264	-2472.049489	-2696.570785	-2555.516814	-2740.060125
40	-3049.251441	-3247.718019	-3723.450127	-3233.787314	-3458.308645	-3317.255550	-3501.798234
60	-4572.714938	-4771.193099	-5246.926285	-4757.263340	-4981.784616	-4840.732140	-5025.273889
80	-6096.202785	-6294.670222	-6770.401949	-6280.739280	-6505.260691	-6364.207429	-6548.750886
100	-7619.679715	-7818.143608	-8293.878417	-7804.214838	-8028.736811	-7887.684663	-8072.226853

Table S2. SCF energy of all the polyyne monomers with different substitutions and chain lengths studied

# C atoms	H/H	H/F	H/CF3	H/CN	H/NO2	H/NMe2	NMe2/CN
2	-77.337670	-176.571873	-414.435812	-169.598784	-281.860737	-211.322814	-303.594357
4	-153.503745	-252.736067	-490.601629	-245.767727	-358.027763	-287.492854	-379.764208
6	-229.673638	-328.905895	-566.771422	-321.938578	-434.198316	-363.665256	-455.935598
8	-305.844996	-405.077271	-642.942577	-398.110301	-510.369974	-439.838134	-532.107692

10	-382.017008	-481.249286	-719.114579	-474.282481	-586.542141	-516.011171	-608.280100
20	-762.879594	-862.111923	-1099.976876	-855.145044	-967.404767	-896.875865	-989.143037
30	-1143.743754	-1242.976051	-1480.840784	-1236.009062	-1348.268883	-1277.740790	-1370.007194
40	-1524.608050	-1623.840376	-1861.705120	-1616.873345	-1729.133100	-1658.605437	-1750.871405
60	-2286.336786	-2385.569123	-2623.433746	-2378.602015	-2490.861733	-2420.334437	-2512.599990
80	-3048.065674	-3147.297901	-3385.162511	-3140.330800	-3252.590470	-3182.063259	-3274.328712
100	-3809.794271	-3909.026359	-4146.891225	-3902.059421	-4014.319287	-3943.792071	-4036.057347

Table S3. BSSE energy of all the polyyne dimers with different substitutions and chain lengths studied

# C atoms	Unsubstituted	F	CF3	CN	NO2	NMe2	NMe2/CN
2	0.000136	0.000458	0.001037	0.000410	0.000836	0.000576	0.000999
4	0.000517	0.000811	0.001321	0.000771	0.001074	0.001120	0.001288
6	0.000878	0.001128	0.001847	0.001070	0.001431	0.001641	0.001511
8	0.001312	0.001528	0.002366	0.001700	0.001799	0.002115	0.001994
10	0.001773	0.002004	0.002867	0.002142	0.002281	0.002585	0.003078
20	0.003429	0.003649	0.004483	0.003697	0.004025	0.004249	0.003956
30	0.005293	0.005532	0.006322	0.005629	0.005877	0.006157	0.005598
40	0.007155	0.007411	0.008077	0.007376	0.007743	0.008011	0.007508
60	0.005520	0.010694	0.011736	0.011066	0.011389	0.011634	0.010296
80	0.013006	0.014685	0.015428	0.014770	0.015061	0.014888	0.015099
100	0.018144	0.018011	0.019089	0.017873	0.018725	0.019025	0.018766

Table S4. Lowest vibrational frequencies of the polyyne dimers with different substitutions having chain lengths up to 80 C atoms. Frequencies of the polyyne dimers with 100 C atoms (50ynes) have not been calculated due to high computational coast. However, since the trends in their geometries are similar to the lower analogues, we assume that the dimers of 50ynes are also minima.

# C atoms	Unsubstituted	F	CF3	CN	NO2	NMe2	NMe2/CN
2	34.20	48.57	34.02	45.12	27.16	45.74	36.16
4	30.48	25.67	20.49	28.36	24.59	15.20	20.92
6	16.28	19.05	23.30	21.51	23.53	15.95	13.32
8	19.44	18.87	12.69	25.07	16.84	18.38	20.06
10	21.89	16.44	20.88	24.64	16.19	15.34	15.49
20	15.88	14.52	13.25	14.07	9.68	6.72	12.12
30	8.99	8.32	7.62	8.13	6.95	7.58	6.96
40	5.95	5.62	5.25	5.52	5.00	5.23	4.82
60	3.61	2.07	3.06	3.22	3.06	3.05	2.79
80	2.32	2.27	2.06	2.24	2.15	1.23	2.00

Table S5. Difference between adjacent single and triple bonds of pentayne derivatives in Å. From top to bottom: from substituted end to H end. In pentayne_CN/NMe_2, from top to bottom lists the BLA patterns from CN end to NMe_2 end.

H/H	H/F	H/CF_3	H/CN	H/NO_2	H/NMe_2	CN/NMe_2
0.128	0.135	0.125	0.104	0.115	0.105	0.100
0.115	0.116	0.112	0.098	0.102	0.098	0.092
0.103	0.105	0.101	0.094	0.095	0.093	0.086
0.100	0.101	0.098	0.093	0.093	0.092	0.084
0.100	0.100	0.099	0.095	0.095	0.094	0.084
0.103	0.103	0.102	0.100	0.100	0.099	0.085
0.115	0.115	0.114	0.114	0.114	0.113	0.091
0.128	0.128	0.128	0.127	0.127	0.127	0.099

Table S6. Coordinates of acetylene dimer

Atom	x	y	z
6	1.443442000	2.178805000	0.000000000
6	1.443442000	0.977750000	0.000000000
1	1.450449000	3.241879000	0.000000000
1	1.434319000	-0.086179000	0.000000000
6	-1.443442000	-2.178805000	0.000000000
6	-1.443442000	-0.977750000	0.000000000
1	-1.450449000	-3.241879000	0.000000000
1	-1.434319000	0.086179000	0.000000000

Table S7. Coordinates of diyne dimer

Atom	x	y	z
6	-0.073873000	1.731026000	0.000000000
6	1.264239000	1.962563000	0.000000000
6	2.456572000	2.170032000	0.000000000
6	0.073873000	-1.731026000	0.000000000
6	-1.264239000	-1.962563000	0.000000000
6	-2.456572000	-2.170032000	0.000000000
6	1.264239000	-1.517284000	0.000000000
1	2.306770000	-1.313179000	0.000000000
6	-1.264239000	1.517284000	0.000000000
1	-2.306770000	1.313179000	0.000000000
1	-3.500790000	-2.365656000	0.000000000
1	3.500790000	2.365656000	0.000000000

Table S8. Coordinates of triyne dimer

Atom	x	y	z
6	-1.635969000	2.435728000	-0.004153000
6	-0.499252000	2.013285000	-0.002474000
6	0.762286000	1.538959000	-0.000868000

6	1.636190000	-2.435068000	-0.003852000
6	0.499323000	-2.012991000	-0.002605000
6	-0.762219000	-1.538740000	-0.001098000
1	2.636440000	-2.792854000	-0.004900000
1	-2.636040000	2.793753000	-0.005294000
6	-1.906316000	-1.111216000	0.000406000
6	1.906343000	1.111319000	0.000672000
6	-3.170660000	-0.644166000	0.002345000
6	3.170562000	0.643838000	0.002459000
6	-4.310998000	-0.229804000	0.004586000
6	4.310719000	0.228941000	0.004287000
1	-5.314938000	0.118021000	0.006179000
1	5.314489000	-0.119430000	0.005781000

Table S9. Coordinates of tetrayne dimer

Atom	x	y	z
6	2.168364000	2.119297000	0.004565000
6	0.845335000	1.880160000	-0.002112000
6	-0.361576000	1.665300000	0.005944000
6	3.363815000	2.331255000	0.008285000
1	4.411021000	2.507730000	0.014980000
6	-1.676433000	1.432596000	-0.007415000
6	-2.884804000	1.226532000	0.001427000
6	-4.211466000	1.007972000	-0.004117000
6	-2.167799000	-2.123593000	0.003587000
6	-0.843791000	-1.889930000	-0.001671000
6	0.362686000	-1.672727000	0.007650000
6	-3.364763000	-2.326192000	0.007251000
1	-4.413012000	-2.495980000	0.011240000
6	1.677073000	-1.437168000	-0.005594000
6	2.884919000	-1.227219000	0.002934000
6	4.210756000	-1.002886000	-0.004212000
6	5.408867000	-0.803507000	-0.009393000
6	-5.410457000	0.815117000	-0.007343000
1	-6.461796000	0.662823000	-0.010370000
1	6.459438000	-0.644607000	-0.014569000

Table S10. Coordinates of pentayne dimer

Atom	x	y	z
6	3.610642000	2.087634000	0.003287000
6	2.275445000	1.943547000	0.006599000
6	1.054562000	1.814091000	-0.003233000
6	4.818664000	2.212529000	0.000605000

6	-0.268915000	1.675644000	0.008623000
6	-1.493528000	1.551324000	-0.007410000
6	-2.817818000	1.419187000	0.004332000
6	-3.610770000	-2.086689000	0.002996000
6	-2.274512000	-1.953193000	0.004748000
6	-1.053128000	-1.828576000	-0.002203000
6	-4.820226000	-2.198937000	0.004072000
6	0.270275000	-1.688943000	0.008261000
6	1.494434000	-1.559908000	-0.012011000
6	2.818092000	-1.421555000	-0.000572000
6	4.039927000	-1.300343000	-0.006581000
6	-4.040253000	1.303621000	-0.003833000
6	-5.378004000	1.185237000	-0.002424000
6	5.377212000	-1.176417000	-0.001966000
1	5.875825000	2.317045000	-0.005328000
1	-5.878768000	-2.288160000	0.005614000
6	-6.588998000	1.085179000	-0.004638000
6	6.587672000	-1.071334000	0.001330000
1	-7.649124000	1.013191000	-0.005320000
1	7.647434000	-0.994654000	0.005150000

Table 11. Coordinates of acetylene fluoride dimer

Atom	x	y	z
6	-1.649991000	-0.204850000	0.000029000
6	-1.472376000	-1.387522000	0.000318000
1	-1.306277000	-2.434546000	0.000690000
6	1.649991000	0.204849000	0.000037000
6	1.472443000	1.387532000	0.000329000
1	1.306411000	2.434567000	0.000628000
9	1.849292000	-1.049423000	-0.000314000
9	-1.849352000	1.049414000	-0.000308000

Table 12. Coordinates of diyne_F dimer

Atom	x	y	z
6	-0.048235000	1.690070000	0.000000000
6	1.308633000	1.648848000	0.000000000
6	2.517795000	1.606449000	0.000000000
6	0.048235000	-1.690070000	0.000000000
6	-1.308633000	-1.648848000	0.000000000
6	-2.517795000	-1.606449000	0.000000000
6	1.251271000	-1.704662000	0.000000000
9	2.517795000	-1.737613000	0.000000000
6	-1.251271000	1.704662000	0.000000000

9	-2.517795000	1.737613000	0.000000000
1	-3.579312000	-1.571581000	0.000000000
1	3.579312000	1.571581000	0.000000000

Table 13. Coordinates of triyne_F dimer

Atom	x	y	z
6	2.658184000	1.530674000	-0.001347000
6	1.455185000	1.615962000	-0.000680000
6	0.110418000	1.700270000	0.000014000
6	-2.658182000	-1.530646000	-0.001328000
6	-1.455184000	-1.615936000	-0.000500000
6	-0.110420000	-1.700293000	0.000323000
9	-3.921867000	-1.457406000	-0.002248000
9	3.921874000	1.457505000	-0.001979000
6	1.107941000	-1.776653000	0.000964000
6	-1.107943000	1.776613000	0.000692000
6	2.454139000	-1.858003000	0.001524000
6	-2.454142000	1.857950000	0.001494000
6	3.665400000	-1.930526000	0.001998000
6	-3.665404000	1.930457000	0.002296000
1	4.725313000	-2.003444000	0.002336000
1	-4.725318000	2.003354000	0.002996000

Table 14. Coordinates of tetrayne_F dimer

Atom	x	y	z
6	2.688634000	-1.617014000	0.000632000
6	1.345255000	-1.663899000	0.003979000
6	0.120837000	-1.706065000	-0.003875000
6	3.894605000	-1.561765000	-0.000541000
9	5.159169000	-1.519020000	-0.003212000
6	-1.214602000	-1.747059000	0.005867000
6	-2.439753000	-1.786067000	-0.002765000
6	-3.784294000	-1.825656000	0.000074000
6	-2.688620000	1.615749000	-0.000622000
6	-1.345263000	1.663592000	0.001397000
6	-0.120857000	1.706257000	-0.006457000
6	-3.894597000	1.560701000	0.000013000
9	-5.159166000	1.518560000	-0.000377000
6	1.214606000	1.747625000	0.003933000
6	2.439777000	1.786221000	-0.003441000
6	3.784309000	1.826189000	0.001087000
6	4.998489000	1.863313000	0.003591000
6	-4.998521000	-1.861813000	0.000991000

1	-6.060156000	-1.903907000	0.002521000
1	6.060094000	1.906209000	0.006595000

Table S15. Coordinates of pentayne_F dimer

Atom	x	y	z
6	3.947718000	1.616557000	-0.009161000
6	2.605444000	1.649829000	-0.008099000
6	1.378663000	1.679933000	0.000404000
6	5.154867000	1.575015000	-0.010206000
6	0.047419000	1.707754000	-0.006908000
6	-1.183124000	1.733219000	0.013888000
6	-2.514064000	1.758921000	0.004149000
6	-3.947862000	-1.621224000	-0.006582000
6	-2.605572000	-1.654203000	-0.002317000
6	-1.378736000	-1.682223000	-0.006778000
6	-5.154975000	-1.578719000	-0.009118000
6	-0.047464000	-1.707859000	0.006684000
6	1.183190000	-1.731870000	-0.007911000
6	2.514135000	-1.757297000	0.008143000
6	3.741792000	-1.781240000	0.004634000
6	-3.741707000	1.783006000	0.011745000
6	-5.084910000	1.808288000	0.010336000
6	5.085060000	-1.804494000	0.011762000
9	6.419427000	1.546857000	-0.012060000
9	-6.419492000	-1.547662000	-0.012321000
6	-6.300079000	1.831235000	0.010310000
6	6.300259000	-1.824963000	0.016543000
1	-7.362105000	1.863235000	0.009080000
1	7.362358000	-1.853989000	0.021246000

Table S16. Coordinates of acetylene_CF_3 dimer

Atom	x	y	z
6	-1.409395000	-1.100944000	-0.002232000
6	-0.634416000	-2.016219000	-0.008706000
1	0.063141000	-2.819512000	-0.013303000
6	1.409320000	1.100882000	-0.003470000
6	0.633994000	2.015886000	-0.008731000
1	-0.063828000	2.818946000	-0.013164000
6	-2.355630000	-0.000590000	0.001501000
9	-3.625115000	-0.436517000	0.003772000
9	-2.198767000	0.782705000	1.084919000
9	-2.203087000	0.785104000	-1.080996000
6	2.355703000	0.000659000	0.001458000

9	2.203914000	-0.785647000	-1.080647000
9	3.625171000	0.436714000	0.004113000
9	2.198244000	-0.782077000	1.085234000

Table S17. Coordinates of diyne_CF_3 dimer

Atom	x	y	z
6	-2.017818000	-0.881295000	-0.000265000
6	-0.956722000	-1.461725000	-0.000644000
6	0.234819000	-2.106231000	-0.001110000
6	2.017714000	0.881115000	-0.000904000
6	0.957023000	1.462265000	-0.000894000
6	-0.234458000	2.106857000	-0.001137000
6	-1.297821000	2.682565000	-0.001323000
6	1.298048000	-2.682219000	-0.001360000
1	-2.240081000	3.175582000	-0.001327000
1	2.240264000	-3.175310000	-0.001783000
6	-3.305311000	-0.218991000	0.000482000
9	-4.316186000	-1.104550000	0.001270000
9	-3.461544000	0.567059000	1.083099000
9	-3.462901000	0.566722000	-1.082240000
6	3.305202000	0.218793000	0.000515000
9	3.462953000	-0.567467000	-1.081886000
9	4.316093000	1.104292000	0.001077000
9	3.461112000	-0.566844000	1.083451000

Table S18. Coordinates of triyne_CF_3 dimer

Atom	x	y	z
6	2.961498000	0.864868000	0.020222000
6	1.804215000	1.224397000	-0.032934000
6	0.522539000	1.625298000	-0.097977000
6	-2.959393000	-0.861012000	0.037022000
6	-1.803648000	-1.224257000	-0.023993000
6	-0.522481000	-1.626449000	-0.091021000
6	0.636420000	-2.008587000	-0.145763000
6	-0.636823000	2.006528000	-0.148981000
6	1.912918000	-2.432256000	-0.208227000
6	-1.913747000	2.429512000	-0.207242000
6	3.062929000	-2.812338000	-0.260639000
6	-3.064257000	2.808522000	-0.256239000
1	4.076285000	-3.131522000	-0.303825000
1	-4.078001000	3.126906000	-0.296122000
6	-4.357192000	-0.494499000	0.113867000
9	-4.769295000	0.140214000	-1.000681000

9	-5.142132000	-1.574786000	0.270001000
9	-4.602214000	0.327838000	1.151105000
6	4.357770000	0.496256000	0.113704000
9	5.143563000	1.576364000	0.266654000
9	4.590138000	-0.315698000	1.161852000
9	4.779633000	-0.150740000	-0.990135000

Table S19. Coordinates of tetrayne_CF_3 dimer

Atom	x	y	z
6	-2.902463000	-1.123574000	-0.004361000
6	-1.587436000	-1.387605000	-0.012467000
6	-0.388869000	-1.645598000	0.005427000
6	-4.093358000	-0.885750000	-0.000477000
6	0.914348000	-1.929855000	-0.001100000
6	2.109826000	-2.200089000	0.012825000
6	3.420298000	-2.495996000	0.015858000
6	2.903139000	1.126905000	-0.007356000
6	1.588781000	1.394079000	0.004596000
6	0.390279000	1.652663000	-0.008897000
6	4.093156000	0.884735000	-0.012061000
6	-0.913099000	1.935847000	0.007248000
6	-2.109506000	2.202359000	0.005250000
6	-3.420840000	2.494353000	0.014799000
6	-4.605439000	2.757850000	0.021973000
6	4.604038000	-2.763381000	0.020501000
1	5.644219000	-2.983355000	0.023235000
1	-5.646230000	2.974867000	0.029492000
6	5.525303000	0.677068000	-0.007225000
9	5.929748000	0.002226000	1.086260000
9	5.935602000	-0.025535000	-1.080635000
9	6.189835000	1.846023000	-0.020778000
6	-5.525688000	-0.679527000	-0.005873000
9	-5.929265000	0.010259000	-1.090150000
9	-6.189052000	-1.849129000	-0.010054000
9	-5.938292000	0.007444000	1.077058000

Table S20. Coordinates of pentayne_CF_3 dimer

Atom	x	y	z
6	-4.080213000	-1.111842000	-0.005680000
6	-2.753057000	-1.296067000	-0.007740000
6	-1.538485000	-1.479157000	0.004116000
6	-5.284135000	-0.947456000	-0.008906000
6	-0.224435000	-1.681942000	-0.005398000

6	0.991539000	-1.874774000	0.010724000
6	2.305205000	-2.082536000	-0.000091000
6	4.080301000	1.112345000	0.003402000
6	2.752988000	1.295573000	0.005817000
6	1.538362000	1.478381000	-0.005393000
6	5.284211000	0.947705000	0.006919000
6	0.224230000	1.680543000	0.004124000
6	-0.991840000	1.872892000	-0.009960000
6	-2.305401000	2.081044000	0.003117000
6	-3.517798000	2.275218000	-0.003558000
6	3.517794000	-2.275358000	0.007151000
6	4.843479000	-2.485967000	0.001461000
6	-4.843405000	2.486353000	0.001905000
6	6.042907000	-2.675349000	-0.003173000
6	-6.042853000	2.675699000	0.005432000
1	7.095645000	-2.824061000	-0.008035000
1	-7.095698000	2.823610000	0.008904000
6	-6.724207000	-0.807289000	-0.000954000
9	-7.155429000	-0.144438000	1.089910000
9	-7.167213000	-0.129736000	-1.077612000
9	-7.336969000	-2.004082000	-0.005674000
6	6.724276000	0.808039000	-0.000344000
9	7.156444000	0.143779000	-1.089739000
9	7.336700000	2.005042000	0.003351000
9	7.166831000	0.132114000	1.077687000

Table S21. Coordinates of acetylene cyanide dimer

Atom	x	y	z
6	-0.077798000	1.688996000	0.000000000
6	-1.284266000	1.672699000	0.000000000
1	-2.348071000	1.637979000	0.000000000
6	0.077798000	-1.688996000	0.000000000
6	1.284266000	-1.672699000	0.000000000
1	2.348071000	-1.637979000	0.000000000
6	-1.284266000	-1.666337000	0.000000000
7	-2.448105000	-1.620534000	0.000000000
6	1.284266000	1.666337000	0.000000000
7	2.448105000	1.620534000	0.000000000

Table S22. Coordinates of diyne_CN dimer

Atom	x	y	z
6	-1.283279000	1.582865000	-0.519882000
6	-0.066468000	1.642155000	-0.500054000

6	1.280093000	1.686529000	-0.471283000
6	1.283279000	-1.582865000	0.519882000
6	0.066468000	-1.642155000	0.500054000
6	-1.280093000	-1.686529000	0.471283000
6	2.632703000	-1.483163000	0.529584000
7	3.795636000	-1.377252000	0.532030000
6	-2.632703000	1.483163000	-0.529584000
7	-3.795636000	1.377252000	-0.532030000
6	-2.491146000	-1.703866000	0.436718000
6	2.491146000	1.703866000	-0.436718000
1	-3.554644000	-1.696460000	0.399636000
1	3.554644000	1.696460000	-0.399636000

Table S23. Coordinates of triyne_CN dimer

Atom	x	y	z
6	-2.523959000	1.599409000	-0.500484000
6	-1.302027000	1.639847000	-0.475208000
6	0.032871000	1.672474000	-0.442724000
6	2.523959000	-1.599409000	0.500484000
6	1.302027000	-1.639847000	0.475208000
6	-0.032871000	-1.672474000	0.442724000
6	3.872270000	-1.525754000	0.518698000
7	5.038327000	-1.444536000	0.529926000
6	-3.872270000	1.525754000	-0.518698000
7	-5.038327000	1.444536000	-0.529926000
6	-1.257217000	-1.687007000	0.407597000
6	1.257217000	1.687007000	-0.407597000
6	-2.600493000	-1.690908000	0.366485000
6	2.600493000	1.690908000	-0.366485000
6	-3.813299000	-1.675594000	0.326801000
6	3.813299000	1.675594000	-0.326801000
1	-4.875679000	-1.640563000	0.277880000
1	4.875679000	1.640563000	-0.277880000

Table S24. Coordinates of tetrayne_CN dimer

Atom	x	y	z
6	-2.685128000	-1.507464000	-0.004058000
6	-1.358442000	-1.620539000	-0.011415000
6	-0.132552000	-1.719974000	0.004661000
6	-3.904716000	-1.395484000	-0.002725000
6	1.193815000	-1.823313000	-0.005788000
6	2.417939000	-1.913268000	0.004525000
6	3.757562000	-1.997529000	0.003926000
6	2.685002000	1.506046000	-0.000614000
6	1.358452000	1.620587000	0.007091000

6	0.132495000	1.719495000	-0.007069000
6	3.904646000	1.394782000	0.001827000
6	-1.193950000	1.821890000	0.004700000
6	-2.418136000	1.910956000	-0.004465000
6	-3.757623000	1.996946000	0.000727000
6	-4.970477000	2.058466000	0.002588000
6	4.970538000	-2.056757000	0.003879000
1	6.034171000	-2.084122000	0.003827000
1	-6.034049000	2.087833000	0.003762000
6	-5.245411000	-1.243107000	0.001774000
7	-6.405304000	-1.093540000	0.004312000
6	5.245499000	1.243830000	-0.000637000
7	6.405705000	1.096811000	-0.004477000

Table S25. Coordinates of pentayne_CN dimer

Atom	x	y	z
6	-3.918215000	1.503896000	0.001078000
6	-2.590649000	1.576981000	0.007036000
6	-1.360129000	1.643646000	-0.004201000
6	-5.141697000	1.429806000	-0.001153000
6	-0.036578000	1.714454000	0.007308000
6	1.194509000	1.783470000	-0.008265000
6	2.520683000	1.854070000	0.003089000
6	3.918276000	-1.505511000	-0.001767000
6	2.590791000	-1.579948000	-0.007255000
6	1.360351000	-1.647675000	0.001809000
6	5.141631000	-1.429437000	-0.001710000
6	0.036920000	-1.718918000	-0.010394000
6	-1.194084000	-1.789924000	0.005689000
6	-2.520372000	-1.858414000	-0.001983000
6	-3.747827000	-1.915463000	0.006135000
6	3.747956000	1.914680000	-0.002318000
6	5.088461000	1.964984000	0.001754000
6	-5.088465000	-1.962307000	0.003835000
6	-6.485999000	1.321209000	-0.002769000
7	-7.650472000	1.209921000	-0.005168000
6	6.485521000	-1.315990000	0.000201000
7	7.649638000	-1.201462000	0.002007000
6	6.303070000	1.991061000	0.003273000
6	-6.303170000	-1.985800000	0.003500000
1	7.366972000	1.987022000	0.005562000
1	-7.367047000	-1.979454000	-0.000784000

Table S26. Coordinates of nitroacetylene dimer

Atom	x	y	z
6	-0.655689000	1.772669000	-0.186117000
6	0.539732000	1.669316000	-0.148641000
1	1.597199000	1.547440000	-0.107027000
6	0.655689000	-1.772669000	0.186117000
6	-0.539732000	-1.669316000	0.148641000
1	-1.597199000	-1.547440000	0.107027000
7	-2.046067000	1.846719000	-0.220706000
8	-2.652122000	0.784870000	-0.098995000
8	-2.545708000	2.951127000	-0.367230000
7	2.046067000	-1.846719000	0.220706000
8	2.545708000	-2.951127000	0.367230000
8	2.652122000	-0.784870000	0.098995000

Table S27. Coordinates of diyne_NO_2 dimer

Atom	x	y	z
6	-2.169285000	1.737210000	-0.571335000
6	-0.959437000	1.711000000	-0.515756000
6	0.386015000	1.643665000	-0.437403000
6	2.169285000	-1.737210000	0.571335000
6	0.959437000	-1.711000000	0.515756000
6	-0.386015000	-1.643665000	0.437403000
6	-1.589508000	-1.541724000	0.346870000
6	1.589508000	1.541724000	-0.346870000
1	-2.643911000	-1.412042000	0.251204000
1	2.643911000	1.412042000	-0.251204000
7	-3.549764000	1.674289000	-0.594278000
8	-4.048398000	0.569387000	-0.372262000
8	-4.161725000	2.707025000	-0.829755000
7	3.549764000	-1.674289000	0.594278000
8	4.161725000	-2.707025000	0.829755000
8	4.048398000	-0.569387000	0.372262000

Table S28. Coordinates of triyne_NO_2 dimer

Atom	x	y	z
6	-3.448048000	1.941206000	-0.620745000
6	-2.234079000	1.905610000	-0.565759000
6	-0.900925000	1.824008000	-0.497782000
6	3.448048000	-1.941206000	0.620745000
6	2.234079000	-1.905610000	0.565759000
6	0.900925000	-1.824008000	0.497782000
6	-0.313407000	-1.694777000	0.415304000
6	0.313407000	1.694777000	-0.415304000
6	-1.640663000	-1.511533000	0.313489000
6	1.640663000	1.511533000	-0.313489000

6	-2.833400000	-1.307842000	0.214645000
6	2.833400000	1.307842000	-0.214645000
1	-3.872827000	-1.087457000	0.111198000
1	3.872827000	1.087457000	-0.111198000
7	-4.824559000	1.880325000	-0.636069000
8	-5.324751000	0.772761000	-0.420088000
8	-5.438718000	2.915576000	-0.859816000
7	4.824559000	-1.880325000	0.636069000
8	5.438718000	-2.915576000	0.859816000
8	5.324751000	-0.772761000	0.420088000

Table S29. Coordinates of tetrayne_NO_2 dimer

Atom	x	y	z
6	-4.021043000	-1.026334000	0.006116000
6	-2.725458000	-1.338725000	-0.014522000
6	-1.518141000	-1.569806000	-0.021926000
6	-5.193907000	-0.698548000	0.018763000
6	-0.205516000	-1.784495000	-0.042532000
6	1.009968000	-1.957513000	-0.034476000
6	2.342243000	-2.116939000	-0.045342000
6	4.021422000	1.028411000	0.024506000
6	2.725443000	1.339732000	0.013210000
6	1.517530000	1.567599000	-0.006392000
6	5.194233000	0.701182000	0.038933000
6	0.204473000	1.780063000	-0.014138000
6	-1.010666000	1.952185000	-0.048124000
6	-2.342499000	2.115100000	-0.064231000
6	-3.552027000	2.230864000	-0.075370000
6	3.552126000	-2.229260000	-0.059380000
1	4.619706000	-2.274528000	-0.072194000
1	-4.619516000	2.278961000	-0.084170000
7	6.477510000	0.204774000	0.038724000
8	6.586241000	-1.023797000	-0.037697000
8	7.402411000	1.004039000	0.113790000
7	-6.477072000	-0.202892000	0.045833000
8	-7.398942000	-1.002646000	0.148477000
8	-6.588752000	1.025065000	-0.035333000

Table S30. Coordinates of pentayne_NO_2 dimer

Atom	x	y	z
6	5.255512000	-1.020629000	0.043590000
6	3.949327000	-1.276609000	0.026460000
6	2.731622000	-1.460713000	0.004001000

6	6.441575000	-0.741291000	0.058386000
6	1.417543000	-1.631857000	-0.005016000
6	0.192976000	-1.774062000	-0.039026000
6	-1.126899000	-1.914611000	-0.047387000
6	-5.255772000	1.022572000	0.044960000
6	-3.949649000	1.278883000	0.029870000
6	-2.731825000	1.462040000	0.008342000
6	-6.441945000	0.743469000	0.058702000
6	-1.417662000	1.632293000	-0.000804000
6	-0.192958000	1.773630000	-0.035331000
6	1.126999000	1.913057000	-0.045455000
6	2.350135000	2.030902000	-0.075177000
6	-2.350010000	-2.033400000	-0.074815000
6	-3.686098000	-2.144552000	-0.093637000
6	3.686231000	2.141404000	-0.096434000
6	-4.899298000	-2.220837000	-0.113967000
6	4.899424000	2.217045000	-0.119285000
1	-5.967406000	-2.237409000	-0.129204000
1	5.967516000	2.233167000	-0.136382000
7	7.743400000	-0.299721000	0.066840000
8	7.906389000	0.920231000	-0.051650000
8	8.632085000	-1.134413000	0.190495000
7	-7.743460000	0.300952000	0.064838000
8	-8.632848000	1.135150000	0.184606000
8	-7.905005000	-0.919066000	-0.051454000

Table S31. Coordinates of acetylene_NMe_2 dimer

Atom	x	y	z
6	-1.958420000	0.867050000	-0.002773000
6	-1.953134000	2.078378000	-0.004416000
1	-2.059335000	3.133951000	-0.005576000
6	1.959462000	-0.866773000	0.000276000
6	1.955858000	-2.078106000	-0.002286000
1	2.063743000	-3.133507000	-0.004829000
7	-1.973102000	-0.465373000	-0.000606000
7	1.972627000	0.465674000	0.002010000
6	-1.598947000	-1.154481000	-1.229536000
1	-0.511274000	-1.277179000	-1.317773000
1	-2.057875000	-2.147149000	-1.234702000
1	-1.971721000	-0.593962000	-2.086845000
6	-1.602562000	-1.150186000	1.231809000
1	-0.515209000	-1.273716000	1.323066000
1	-1.976688000	-0.585931000	2.086078000
1	-2.062594000	-2.142323000	1.239781000
6	1.602244000	1.153243000	-1.228984000

1	0.514688000	1.272997000	-1.322384000
1	2.058536000	2.147124000	-1.232440000
1	1.980641000	0.593305000	-2.084223000
6	1.596736000	1.150846000	1.232584000
1	0.508908000	1.272074000	1.320545000
1	1.969634000	0.588333000	2.088540000
1	2.054449000	2.144045000	1.240894000

Table S32. Coordinates of diyne_NMe_2 dimer

Atom	x	y	z
6	1.304838000	4.083498000	0.000000000
6	1.485509000	2.881110000	0.000000000
6	1.645633000	1.539907000	0.000000000
6	-1.304838000	-4.083498000	0.000000000
6	-1.485509000	-2.881110000	0.000000000
6	-1.645633000	-1.539907000	0.000000000
1	-1.195660000	-5.139576000	0.000000000
1	1.195660000	5.139576000	0.000000000
6	-1.762373000	-0.323531000	0.000000000
6	1.762373000	0.323531000	0.000000000
7	1.955332000	-0.979869000	0.000000000
7	-1.955332000	0.979869000	0.000000000
6	1.762373000	-1.724955000	1.239531000
1	2.066568000	-1.106327000	2.083035000
1	0.718008000	-2.030066000	1.369790000
1	2.388172000	-2.620633000	1.214702000
6	1.762373000	-1.724955000	-1.239531000
1	0.718008000	-2.030066000	-1.369790000
1	2.066568000	-1.106327000	-2.083035000
1	2.388172000	-2.620633000	-1.214702000
6	-1.762373000	1.724955000	-1.239531000
1	-2.066568000	1.106327000	-2.083035000
1	-2.388172000	2.620633000	-1.214702000
1	-0.718008000	2.030066000	-1.369790000
6	-1.762373000	1.724955000	1.239531000
1	-0.718008000	2.030066000	1.369790000
1	-2.388172000	2.620633000	1.214702000
1	-2.066568000	1.106327000	2.083035000

Table S33. Coordinates of triyne_NMe_2 dimer

Atom	x	y	z
6	-5.839422000	-0.837725000	-0.001775000
6	-4.650963000	-1.099198000	-0.001758000

6	-3.329709000	-1.353337000	-0.001814000
6	5.837360000	0.828323000	-0.002171000
6	4.649951000	1.094292000	-0.002845000
6	3.329612000	1.352894000	-0.002532000
1	6.881216000	0.633482000	-0.001084000
1	-6.884052000	-0.646918000	-0.003908000
6	2.113080000	1.530557000	-0.001054000
6	-2.112792000	-1.528541000	-0.001259000
6	0.791004000	1.720337000	-0.000809000
6	-0.790319000	-1.715639000	-0.000939000
6	-0.429116000	1.845215000	0.000236000
6	0.429729000	-1.841167000	0.000606000
7	-1.724235000	2.036504000	0.001385000
7	1.724666000	-2.033444000	0.001919000
6	-2.484726000	1.951026000	1.242775000
1	-2.953055000	0.966757000	1.349650000
1	-1.820438000	2.127150000	2.087162000
1	-3.266486000	2.715768000	1.238888000
6	-2.486688000	1.953224000	-1.239027000
1	-2.950596000	0.967245000	-1.349802000
1	-3.271987000	2.714319000	-1.230107000
1	-1.824993000	2.136789000	-2.083801000
6	2.487086000	-1.953791000	-1.238492000
1	2.957395000	-0.970721000	-1.348143000
1	3.267455000	-2.720047000	-1.230689000
1	1.823725000	-2.131860000	-2.083356000
6	2.485363000	-1.948309000	1.243323000
1	2.953229000	-0.964139000	1.351086000
1	1.821603000	-2.125640000	2.087619000
1	3.267262000	-2.712577000	1.238577000

Table S34. Coordinates of tetrayne_NMe_2 dimer

Atom	x	y	z
6	-1.335124000	6.249631000	0.007958000
6	-1.421999000	5.034523000	0.007281000
6	-1.499224000	3.693892000	0.011914000
6	1.335124000	-6.249631000	-0.007958000
6	1.421999000	-5.034523000	-0.007281000
6	1.499224000	-3.693892000	-0.011914000
1	1.310834000	-7.311506000	-0.008559000
1	-1.310834000	7.311506000	0.008559000
6	1.572093000	-2.465114000	-0.005806000
6	-1.572093000	2.465114000	0.005806000
6	1.655846000	-1.137846000	-0.017702000
6	-1.655846000	1.137846000	0.017702000

6	1.723037000	0.093500000	-0.000513000
6	-1.723037000	-0.093500000	0.000513000
7	1.839875000	3.956682000	-0.008649000
7	-1.839875000	-3.956682000	0.008649000
6	1.937177000	4.708659000	1.233366000
1	1.230698000	5.543229000	1.204673000
1	1.681330000	4.060230000	2.069590000
1	2.950341000	5.101719000	1.381388000
6	1.924421000	4.706152000	-1.253091000
1	2.936398000	5.097646000	-1.413010000
1	1.658537000	4.056593000	-2.085309000
1	1.219455000	5.541722000	-1.217935000
6	-1.937177000	-4.708659000	-1.233366000
1	-1.230698000	-5.543229000	-1.204673000
1	-2.950341000	-5.101719000	-1.381388000
1	-1.681330000	-4.060230000	-2.069590000
6	-1.924421000	-4.706152000	1.253091000
1	-1.219455000	-5.541722000	1.217935000
1	-1.658537000	-4.056593000	2.085309000
1	-2.936398000	-5.097646000	1.413010000
6	1.792569000	1.422509000	-0.007680000
6	1.828948000	2.649552000	-0.006741000
6	-1.792569000	-1.422509000	0.007680000
6	-1.828948000	-2.649552000	0.006741000

Table S35. Coordinates of pentayne_NMe_2 dimer

Atom	x	y	z
6	4.769110000	-2.222895000	0.032064000
6	3.547178000	-2.064809000	0.033293000
6	2.228148000	-1.918214000	0.019723000
6	-4.769110000	2.222895000	-0.032064000
6	-3.547178000	2.064809000	-0.033293000
6	-2.228148000	1.918214000	-0.019723000
6	-0.997554000	1.802441000	-0.030290000
6	0.997554000	-1.802441000	0.030290000
6	0.321370000	1.688975000	-0.018588000
6	-0.321370000	-1.688975000	0.018588000
6	1.552493000	1.581891000	-0.031056000
6	-1.552493000	-1.581891000	0.031056000
7	5.398761000	1.224618000	-0.042828000
7	-5.398761000	-1.224618000	0.042828000
6	6.120422000	0.967499000	-1.283311000
1	6.449486000	-0.076088000	-1.330173000
1	5.470485000	1.177038000	-2.130587000
1	6.998629000	1.617895000	-1.337069000

6	6.139861000	1.036320000	1.198376000
1	7.019807000	1.686465000	1.200872000
1	5.503955000	1.295247000	2.042612000
1	6.468155000	-0.004018000	1.299070000
6	-6.120422000	-0.967499000	1.283311000
1	-6.449486000	0.076088000	1.330173000
1	-6.998629000	-1.617895000	1.337069000
1	-5.470485000	-1.177038000	2.130587000
6	-6.139861000	-1.036320000	-1.198376000
1	-6.468155000	0.004018000	-1.299070000
1	-5.503955000	-1.295247000	-2.042612000
1	-7.019807000	-1.686465000	-1.200872000
6	2.875292000	1.465691000	-0.029457000
6	4.096438000	1.330326000	-0.036076000
6	-2.875292000	-1.465691000	0.029457000
6	-4.096438000	-1.330326000	0.036076000
6	-6.096626000	2.421702000	-0.036489000
6	-7.303906000	2.583357000	-0.037113000
1	-8.351570000	2.758587000	-0.037238000
6	6.096626000	-2.421702000	0.036489000
6	7.303906000	-2.583357000	0.037113000
1	8.351570000	-2.758587000	0.037238000

Table S36. Coordinates of acetylene_CN/NMe_2 dimer

Atom	x	y	z
6	1.905335000	1.045148000	0.002109000
6	0.789931000	1.543306000	0.002528000
6	-1.906705000	-1.047505000	0.001122000
6	-0.790987000	-1.544850000	-0.000841000
7	3.127255000	0.576537000	0.000715000
7	-3.129072000	-0.579397000	0.001324000
6	3.682966000	0.030722000	1.237530000
1	3.473709000	-1.041446000	1.311469000
1	4.763422000	0.194200000	1.240278000
1	3.245181000	0.546704000	2.090776000
6	3.681841000	0.036337000	-1.239065000
1	3.471273000	-1.035212000	-1.318454000
1	3.244520000	0.557311000	-2.089495000
1	4.762495000	0.198477000	-1.241245000
6	-3.679760000	-0.029561000	1.238861000
1	-3.458167000	1.039919000	1.315589000
1	-4.761997000	-0.180313000	1.239361000
1	-3.249495000	-0.553010000	2.091486000
6	-3.682479000	-0.036150000	-1.237910000
1	-3.456635000	1.031769000	-1.323585000

1	-3.258458000	-0.567940000	-2.088436000
1	-4.765289000	-0.182035000	-1.232487000
6	-0.499363000	1.940034000	-0.000639000
7	-1.621081000	2.277415000	-0.003539000
6	0.499017000	-1.939480000	0.000769000
7	1.621565000	-2.274045000	-0.001648000

Table S37. Coordinates of diyne_CN/NMe_2 dimer

Atom	x	y	z
6	0.662442000	1.897517000	0.003456000
6	-0.540699000	1.655166000	0.001697000
6	-1.844437000	1.380309000	-0.000112000
6	-0.662526000	-1.897186000	0.003848000
6	0.540619000	-1.654850000	0.003700000
6	1.844358000	-1.380016000	0.004104000
6	-1.993993000	-2.094919000	0.003602000
7	-3.155793000	-2.252280000	0.003426000
6	1.993954000	2.094974000	0.005204000
7	3.155790000	2.252061000	0.006599000
6	3.022514000	-1.038047000	0.000366000
6	-3.022474000	1.037909000	-0.001805000
7	-4.288570000	0.717686000	-0.003141000
7	4.288551000	-0.717676000	-0.004129000
6	-4.919771000	0.267616000	-1.242008000
1	-4.400245000	0.704157000	-2.093363000
1	-4.881834000	-0.824212000	-1.312306000
1	-5.961051000	0.598922000	-1.250576000
6	-4.923592000	0.272564000	1.235567000
1	-4.886119000	-0.818994000	1.310200000
1	-4.406491000	0.712257000	2.086765000
1	-5.964813000	0.604141000	1.239731000
6	4.927063000	-0.273334000	1.233069000
1	4.411800000	-0.712874000	2.085461000
1	5.968070000	-0.605627000	1.234521000
1	4.890498000	0.818226000	1.308067000
6	4.916465000	-0.267225000	-1.244499000
1	4.878459000	0.824636000	-1.314304000
1	5.957692000	-0.598619000	-1.255973000
1	4.394652000	-0.703409000	-2.094634000

Table S38. Coordinates of triyne_CN/NMe_2 dimer

Atom	x	y	z
6	2.047839000	1.995899000	0.041203000

6	0.827232000	1.852843000	0.021125000
6	-0.490132000	1.690052000	0.013534000
6	-2.047341000	-1.996839000	0.024970000
6	-0.826239000	-1.856759000	0.021534000
6	0.491376000	-1.696844000	0.004875000
6	-3.388137000	-2.103615000	0.031788000
7	-4.558048000	-2.182529000	0.036613000
6	3.388371000	2.105571000	0.048798000
7	4.558249000	2.185117000	0.051085000
6	1.712878000	-1.519920000	0.011151000
6	-1.710842000	1.509976000	-0.015914000
6	3.023352000	-1.307602000	-0.007652000
6	-3.022451000	1.303985000	-0.015708000
6	4.224708000	-1.047998000	-0.017320000
6	-4.224660000	1.048081000	-0.024381000
7	5.506115000	-0.807010000	-0.034667000
7	-5.506152000	0.807864000	-0.024225000
6	6.200847000	-0.456604000	1.202144000
1	6.263882000	0.631575000	1.303364000
1	5.659795000	-0.868612000	2.052218000
1	7.207746000	-0.881152000	1.178375000
6	6.153564000	-0.382326000	-1.273904000
1	6.233570000	0.709225000	-1.301915000
1	7.151779000	-0.824600000	-1.325536000
1	5.567358000	-0.723443000	-2.125174000
6	-6.175280000	0.409475000	-1.260488000
1	-6.242755000	-0.681578000	-1.317975000
1	-7.179910000	0.839721000	-1.277495000
1	-5.612757000	0.782772000	-2.114434000
6	-6.182874000	0.441226000	1.217784000
1	-6.259968000	-0.647627000	1.297911000
1	-5.619591000	0.826990000	2.065671000
1	-7.183560000	0.881028000	1.222109000

Table S39. Coordinates of tetrayne_CN/NMe_2 dimer

Atom	x	y	z
6	-3.390397000	-2.017113000	-0.000057000
6	-2.164592000	-1.920235000	-0.002183000
6	-0.843750000	-1.810171000	-0.012054000
6	3.390239000	2.017572000	0.001607000
6	2.164260000	1.922928000	-0.000848000
6	0.843096000	1.816595000	-0.010486000
6	4.733279000	2.085674000	0.006321000
7	5.904963000	2.131314000	0.009914000
6	-4.733313000	-2.087402000	0.005272000
7	-5.904934000	-2.134636000	0.009371000

6	-0.388497000	1.707574000	0.001464000
6	0.387996000	-1.703050000	0.000943000
6	-1.704364000	1.584757000	-0.012381000
6	1.703802000	-1.579409000	-0.010056000
6	-2.934573000	1.454868000	-0.004076000
6	2.934296000	-1.452671000	0.002617000
7	-6.749013000	0.876536000	0.001730000
7	6.749390000	-0.879193000	0.001166000
6	-7.433866000	0.526286000	1.244234000
1	-7.542693000	-0.560139000	1.320653000
1	-6.857844000	0.892720000	2.092017000
1	-8.421369000	0.994662000	1.251940000
6	-7.440068000	0.518580000	-1.235137000
1	-8.427136000	0.987898000	-1.241396000
1	-6.867651000	0.878662000	-2.088043000
1	-7.550391000	-0.568212000	-1.303754000
6	7.430534000	-0.523560000	-1.241847000
1	7.539466000	0.563157000	-1.313693000
1	8.417901000	-0.992120000	-1.254579000
1	6.851841000	-0.886055000	-2.089482000
6	7.444382000	-0.527396000	1.237550000
1	7.555661000	0.559012000	1.310616000
1	6.874134000	-0.890693000	2.090552000
1	8.431096000	-0.997504000	1.239037000
6	-4.249678000	1.289789000	-0.005820000
6	-5.461355000	1.075701000	-0.001983000
6	4.249744000	-1.290442000	0.001082000
6	5.461847000	-1.078796000	0.007650000

Table S40. Coordinates of pentayne_CN/NMe_2 dimer

Atom	x	y	z
6	-0.393721000	-1.695568000	0.025482000
6	0.393358000	1.691752000	0.027340000
6	1.630694000	1.616792000	0.017785000
6	-1.630927000	-1.618609000	0.014505000
6	2.946691000	1.527170000	0.024623000
6	-2.946825000	-1.527130000	0.017635000
6	4.181210000	1.429287000	0.003466000
6	-4.181330000	-1.429382000	-0.004524000
7	8.005152000	0.928864000	-0.031216000
7	-8.005052000	-0.927018000	-0.028456000
6	8.689041000	0.581204000	-1.274893000
1	8.822623000	-0.503221000	-1.339892000
1	8.098546000	0.924633000	-2.122192000
1	9.665456000	1.071901000	-1.294896000

6	8.717463000	0.611199000	1.204763000
1	9.690159000	1.109674000	1.195018000
1	8.141862000	0.966388000	2.057506000
1	8.861381000	-0.470479000	1.288116000
6	-8.710441000	-0.609779000	1.211672000
1	-8.849058000	0.472353000	1.298901000
1	-9.685465000	-1.103738000	1.204545000
1	-8.132777000	-0.970340000	2.060824000
6	-8.694830000	-0.576832000	-1.268188000
1	-8.827555000	0.507846000	-1.331091000
1	-8.108957000	-0.919685000	-2.118937000
1	-9.671874000	-1.066415000	-1.284007000
6	5.498640000	1.296023000	-0.002928000
6	6.714998000	1.105699000	-0.018495000
6	-5.498903000	-1.297271000	-0.010125000
6	-6.715087000	-1.105575000	-0.022105000
6	-0.923827000	1.769855000	0.017252000
6	-2.158829000	1.845087000	0.029291000
6	0.923491000	-1.773315000	0.016474000
6	2.158520000	-1.848059000	0.029416000
6	-3.480694000	1.931739000	0.015835000
6	-4.707906000	2.011203000	0.013319000
6	-6.051624000	2.064933000	0.007929000
7	-7.223701000	2.098303000	0.004337000
6	3.480522000	-1.933284000	0.018037000
6	4.707801000	-2.011865000	0.015909000
6	6.051617000	-2.063778000	0.010968000
7	7.223752000	-2.095563000	0.007255000