Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

How aromatic system size affects impact sensitivities of highly energetic molecules?

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1. The numbering system in the aromatic molecules

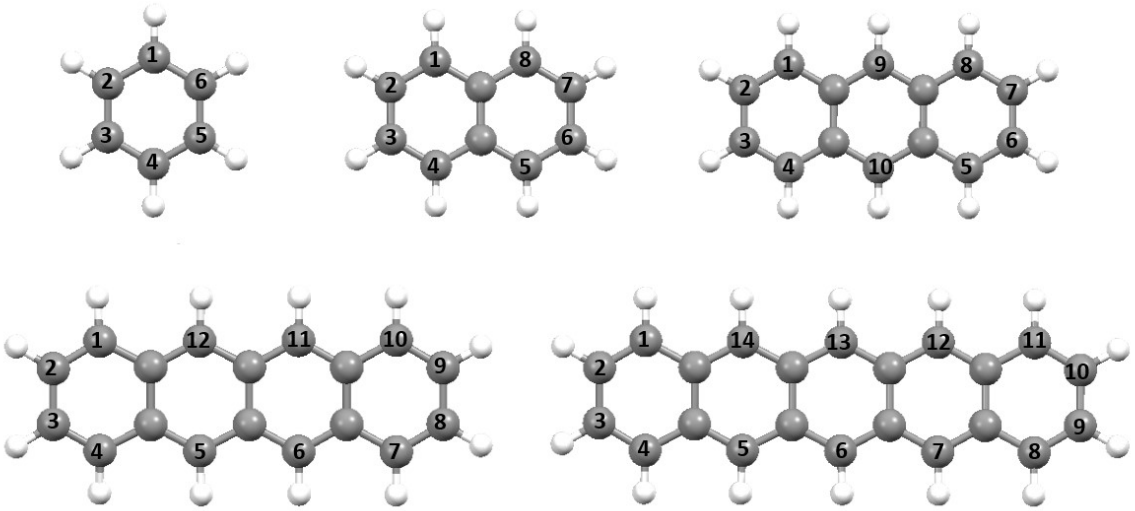

Figure S1. The numbering system in the aromatic molecules studied in this work.

2. Electrostatic Potential Maps for polycyclic nitroaromatic compounds with alifatic rings

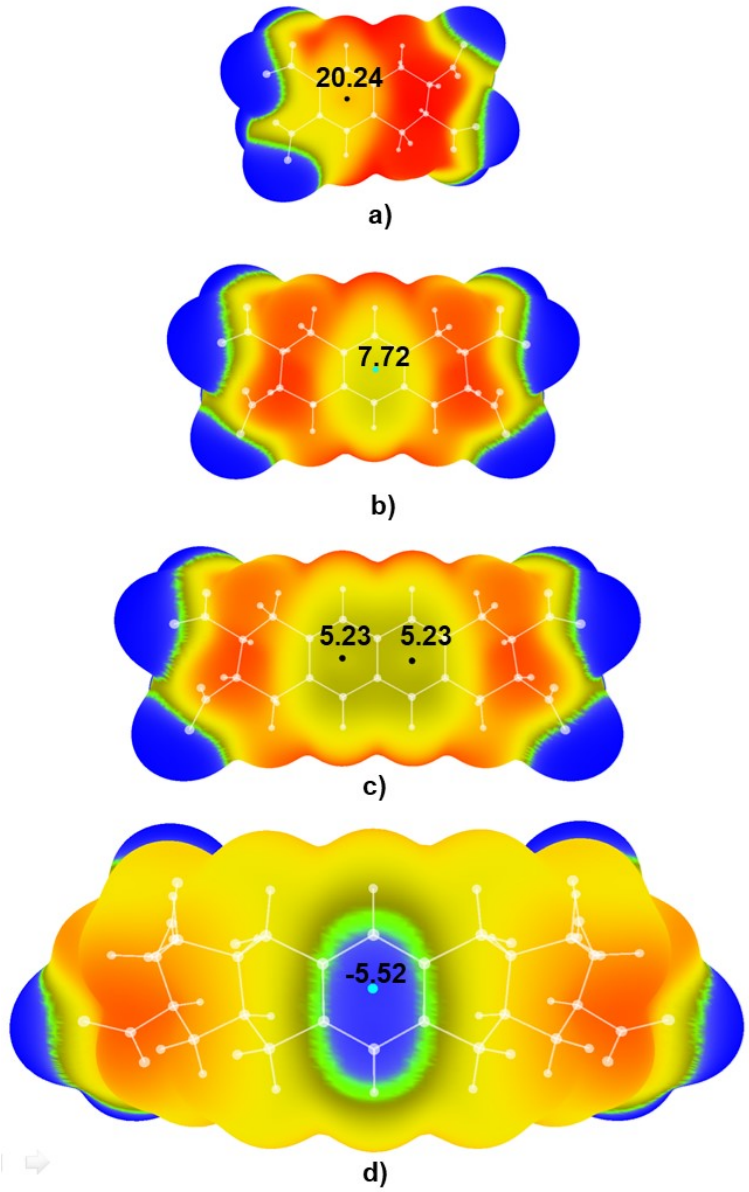

Figure S2. Electrostatic potential maps for the polycyclic nitroaromatic compounds with a) two rings (one aromatic ring (left) and one aliphatic ring (right), b) three rings (one aromatic ring in the center and two aliphatic rings - one on each side), c) four rings (two condensed aromatic rings in the center and two aliphatic rings – one on each side) and d) five rings (one aromatic ring in the center and four aliphatic rings – two on each side). Values of energies in the critical points are given in kcal/mol. Colour ranges, in kcal/mol, are: red, greater than 25.10; yellow, from 0.00 to 25.10; green, from -2.13 to 0.00; blue, more negative than -2.13. Black dots refer to local maxima on the molecular surfaces.

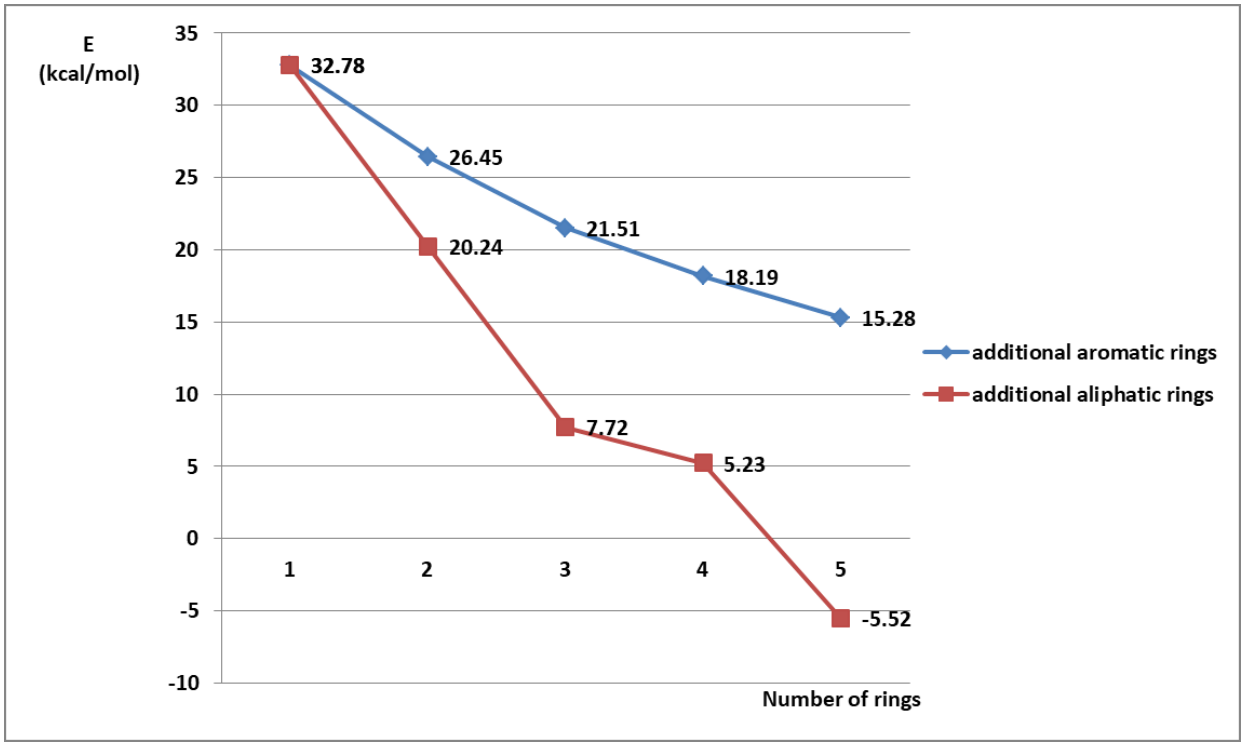

Figure S3. Electrostatic potential maps for the polycyclic nitroaromatic compounds with a) two rings (one aromatic ring and one aliphatic ring), b) three rings (one aromatic ring in the center and two aliphatic rings - one on each side), c) four rings (two condensed aromatic rings in the center and two aliphatic rings – one on each side) and d) five rings (one aromatic ring in the center and four aliphatic rings – two on each side).

3. Cartesian coordinates

Table S1. Cartesian coordinates for 1,2,4,5-tetranitrobenzene

atom	x	y	z
C	0.0000030000	-1.4016970000	0.0000020000
C	-1.2026570000	-0.6999580000	-0.0060310000
C	-1.2026610000	0.7001870000	0.0061150000
C	1.2026600000	-0.6999510000	0.0060350000
C	1.2026530000	0.7001920000	-0.0061190000
C	-0.0000070000	1.4018940000	-0.0000060000
N	-2.4576850000	-1.4986580000	-0.1139160000
O	-3.3021710000	-1.0783320000	-0.8982630000
O	-2.5057540000	-2.5273380000	0.5547630000
N	-2.4577970000	1.4986510000	0.1139410000
O	-2.5048740000	2.5290160000	-0.5522650000
O	-3.3037110000	1.0763660000	0.8957620000
N	2.4577900000	1.4986560000	-0.1139340000
O	3.3037610000	1.0763090000	-0.8956600000
O	2.5048150000	2.5290830000	0.5521790000
N	2.4576920000	-1.4986430000	0.1139100000
O	3.3021910000	-1.0782970000	0.8982320000
O	2.5057510000	-2.5273380000	-0.5547450000
H	-0.0000010000	-2.4924250000	0.0000000000
H	-0.0000040000	2.4926250000	-0.0000100000

Table S2. Cartesian coordinates for 1,4,5,8-tetranitronaphthalene

atom	x	y	z
C	1.3801720000	1.2631390000	-0.1369700000
C	0.7219580000	0.0000130000	0.0000420000
C	-0.7219620000	-0.0000040000	0.0000300000
C	-1.3802030000	1.2631140000	0.1369680000
C	-0.6971180000	2.4582590000	0.0915240000
C	0.6970630000	2.4582730000	-0.0915740000
C	1.3801980000	-1.2631070000	0.1369860000
C	0.6971140000	-2.4582540000	0.0915390000
C	-0.6970700000	-2.4582630000	-0.0915480000
C	-1.3801800000	-1.2631300000	-0.1369430000
N	2.8156080000	1.3660530000	-0.5314110000
O	3.2235170000	0.5107860000	-1.3211920000
O	3.4485970000	2.3303850000	-0.1144300000
N	-2.8156390000	1.3660110000	0.5314040000
O	-3.4486290000	2.3303480000	0.1144310000
O	-3.2235180000	0.5107860000	1.3212460000
N	2.8156460000	-1.3660190000	0.5313860000
O	3.2235550000	-0.5107650000	1.3211770000
O	3.4485970000	-2.3303900000	0.1144490000
N	-2.8156140000	-1.3660380000	-0.5314000000
O	-3.2235020000	-0.5107890000	-1.3212100000
O	-3.4485970000	-2.3304000000	-0.1144740000
H	-1.2557460000	3.3891540000	0.1909210000
H	1.2556650000	3.3891790000	-0.1910160000
H	1.2557400000	-3.3891500000	0.1909270000
H	-1.2556760000	-3.3891660000	-0.1909890000

Table S3. Cartesian coordinates for 2,3,6,7-tetranitronaphthalene

atom	x	y	z
C	1.2397860000	1.4098800000	-0.0080400000
C	-0.0000330000	0.7189650000	-0.0000450000
C	-0.0000200000	-0.7189040000	0.0000380000
C	1.2398090000	-1.4098160000	0.0080480000
C	2.4254550000	-0.7091570000	0.0113610000
C	2.4254420000	0.7092250000	-0.0113830000
C	-1.2398630000	1.4098730000	0.0079160000
C	-2.4255070000	0.7092150000	0.0113420000
C	-2.4254900000	-0.7091890000	-0.0113180000
C	-1.2398450000	-1.4098320000	-0.0079180000
N	-3.6824400000	1.4891350000	0.1829490000
O	-3.7556020000	2.5612260000	-0.4132550000
O	-4.5121220000	1.0146340000	0.9551910000
N	-3.6824430000	-1.4891870000	-0.1829360000
O	-4.5118510000	-1.0150030000	-0.9556520000
O	-3.7557880000	-2.5609910000	0.4136990000
N	3.6823990000	1.4890960000	-0.1829530000
O	3.7556270000	2.5611620000	0.4132510000
O	4.5121300000	1.0145090000	-0.9551190000
N	3.6824690000	-1.4890900000	0.1829470000
O	3.7560090000	-2.5607760000	-0.4138630000
O	4.5118190000	-1.0149290000	0.9557380000
H	1.2718930000	2.5007950000	-0.0243620000
H	1.2718660000	-2.5007290000	0.0243680000
H	-1.2719520000	2.5007920000	0.0241800000
H	-1.2718840000	-2.5007510000	-0.0241790000

Table S4. Cartesian coordinates for 1,4,9,10-tetranitroanthracene

atom	x	y	z
C	-1.3842550000	-1.8668210000	-0.1102230000
C	-0.7269330000	-0.5896740000	0.0025020000
C	-1.3870160000	0.6538870000	0.1248090000
C	-0.7202880000	1.8965690000	0.0946740000
C	-1.3911710000	3.1543900000	0.2333220000
C	-0.6985950000	4.3360110000	0.1276520000
C	0.6984430000	4.3359710000	-0.1290540000
C	1.3910220000	3.1543010000	-0.2341310000
C	0.7201330000	1.8965540000	-0.0949120000
C	1.3869620000	0.6539310000	-0.1244900000
C	0.7269680000	-0.5896760000	-0.0025000000
C	1.3842580000	-1.8668920000	0.1097780000
C	0.7010620000	-3.0567030000	0.0701520000
C	-0.7011000000	-3.0566680000	-0.0710660000
N	-2.8272360000	-2.0029020000	-0.4630380000
O	-3.2507270000	-1.2200360000	-1.3170990000
O	-3.4513440000	-2.9274540000	0.0489440000
N	2.8272090000	-2.0031620000	0.4625560000
O	3.2505480000	-1.2208620000	1.3172160000
O	3.4514130000	-2.9273320000	-0.0499950000
N	-2.8432320000	0.6686430000	0.4428740000
O	-3.5819120000	1.3990990000	-0.2114000000
O	-3.1821280000	-0.0384020000	1.3962680000
N	2.8433960000	0.6690540000	-0.4416010000
O	3.1830220000	-0.0372810000	-1.3952390000
O	3.5814360000	1.3991740000	0.2137520000
H	-1.2316540000	5.2833350000	0.2291830000
H	1.2314720000	5.2832540000	-0.2311080000
H	1.2592590000	-3.9896310000	0.1486250000
H	-1.2592980000	-3.9895550000	-0.1499830000
H	-2.4671470000	3.1724730000	0.3914590000
H	2.4669920000	3.1723750000	-0.3923560000

Table S5. Cartesian coordinates for 1,4,5,8-tetranitroanthracene

atom	x	y	z
C	2.5024240000	1.3924500000	0.0268060000
C	1.2275520000	0.7273320000	0.0192560000
C	0.0001940000	1.4078010000	-0.0000120000
C	-1.2273230000	0.7276440000	-0.0192190000
C	-2.5019520000	1.3932070000	-0.0267670000
C	-3.6933330000	0.7062110000	-0.0009540000
C	-3.6935870000	-0.7049070000	0.0007430000
C	-2.5025080000	-1.3924300000	0.0267310000
C	-1.2275770000	-0.7273770000	0.0192750000
C	-0.0002210000	-1.4078450000	0.0000860000
C	1.2273220000	-0.7277000000	-0.0191650000
C	2.5019960000	-1.3931890000	-0.0266500000
C	3.6933400000	-0.7061040000	-0.0007210000
C	3.6935500000	0.7050160000	0.0009850000
N	2.6237800000	2.8777820000	0.0864990000
O	1.7826370000	3.4980240000	0.7414260000
O	3.5857170000	3.3776260000	-0.4978890000
N	2.6229330000	-2.8785910000	-0.0865740000
O	1.7818360000	-3.4984860000	-0.7418660000
O	3.5845560000	-3.3788790000	0.4979650000
N	-2.6226560000	2.8785530000	-0.0864960000
O	-3.5841700000	3.3788650000	0.4981910000
O	-1.7814890000	3.4983060000	-0.7418580000
N	-2.6240310000	-2.8777460000	0.0865430000
O	-3.5861740000	-3.3775040000	-0.4975890000
O	-1.7828340000	-3.4980600000	0.7413360000
H	0.0003390000	2.4927550000	-0.0000570000
H	-0.0003970000	-2.4927910000	0.0001420000
H	-4.6283630000	1.2658260000	0.0199100000
H	-4.6288100000	-1.2642000000	-0.0201990000
H	4.6283730000	-1.2657030000	0.0201410000
H	4.6287600000	1.2643310000	-0.0198500000

Table S6. Cartesian coordinates for 2,3,6,7-tetranitroanthracene

atom	x	y	z
C	2.4733820000	-1.4107700000	0.0155320000
C	1.2223600000	-0.7244470000	-0.0001500000
C	0.0000350000	-1.4147830000	-0.0000990000
C	-1.2223210000	-0.7244680000	-0.0000310000
C	-2.4732870000	-1.4108520000	-0.0157510000
C	-3.6544310000	-0.7136130000	-0.0161720000
C	-3.6544750000	0.7134530000	0.0160590000
C	-2.4733800000	1.4107650000	0.0155230000
C	-1.2223640000	0.7244380000	-0.0001560000
C	-0.0000300000	1.4147730000	-0.0001010000
C	1.2223180000	0.7244580000	-0.0000200000
C	2.4732940000	1.4108370000	-0.0157150000
C	3.6544360000	0.7136040000	-0.0161500000
C	3.6544800000	-0.7134690000	0.0160760000
N	-4.9075190000	-1.4860660000	-0.2219040000
O	-5.7345680000	-0.9823820000	-0.9802870000
O	-4.9870450000	-2.5825010000	0.3292090000
N	-4.9075350000	1.4859540000	0.2220050000
O	-4.9879580000	2.5814280000	-0.3308240000
O	-5.7334080000	0.9832970000	0.9823220000
N	4.9075450000	-1.4859600000	0.2220100000
O	4.9878750000	-2.5815470000	-0.3306190000
O	5.7335510000	-0.9831600000	0.9820920000
N	4.9075140000	1.4860730000	-0.2218930000
O	5.7344480000	0.9824940000	-0.9804710000
O	4.9870890000	2.5824310000	0.3293620000
H	2.5074010000	-2.5015130000	0.0461050000
H	0.0000260000	-2.5077180000	-0.0001140000
H	-2.5073570000	-2.5015920000	-0.0464410000
H	-2.5073980000	2.5015090000	0.0460860000
H	-0.0000280000	2.5077080000	-0.0001110000
H	2.5073470000	2.5015770000	-0.0463850000

Table S7. Cartesian coordinates for 1,4,5,12-tetranitrotetracene

atom	x	y	z
C	2.6569100000	1.3881170000	0.0185970000
C	1.3732090000	0.7329100000	-0.0150200000
C	0.1342750000	1.3943060000	0.0282420000
C	-1.1201780000	0.7302330000	-0.0362830000
C	-2.3597810000	1.4087040000	-0.0311030000
C	-2.3597480000	-1.4087420000	-0.0307490000
C	-1.1201450000	-0.7302560000	-0.0361880000
C	0.1343150000	-1.3943060000	0.0281540000
C	1.3732370000	-0.7329030000	-0.0150440000
C	2.6569750000	-1.3880360000	0.0186100000
C	3.8303050000	-0.7055000000	0.2193070000
C	3.8302900000	0.7056640000	0.2192730000
C	-4.8312870000	1.4158330000	-0.0356430000
C	-6.0126390000	0.7150240000	-0.0364370000
C	-6.0126180000	-0.7151700000	-0.0361150000
C	-3.5770860000	0.7245860000	-0.0309740000
C	-3.5770620000	-0.7246460000	-0.0307100000
C	-4.8312440000	-1.4159400000	-0.0350490000
N	2.8384340000	-2.8240880000	-0.3351820000
O	3.7021990000	-3.4532640000	0.2695210000
O	2.1543680000	-3.2394680000	-1.2738640000
N	0.1061620000	-2.8524090000	0.3272610000
O	-0.5566000000	-3.5864220000	-0.4018770000
O	0.7293400000	-3.2039740000	1.3323510000
N	2.8382350000	2.8241930000	-0.3352410000
O	3.7019980000	3.4534480000	0.2693690000
O	2.1540790000	3.2395170000	-1.2738920000
N	0.1060800000	2.8523420000	0.3275270000
O	0.7293020000	3.2037950000	1.3326310000
O	-0.5567150000	3.5864470000	-0.4014870000
H	-4.8274600000	2.5084410000	-0.0383350000
H	-4.8273860000	-2.5085480000	-0.0372870000
H	-2.3759160000	2.4972200000	-0.0507470000
H	-2.3759420000	-2.4972600000	-0.0501380000
H	4.7624060000	-1.2672950000	0.2821620000
H	4.7624010000	1.2674440000	0.2820140000
H	-6.9653260000	1.2489330000	-0.0390230000
H	-6.9652900000	-1.2491080000	-0.0384230000

Table S8. Cartesian coordinates for 5,6,11,12-tetranitrotetracene

atom	x	y	z
C	3.7576350000	1.4033240000	-0.1495290000
C	2.4967350000	0.7240390000	-0.0556900000
C	1.2593780000	1.3886240000	-0.0769370000
C	-0.0000030000	0.7310550000	0.0000090000
C	-1.2593940000	1.3886070000	0.0769200000
C	-1.2594100000	-1.3886840000	-0.0768560000
C	0.0000070000	-0.7311440000	0.0000320000
C	1.2594340000	-1.3886630000	0.0769320000
C	2.4967670000	-0.7240180000	0.0555750000
C	3.7577090000	-1.4032320000	0.1493870000
C	4.9373750000	-0.7067610000	0.0843530000
C	4.9373380000	0.7069150000	-0.0845430000
C	-3.7576470000	1.4032840000	0.1494630000
C	-4.9373420000	0.7068610000	0.0844770000
C	-4.9373610000	-0.7068210000	-0.0843720000
C	-2.4967410000	0.7240060000	0.0556770000
C	-2.4967530000	-0.7240550000	-0.0555390000
C	-3.7576880000	-1.4032830000	-0.1493580000
N	1.3206500000	2.8535660000	-0.3353880000
O	1.9619990000	3.5577070000	0.4410640000
O	0.7592640000	3.2323640000	-1.3664550000
N	1.3208320000	-2.8535680000	0.3355710000
O	1.9619010000	-3.5578180000	-0.4410130000
O	0.7597480000	-3.2322460000	1.3668470000
N	-1.3206980000	2.8535590000	0.3353040000
O	-0.7593460000	3.2324140000	1.3663680000
O	-1.9620530000	3.5576490000	-0.4411900000
N	-1.3207750000	-2.8535970000	-0.3354620000
O	-0.7596970000	-3.2322830000	-1.3667380000
O	-1.9618570000	-3.5578390000	0.4411190000
H	3.7772340000	2.4871260000	-0.2451860000
H	3.7773690000	-2.4870300000	0.2450660000
H	5.8851770000	-1.2443260000	0.1517480000
H	5.8851120000	1.2445280000	-0.1519600000
H	-3.7772560000	2.4870900000	0.2450780000
H	-5.8851220000	1.2444680000	0.1518540000
H	-5.8851570000	-1.2443960000	-0.1517730000
H	-3.7773370000	-2.4870830000	-0.2450060000

Table S9. Cartesian coordinates for 1,4,7,10-tetranitrotetracene

atom	x	y	z
C	-3.7347640000	-1.3945850000	0.0001270000
C	-2.4543670000	-0.7346430000	0.0367260000
C	-1.2308440000	-1.4127120000	0.0258930000
C	-0.0013890000	-0.7216590000	0.0128060000
C	1.2279700000	-1.4125180000	-0.0091550000
C	1.2284510000	1.4131010000	0.0107210000
C	-0.0012580000	0.7223550000	0.0164370000
C	-1.2307770000	1.4134300000	0.0293180000
C	-2.4544050000	0.7353540000	0.0363560000
C	-3.7350790000	1.3947660000	-0.0036810000
C	-4.9221260000	0.7062260000	-0.0780590000
C	-4.9220670000	-0.7066960000	-0.0755540000
C	3.7329050000	-1.3953280000	-0.0161920000
C	4.9222880000	-0.7067590000	-0.0182800000
C	4.9221690000	0.7051590000	-0.0634100000
C	2.4519500000	-0.7350310000	-0.0232240000
C	2.4524160000	0.7354630000	-0.0054350000
C	3.7335460000	1.3948040000	-0.0416910000
N	-3.8625770000	-2.8793530000	0.0487990000
O	-3.0213440000	-3.5122470000	0.6935180000
O	-4.8267530000	-3.3738590000	-0.5379930000
N	-3.8637170000	2.8796400000	0.0383770000
O	-4.8272170000	3.3709730000	-0.5523240000
O	-3.0237350000	3.5159950000	0.6812170000
N	3.8628260000	-2.8810830000	-0.0206800000
O	4.8430390000	-3.3537460000	0.5570960000
O	3.0082090000	-3.5371010000	-0.6233460000
N	3.8652260000	2.8804950000	-0.0461260000
O	3.0226170000	3.5407530000	0.5685060000
O	4.8351440000	3.3492010000	-0.6444030000
H	-1.2182510000	-2.5011040000	0.0368050000
H	1.2159070000	-2.5004730000	-0.0371240000
H	1.2174570000	2.5009130000	0.0439250000
H	-1.2183840000	2.5017710000	0.0450290000
H	-5.8559800000	1.2648080000	-0.1372510000
H	-5.8558660000	-1.2656580000	-0.1319940000
H	5.8580580000	-1.2642180000	0.0153530000
H	5.8573460000	1.2619550000	-0.1177150000

Table S10. Cartesian coordinates for 2,3,8,9-tetranitrotetracene

atom	x	y	z
C	3.7055140000	1.4120170000	-0.0185620000
C	2.4504900000	0.7272370000	-0.0003870000
C	1.2346030000	1.4149940000	-0.0030760000
C	-0.0000040000	0.7284940000	-0.0000290000
C	-1.2346060000	1.4149950000	0.0030130000
C	-1.2346030000	-1.4149920000	-0.0030610000
C	-0.0000020000	-0.7284920000	-0.0000240000
C	1.2346060000	-1.4149940000	0.0030200000
C	2.4504920000	-0.7272400000	0.0003420000
C	3.7055260000	-1.4120100000	0.0185220000
C	4.8848070000	-0.7158400000	0.0187250000
C	4.8848120000	0.7158640000	-0.0187420000
C	-3.7055250000	1.4120110000	0.0185230000
C	-4.8848110000	0.7158440000	0.0187300000
C	-4.8848140000	-0.7158600000	-0.0187350000
C	-2.4504970000	0.7272370000	0.0003410000
C	-2.4504950000	-0.7272330000	-0.0003760000
C	-3.7055170000	-1.4120140000	-0.0185470000
N	-6.1347620000	1.4839480000	0.2442580000
O	-6.2174780000	2.5932150000	-0.2816630000
O	-6.9606480000	0.9649070000	0.9947620000
N	6.1347710000	1.4839480000	-0.2442180000
O	6.2173940000	2.5933360000	0.2814780000
O	6.9608310000	0.9647910000	-0.9944520000
N	6.1347620000	-1.4839470000	0.2442500000
O	6.9606090000	-0.9649430000	0.9948190000
O	6.2175030000	-2.5931830000	-0.2817280000
N	-6.1347670000	-1.4839510000	-0.2442260000
O	-6.9607750000	-0.9648370000	-0.9945470000
O	-6.2174220000	-2.5932990000	0.2815450000
H	3.7403460000	2.5025410000	-0.0568970000
H	3.7403510000	-2.5025350000	0.0568350000
H	-3.7403520000	2.5025360000	0.0568400000
H	-3.7403450000	-2.5025380000	-0.0568740000
H	1.2359440000	2.5082780000	-0.0058690000
H	-1.2359420000	2.5082790000	0.0057880000
H	-1.2359430000	-2.5082760000	-0.0058450000
H	1.2359420000	-2.5082780000	0.0058020000

Table S11. Cartesian coordinates for 1,4,5,14-tetranitropentacene

atom	x	y	z
C	5.1337650000	-0.7194850000	0.1241740000
C	5.1337810000	0.7193600000	-0.1240710000
C	6.3935490000	-1.3947390000	0.2401400000
C	3.9178630000	-1.3947240000	0.2406860000
C	6.3935790000	1.3946110000	-0.2399230000
C	3.9178940000	1.3946010000	-0.2406890000
C	7.5743920000	0.7054930000	-0.1210700000
C	7.5743760000	-0.7056260000	0.1213860000
C	2.6813710000	-0.7173330000	0.1243830000
C	2.6813870000	0.7172090000	-0.1244910000
C	1.4551340000	-1.3934670000	0.2247480000
C	1.4551690000	1.3933470000	-0.2249670000
C	0.2226280000	-0.7269370000	0.0964340000
C	0.2226480000	0.7268190000	-0.0967320000
C	-1.0345030000	-1.3920460000	0.1233850000
C	-1.0344110000	1.3920240000	-0.1236940000
C	-2.2667050000	-0.7312490000	-0.0016520000
C	-2.2666710000	0.7313160000	0.0014560000
C	-3.5487370000	-1.3846300000	-0.1353600000
C	-3.5486360000	1.3846880000	0.1356850000
C	-4.7351620000	-0.7012600000	-0.0870670000
C	-4.7350960000	0.7013110000	0.0882110000
N	-1.0274260000	2.8513070000	-0.4220950000
O	-0.2865300000	3.5845510000	0.2281840000
O	-1.7516500000	3.2044750000	-1.3577090000
N	-1.0276760000	-2.8513300000	0.4218910000
O	-1.7519880000	-3.2043610000	1.3574540000
O	-0.2867980000	-3.5846490000	-0.2283200000
N	-3.6855780000	2.8177930000	0.5260160000
O	-2.8907710000	3.2267980000	1.3763580000
O	-4.6218480000	3.4500750000	0.0449150000
N	-3.6858120000	-2.8176070000	-0.5260770000
O	-4.6221260000	-3.4499540000	-0.0450930000
O	-2.8910790000	-3.2264830000	-1.3765340000
H	6.3922520000	-2.4718300000	0.4256260000
H	6.3922990000	2.4717020000	-0.4254060000
H	8.5271240000	1.2317890000	-0.2113680000
H	8.5270960000	-1.2319290000	0.2117670000
H	1.4745680000	-2.4729010000	0.3646600000
H	1.4746170000	2.4727780000	-0.3649230000
H	-5.6686470000	-1.2553050000	-0.1850780000
H	-5.6685280000	1.2553620000	0.1867040000

H	3.9156290000	-2.4728130000	0.4243170000
H	3.9156720000	2.4726920000	-0.4243110000

Table S12. Cartesian coordinates for 5,6,13,14-tetranitropentacene

atom	x	y	z
C	3.2660290000	0.7246230000	-0.0615960000
C	3.2659800000	-0.7248510000	0.0615590000
C	4.5287070000	1.4019000000	-0.1648790000
C	2.0312860000	1.3895050000	-0.0849220000
C	4.5286010000	-1.4022090000	0.1649710000
C	2.0311560000	-1.3896190000	0.0848010000
C	5.7073530000	-0.7066740000	0.0929610000
C	5.7074030000	0.7062730000	-0.0928500000
C	0.7677850000	0.7330980000	0.0004040000
C	0.7677300000	-0.7330750000	-0.0006580000
C	-0.4839780000	1.3912280000	0.0801960000
C	-0.4840830000	-1.3911020000	-0.0804520000
C	-1.7318160000	0.7278810000	0.0558430000
C	-1.7318580000	-0.7276930000	-0.0560900000
C	-2.9744800000	1.4029730000	0.1399440000
C	-2.9744970000	-1.4028040000	-0.1401040000
C	-4.1887520000	0.7219100000	0.0791970000
C	-4.1887690000	-0.7217610000	-0.0792310000
C	-5.4451320000	1.4082230000	0.1539130000
C	-5.4451520000	-1.4080740000	-0.1537790000
C	-6.6253240000	0.7118270000	0.0782360000
C	-6.6253340000	-0.7116780000	-0.0779340000
N	-0.5404200000	-2.8550100000	-0.3380650000
O	-1.1878510000	-3.5615320000	0.4322270000
O	0.0311860000	-3.2350470000	-1.3633290000
N	-0.5401160000	2.8550970000	0.3379190000
O	-1.1872810000	3.5618700000	-0.4323660000
O	0.0313980000	3.2349330000	1.3633200000
N	2.0914980000	-2.8510180000	0.3605100000
O	1.5215090000	-3.2193560000	1.3909620000
O	2.7397550000	-3.5644710000	-0.4021490000
N	2.0918650000	2.8509290000	-0.3603800000
O	2.7402300000	3.5641750000	0.4023720000
O	1.5219040000	3.2195410000	-1.3907610000
H	4.5484890000	2.4845560000	-0.2721650000
H	4.5482720000	-2.4848550000	0.2723550000
H	6.6553380000	-1.2430640000	0.1670730000

H	6.6554230000	1.2426080000	-0.1669270000
H	-7.5782830000	1.2421280000	0.1362010000
H	-7.5783020000	-1.2419790000	-0.1357540000
H	-2.9957810000	2.4888850000	0.2209630000
H	-2.9957340000	-2.4887230000	-0.2211490000
H	-5.4415550000	2.4946220000	0.2706140000
H	-5.4415970000	-2.4944740000	-0.2704780000

Table S13. Cartesian coordinates for 5,7,12,14-tetranitropentacene

atom	x	y	z
C	-3.7195950000	0.7295330000	-0.0206720000
C	-3.7196240000	-0.7295230000	-0.0209800000
C	-4.9804460000	1.4140860000	-0.0487980000
C	-2.4850250000	1.3926360000	-0.0228740000
C	-4.9805220000	-1.4139750000	-0.0495440000
C	-2.4850810000	-1.3926960000	-0.0233520000
C	-6.1584920000	-0.7132140000	-0.0836970000
C	-6.1584610000	0.7134160000	-0.0832890000
C	-1.2278060000	0.7286820000	-0.0276300000
C	-1.2278410000	-0.7287300000	-0.0277430000
C	-0.0000120000	1.4103510000	-0.0000900000
C	0.0000150000	-1.4102570000	-0.0000220000
C	1.2278570000	0.7288180000	0.0275100000
C	1.2277980000	-0.7285750000	0.0276430000
C	2.4851180000	1.3927440000	0.0227940000
C	2.4849650000	-1.3926070000	0.0232950000
C	3.7196670000	0.7295100000	0.0207240000
C	3.7195580000	-0.7295470000	0.0210450000
C	4.9806700000	1.4138030000	0.0490810000
C	4.9803180000	-1.4142550000	0.0496480000
C	6.1585600000	0.7129070000	0.0836170000
C	6.1584150000	-0.7137160000	0.0838860000
N	2.4867670000	-2.8758890000	0.0331040000
O	1.9110220000	-3.4299440000	0.9725940000
O	3.0652920000	-3.4459210000	-0.8938300000
N	2.4870560000	2.8761100000	0.0320290000
O	1.9112000000	3.4306490000	0.9711640000
O	3.0658140000	3.4457650000	-0.8949910000
N	-2.4870180000	-2.8760150000	-0.0331900000
O	-1.9103370000	-3.4301240000	-0.9720930000
O	-3.0664580000	-3.4460220000	0.8932000000
N	-2.4869030000	2.8759960000	-0.0321750000

O	-1.9109280000	3.4303920000	-0.9713100000
O	-3.0655600000	3.4456150000	0.8949370000
H	-4.9949970000	2.5030630000	-0.0326660000
H	-4.9951460000	-2.5029570000	-0.0339820000
H	-7.1075770000	-1.2523070000	-0.1080170000
H	-7.1075240000	1.2525580000	-0.1072740000
H	-0.0000910000	2.4977840000	-0.0001490000
H	0.0000820000	-2.4976960000	-0.0000700000
H	4.9954880000	2.5027660000	0.0330900000
H	4.9947680000	-2.5032430000	0.0340890000
H	7.1076960000	1.2519170000	0.1077420000
H	7.1074230000	-1.2529370000	0.1082010000

Table S14. Cartesian coordinates for 1,4,8,11-tetranitropentacene

atom	x	y	z
C	3.6844330000	-0.7366040000	-0.0316690000
C	3.6844840000	0.7366030000	-0.0331270000
C	4.9665460000	-1.3956220000	0.0101700000
C	2.4633060000	-1.4129650000	-0.0251100000
C	4.9666750000	1.3955790000	0.0084000000
C	2.4633440000	1.4130160000	-0.0287350000
C	6.1529460000	0.7068960000	0.0855050000
C	6.1529010000	-0.7070240000	0.0862150000
C	1.2265550000	-0.7276940000	-0.0171560000
C	1.2265640000	0.7277840000	-0.0195470000
C	0.0012550000	-1.4171080000	-0.0065740000
C	0.0012390000	1.4172200000	-0.0130060000
C	-1.2239910000	-0.7275310000	0.0014300000
C	-1.2240170000	0.7276820000	-0.0025920000
C	-2.4606730000	-1.4126980000	0.0166020000
C	-2.4608110000	1.4128520000	-0.0018700000
C	-3.6822620000	-0.7368190000	0.0232230000
C	-3.6824100000	0.7369610000	0.0075530000
C	-4.9652100000	-1.3959690000	0.0075860000
C	-4.9651900000	1.3959740000	0.0391900000
C	-6.1535700000	-0.7065230000	0.0059990000
C	-6.1533570000	0.7062900000	0.0541940000
N	-5.0984980000	-2.8809750000	0.0056030000
O	-4.2429950000	-3.5434400000	0.6009570000
O	-6.0816910000	-3.3501450000	-0.5708820000
N	-5.0988040000	2.8809530000	0.0449800000
O	-6.0756970000	3.3488610000	0.6332120000

O	-4.2500510000	3.5448070000	-0.5583250000
N	5.0971250000	-2.8797570000	-0.0335900000
O	4.2539930000	-3.5183660000	-0.6711090000
O	6.0647360000	-3.3714980000	0.5507790000
N	5.0975390000	2.8796640000	-0.0363480000
O	4.2545160000	3.5181350000	-0.6741050000
O	6.0652780000	3.3715630000	0.5477430000
H	2.4536140000	-2.5014100000	-0.0369150000
H	2.4537880000	2.5014200000	-0.0435490000
H	7.0869570000	1.2651560000	0.1440270000
H	7.0868840000	-1.2653170000	0.1450170000
H	0.0011570000	-2.5104210000	-0.0054670000
H	0.0011180000	2.5105160000	-0.0187670000
H	-2.4516500000	-2.5006350000	0.0465110000
H	-2.4522800000	2.5007520000	-0.0330290000
H	-7.0895180000	-1.2631580000	-0.0337040000
H	-7.0888380000	1.2627780000	0.1050980000

Table S15. Cartesian coordinates for 2,3,9,10-tetranitropentacene

atom	**x**	**y**	**z**
C	0.7282210000	0.0322720000	-3.6803040000
C	-0.7280260000	-0.0324950000	-3.6802870000
C	1.4119790000	0.0433830000	-4.9372490000
C	1.4149080000	0.0596500000	-2.4676580000
C	-1.4118760000	-0.0432630000	-4.9371820000
C	-1.4146890000	-0.0600080000	-2.4676350000
C	-0.7172930000	-0.0118270000	-6.1159640000
C	0.7172780000	0.0123630000	-6.1159870000
C	0.7299920000	0.0318920000	-1.2279900000
C	-0.7297550000	-0.0322940000	-1.2279860000
C	1.4135410000	0.0623900000	0.0000000000
C	-1.4133070000	-0.0627880000	0.0000000000
C	0.7299920000	0.0318920000	1.2279900000
C	-0.7297550000	-0.0322940000	1.2279860000
C	1.4149080000	0.0596500000	2.4676580000
C	-1.4146890000	-0.0600080000	2.4676350000
C	0.7282210000	0.0322720000	3.6803040000
C	-0.7280260000	-0.0324950000	3.6802870000
C	1.4119790000	0.0433830000	4.9372490000
C	-1.4118760000	-0.0432630000	4.9371820000
C	0.7172780000	0.0123630000	6.1159870000
C	-0.7172930000	-0.0118270000	6.1159640000

N	-1.4932190000	0.1903090000	7.3633680000
O	-2.5865750000	-0.3691350000	7.4462600000
O	-0.9993400000	0.9572990000	8.1903150000
N	1.4930830000	-0.1900040000	7.3634700000
O	2.5866650000	0.3688740000	7.4465020000
O	0.9986710000	-0.9568200000	8.1903220000
N	-1.4932190000	0.1903090000	-7.3633680000
O	-0.9993400000	0.9572990000	-8.1903150000
O	-2.5865750000	-0.3691350000	-7.4462600000
N	1.4930830000	-0.1900040000	-7.3634700000
O	0.9986710000	-0.9568200000	-8.1903220000
O	2.5866650000	0.3688740000	-7.4465020000
H	2.5031620000	0.0491710000	-4.9725650000
H	2.5073390000	0.1051360000	-2.4693890000
H	-2.5030590000	-0.0494450000	-4.9723390000
H	-2.5071260000	-0.1053970000	-2.4693380000
H	2.5060800000	0.1106590000	0.0000000000
H	-2.5058470000	-0.1110330000	0.0000000000
H	2.5073390000	0.1051360000	2.4693890000
H	-2.5071260000	-0.1053970000	2.4693380000
H	2.5031620000	0.0491710000	4.9725650000
H	-2.5030590000	-0.0494450000	4.9723390000