

Supplemental information

1.0 Total energies for all DFT calculations

	Closed shell restricted	Singlet unrestricted	Triplet unrestricted	Triplet restricted-open	Model
Fulminene	-1000.495302	-1000.495302	-1000.401658	-1000.398281	B3LYP/6-31g(d,p)
Hexacene	-1000.458642	-1000.45881	-1000.441285	-1000.43723	B3LYP/6-31g(d,p)
Zethrene	-923.0576062	-923.0576058	-923.029753	-923.024469	B3LYP/6-31g(d,p)
Uthrene	-922.9988346	-923.0224395	-923.0302767	-923.0226217	B3LYP/6-31g(d,p)
Triangulene	N.C.	-845.6194833	-845.6306501	-845.6226249	B3LYP/6-31g(d,p)

Fulminene	-999.9084356	-999.9084359	-999.8083351	-999.8002681	CAM-B3LYP/6-31g(d,p)
Hexacene	-999.8624695	-999.8667273	-999.8453742	-999.8374288	CAM-B3LYP/6-31g(d,p)
Zethrene	-922.5136961	-922.5136961	-922.4873616	-922.4763602	CAM-B3LYP/6-31g(d,p)
Uthrene	-922.441056	-922.4791934	-922.4914136	-922.4757001	CAM-B3LYP/6-31g(d,p)
Triangulene	-845.0850809	-845.1220831	-845.1399606	-845.1232147	CAM-B3LYP/6-31g(d,p)

Fulminene	-999.4096562	-999.4096562	-999.3157966	-999.3114248	HSE06/6-31g(d,p)
Hexacene	-999.3701944	-999.3719311	-999.3554736	-999.3504171	HSE06/6-31g(d,p)
Zethrene	-922.0591741	-922.059174	-922.0332122	-922.0263179	HSE06/6-31g(d,p)
Uthrene	N.C.	-922.0260061	-922.0351929	-922.0251611	HSE06/6-31g(d,p)
Triangulene	N.C.	-844.7101277	-844.7229774	-844.7124661	HSE06/6-31g(d,p)

Graphene*	-76.16057549				HSE06/6-31g(d,p)
Molecular Hydrogen	-1.167279086				HSE06/6-31g(d,p)

Table S1. Total energies in Hartree for all geometry optimized calculations at all levels.

*: Graphene has two carbon atoms per unit cell.

N.C.: Calculation Not Converged.

2.0 Molecular pictures of open-shell ground state geometries optimized at the CAM-B3LYP/6-31g(d,p) level

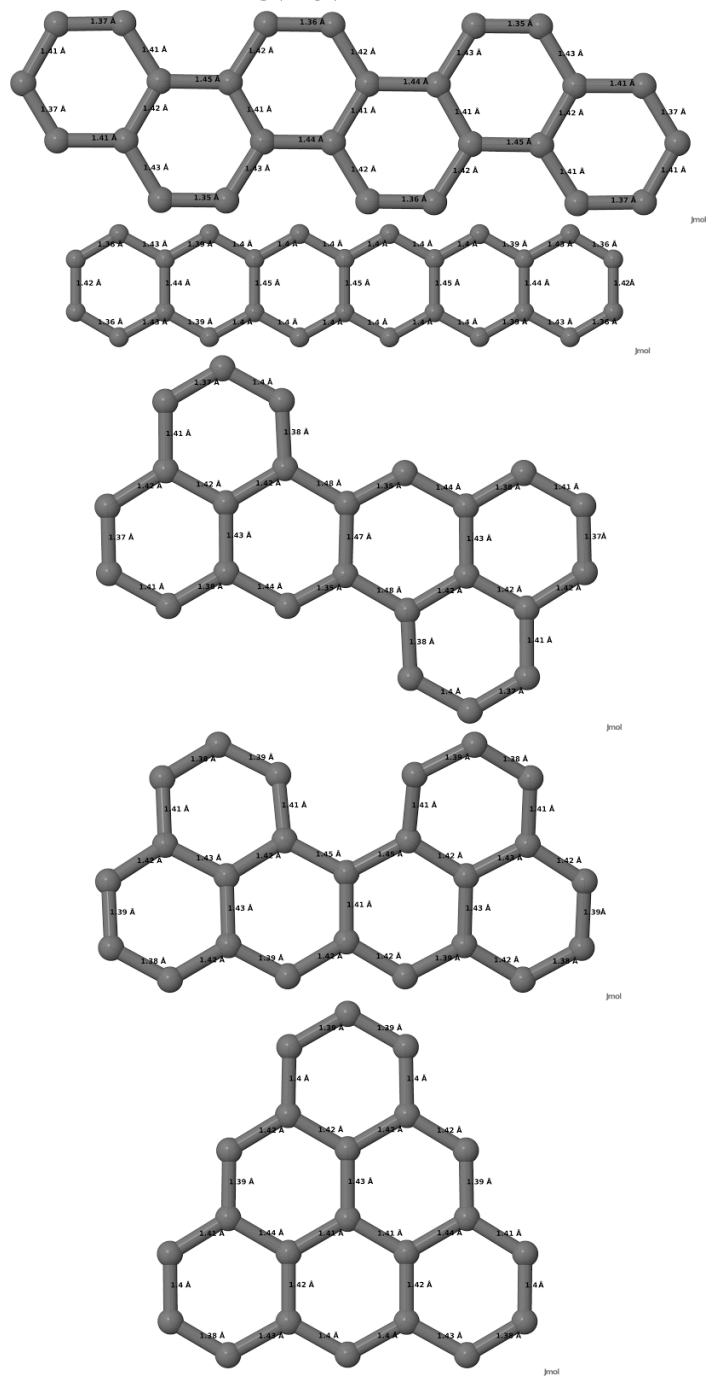


Figure S1. Geometries optimized at the CAM-B3LYP/6-31g(d,p) level singlet unrestricted

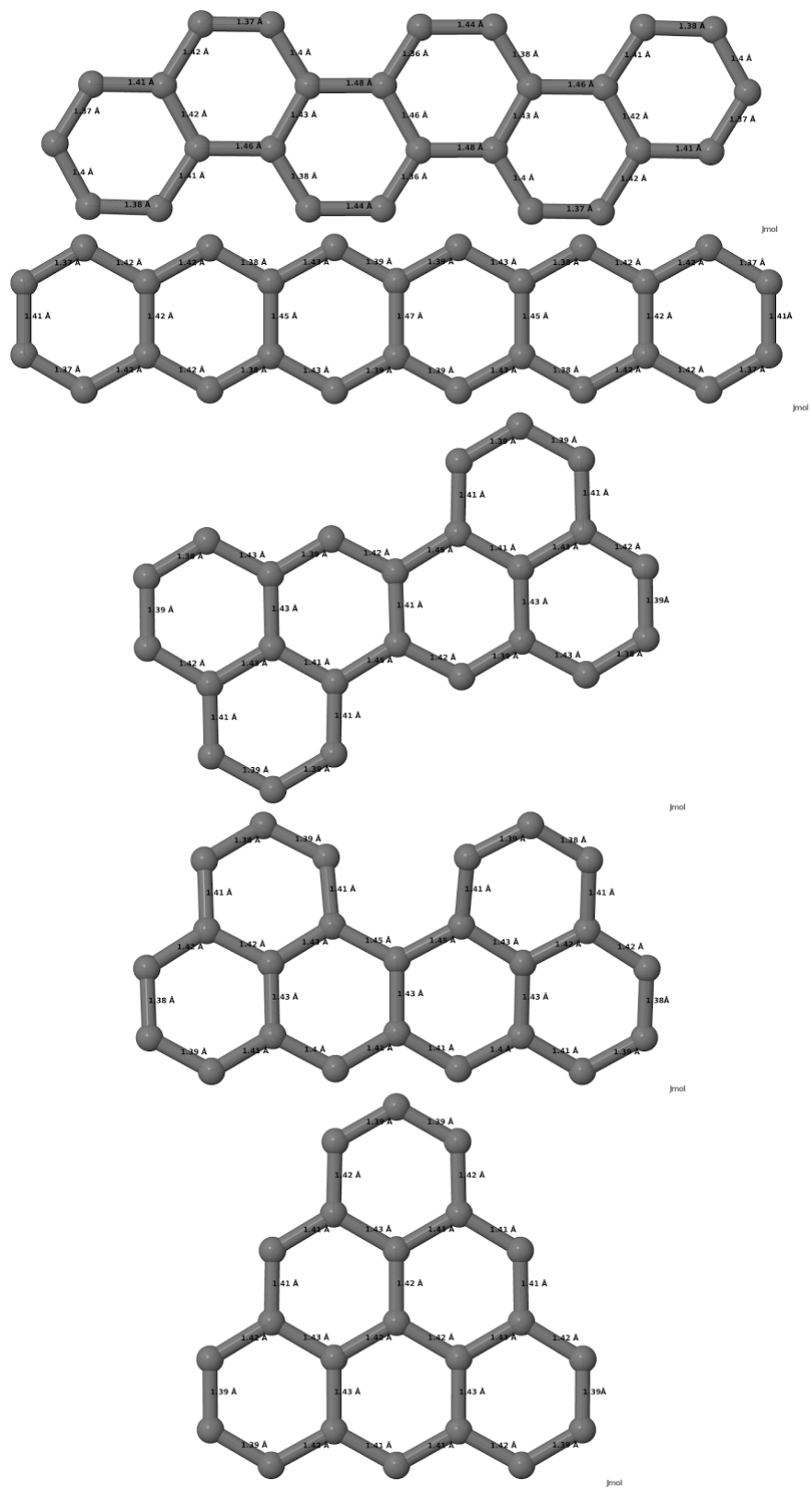


Figure S2. Geometries optimized at the CAM-B3LYP/6-31g(d,p) level triplet unrestricted

3.0 Geometries optimized at the CAM-B3LYP/6-31g(d,p) level, XYZ cartesian coordinates.

closed_shell_restricted_fulminene.xyz:

C	2.18901	-3.71591	0.00000
C	2.05902	-2.36793	0.00000
C	1.77287	0.56166	0.00000
C	1.64552	1.91477	0.00000
C	1.35562	4.86863	0.00000
C	1.19253	6.23318	0.00000
C	-0.09425	6.79788	0.00000
C	-1.19253	5.97581	0.00000
C	-2.18901	3.71591	0.00000
C	-2.05902	2.36793	0.00000
C	-1.77287	-0.56166	0.00000
C	-1.64552	-1.91477	0.00000
C	-1.35562	-4.86863	0.00000
C	-1.19253	-6.23318	0.00000
C	0.09425	-6.79788	0.00000
C	1.19253	-5.97581	0.00000
C	-1.04763	4.57205	0.00000
C	0.24458	3.99493	0.00000
C	-0.77335	1.73673	0.00000
C	0.37380	2.54991	0.00000
C	-0.63908	0.29810	0.00000
C	0.63908	-0.29810	0.00000
C	-0.37380	-2.54991	0.00000
C	0.77335	-1.73673	0.00000
C	-0.24458	-3.99493	0.00000
C	1.04763	-4.57205	0.00000
H	3.17575	-4.16923	0.00000
H	2.95581	-1.76297	0.00000
H	2.77042	0.14315	0.00000
H	2.54624	2.51496	0.00000
H	2.36172	4.46852	0.00000
H	2.06495	6.87846	0.00000
H	-0.21509	7.87608	0.00000
H	-2.19486	6.39403	0.00000
H	-3.17575	4.16923	0.00000
H	-2.95581	1.76297	0.00000
H	-2.77042	-0.14315	0.00000

H	-2.54624	-2.51496	0.00000
H	-2.36172	-4.46852	0.00000
H	-2.06495	-6.87846	0.00000
H	0.21509	-7.87608	0.00000
H	2.19486	-6.39403	0.00000

closed_shell_restricted_hexacene.xyz:

C	0.00000	7.31589	0.71805
C	0.00000	6.15068	1.40725
C	0.00000	4.88390	0.72499
C	0.00000	4.88390	-0.72499
C	0.00000	6.15068	-1.40725
C	0.00000	7.31589	-0.71805
C	0.00000	3.68642	1.40290
C	0.00000	3.68642	-1.40290
C	0.00000	2.44210	-0.72471
C	0.00000	2.44210	0.72471
C	0.00000	1.22836	1.40288
H	0.00000	1.22860	2.48947
C	0.00000	0.00000	0.72481
C	0.00000	0.00000	-0.72481
C	0.00000	1.22836	-1.40288
H	0.00000	3.68667	2.48960
H	0.00000	8.26352	1.24645
H	0.00000	6.14740	2.49317
H	0.00000	6.14740	-2.49317
H	0.00000	8.26352	-1.24645
H	0.00000	3.68667	-2.48960
H	0.00000	1.22860	-2.48947
C	0.00000	-1.22836	-1.40288
C	0.00000	-1.22836	1.40288
C	0.00000	-2.44210	0.72471
C	0.00000	-2.44210	-0.72471
H	0.00000	-1.22860	2.48947
H	0.00000	-1.22860	-2.48947
C	0.00000	-3.68642	-1.40290
C	0.00000	-3.68642	1.40290
C	0.00000	-4.88390	0.72499
C	0.00000	-4.88390	-0.72499
H	0.00000	-3.68667	-2.48960
H	0.00000	-3.68667	2.48960

C	0.00000	-6.15068	-1.40725
C	0.00000	-6.15068	1.40725
C	0.00000	-7.31589	-0.71805
H	0.00000	-8.26352	-1.24645
C	0.00000	-7.31589	0.71805
H	0.00000	-8.26352	1.24645
H	0.00000	-6.14740	-2.49317
H	0.00000	-6.14740	2.49317

closed_shell_restricted_triangulene.xyz:

C	0.00000	-1.20061	3.52216
C	0.00000	-1.22691	2.11565
C	0.00000	0.00000	1.40771
C	0.00000	1.22691	2.11565
C	0.00000	1.20061	3.52216
C	0.00000	0.00000	4.22002
H	0.00000	-2.14169	4.06506
H	0.00000	2.14169	4.06506
H	0.00000	0.00000	5.30396
C	0.00000	0.00000	-0.00705
C	0.00000	-1.23006	-0.71420
C	0.00000	-2.48090	0.00623
C	0.00000	-1.22383	-2.14639
C	0.00000	-3.70032	-0.70441
C	0.00000	-2.48494	-2.79778
C	0.00000	-3.67590	-2.08974
H	0.00000	-2.50257	-3.88296
H	0.00000	-4.61336	-2.63813
C	0.00000	1.23006	-0.71420
C	0.00000	1.22383	-2.14639
C	0.00000	2.48090	0.00623
C	0.00000	2.48494	-2.79778
C	0.00000	3.70032	-0.70441
C	0.00000	3.67590	-2.08974
H	0.00000	2.50257	-3.88296
H	0.00000	4.63655	-0.15740
H	0.00000	4.61336	-2.63813
C	0.00000	2.44081	1.40478
C	0.00000	-2.44081	1.40478
C	0.00000	0.00000	-2.82686
H	0.00000	3.37607	1.95828

H	0.00000	-3.37607	1.95828
H	0.00000	0.00000	-3.91206
H	0.00000	-4.63655	-0.15740

closed_shell_restricted_uthrene.xyz:

C	-0.17476	-1.23335	2.15623
C	0.17476	1.23335	2.15623
C	0.47700	3.68987	2.10195
C	0.44911	4.88657	1.39719
C	0.16454	4.91578	0.04284
C	-0.45706	3.68431	-2.00231
C	-0.78551	2.50587	-2.63693
C	-0.67961	1.29183	-1.95792
C	0.67961	-1.29183	-1.95792
C	0.78551	-2.50587	-2.63693
C	0.45706	-3.68431	-2.00231
C	-0.16454	-4.91578	0.04284
C	-0.44911	-4.88657	1.39719
C	-0.47700	-3.68987	2.10195
C	-0.08567	3.70605	-0.63925
C	0.00000	2.46966	0.05778
C	-0.20644	1.24678	-0.63496
C	0.00000	0.00000	0.06391
C	0.24407	2.45011	1.46803
C	0.00000	0.00000	1.49719
C	0.20644	-1.24678	-0.63496
C	0.00000	-2.46966	0.05778
C	0.08567	-3.70605	-0.63925
C	-0.24407	-2.45011	1.46803
H	-0.27632	-1.23123	3.23661
H	0.27632	1.23123	3.23661
H	0.66611	3.69780	3.17084
H	0.63720	5.81606	1.92564
H	0.11933	5.85377	-0.49992
H	-0.53179	4.62796	-2.53523
H	-1.14737	2.51917	-3.65923
H	-1.02165	0.38497	-2.43791
H	1.02165	-0.38497	-2.43791
H	1.14737	-2.51917	-3.65923
H	0.53179	-4.62796	-2.53523
H	-0.11933	-5.85377	-0.49992

H	-0.63720	-5.81606	1.92564
H	-0.66611	-3.69780	3.17084

closed_shell_restricted_zethrene.xyz:

C	-1.64983	0.78982	0.00000
C	-1.06713	-1.62278	0.00000
C	-0.34393	-3.98471	0.00000
C	0.71136	-4.93349	0.00000
C	2.01869	-4.52545	0.00000
C	2.37802	2.06840	0.00000
C	2.69186	3.43617	0.00000
C	1.69945	4.38161	0.00000
C	-0.71136	4.93349	0.00000
C	-2.01869	4.52545	0.00000
C	-2.33264	3.15491	0.00000
C	2.33264	-3.15491	0.00000
C	1.33662	-2.19737	0.00000
C	1.64983	-0.78982	0.00000
C	0.71136	0.18532	0.00000
C	-0.03047	-2.59946	0.00000
C	-0.71136	-0.18532	0.00000
C	1.06713	1.62278	0.00000
C	0.03047	2.59946	0.00000
C	0.34393	3.98471	0.00000
C	-1.33662	2.19737	0.00000
H	-2.70426	0.53868	0.00000
H	0.46155	-5.98998	0.00000
H	2.81894	-5.25817	0.00000
H	3.19738	1.36019	0.00000
H	3.73373	3.73939	0.00000
H	1.94009	5.44022	0.00000
H	-0.46155	5.98998	0.00000
H	-2.81894	5.25817	0.00000
H	-3.37158	2.83917	0.00000
C	-2.37802	-2.06840	0.00000
C	-1.69945	-4.38161	0.00000
C	-2.69186	-3.43617	0.00000
H	-3.73373	-3.73939	0.00000
H	-3.19738	-1.36019	0.00000
H	-1.94009	-5.44022	0.00000
H	2.70426	-0.53868	0.00000

H	3.37158	-2.83917	0.00000
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singlet_open_shell_unrestricted_fulminene.xyz:

C	2.18923	-3.71571	0.00000
C	2.05928	-2.36783	0.00000
C	1.77286	0.56193	0.00000
C	1.64540	1.91491	0.00000
C	1.35550	4.86820	0.00000
C	1.19254	6.23276	0.00000
C	-0.09416	6.79754	0.00000
C	-1.19254	5.97558	0.00000
C	-2.18923	3.71571	0.00000
C	-2.05928	2.36783	0.00000
C	-1.77286	-0.56193	0.00000
C	-1.64540	-1.91491	0.00000
C	-1.35550	-4.86820	0.00000
C	-1.19254	-6.23276	0.00000
C	0.09416	-6.79754	0.00000
C	1.19254	-5.97558	0.00000
C	-1.04773	4.57187	0.00000
C	0.24437	3.99476	0.00000
C	-0.77345	1.73662	0.00000
C	0.37354	2.54977	0.00000
C	-0.63910	0.29799	0.00000
C	0.63910	-0.29799	0.00000
C	-0.37354	-2.54977	0.00000
C	0.77345	-1.73662	0.00000
C	-0.24437	-3.99476	0.00000
C	1.04773	-4.57187	0.00000
H	3.17591	-4.16916	0.00000
H	2.95599	-1.76278	0.00000
H	2.77044	0.14356	0.00000
H	2.54597	2.51537	0.00000
H	2.36157	4.46791	0.00000
H	2.06506	6.87790	0.00000
H	-0.21502	7.87575	0.00000
H	-2.19481	6.39393	0.00000
H	-3.17591	4.16916	0.00000
H	-2.95599	1.76278	0.00000
H	-2.77044	-0.14356	0.00000
H	-2.54597	-2.51537	0.00000

H	-2.36157	-4.46791	0.00000
H	-2.06506	-6.87790	0.00000
H	0.21502	-7.87575	0.00000
H	2.19481	-6.39393	0.00000

singlet_open_shell_unrestricted_hexacene.xyz:

C	0.00000	7.33019	0.71203
C	0.00000	6.15502	1.40212
C	0.00000	4.90130	0.71917
C	0.00000	4.90130	-0.71917
C	0.00000	6.15502	-1.40212
C	0.00000	7.33019	-0.71203
C	0.00000	3.68551	1.40070
C	0.00000	3.68551	-1.40070
C	0.00000	2.45544	-0.72368
C	0.00000	2.45544	0.72368
C	0.00000	1.22710	1.40441
H	0.00000	1.22784	2.49083
C	0.00000	0.00000	0.72639
C	0.00000	0.00000	-0.72639
C	0.00000	1.22710	-1.40441
H	0.00000	3.68669	2.48735
H	0.00000	8.27550	1.24466
H	0.00000	6.15133	2.48811
H	0.00000	6.15133	-2.48811
H	0.00000	8.27550	-1.24466
H	0.00000	3.68669	-2.48735
H	0.00000	1.22784	-2.49083
C	0.00000	-1.22710	-1.40441
C	0.00000	-1.22710	1.40441
C	0.00000	-2.45544	0.72368
C	0.00000	-2.45544	-0.72368
H	0.00000	-1.22784	2.49083
H	0.00000	-1.22784	-2.49083
C	0.00000	-3.68551	-1.40070
C	0.00000	-3.68551	1.40070
C	0.00000	-4.90130	0.71917
C	0.00000	-4.90130	-0.71917
H	0.00000	-3.68669	-2.48735
H	0.00000	-3.68669	2.48735
C	0.00000	-6.15502	-1.40212

C	0.00000	-6.15502	1.40212
C	0.00000	-7.33019	-0.71203
H	0.00000	-8.27550	-1.24466
C	0.00000	-7.33019	0.71203
H	0.00000	-8.27550	1.24466
H	0.00000	-6.15133	-2.48811
H	0.00000	-6.15133	2.48811

singlet_open_shell_unrestricted_triangulene.xyz:

C	0.00000	1.20516	-3.54169
C	0.00000	1.23035	-2.13811
C	0.00000	0.00000	-1.42947
C	0.00000	-1.23035	-2.13811
C	0.00000	-1.20516	-3.54169
C	0.00000	0.00000	-4.22853
H	0.00000	2.14463	-4.08566
H	0.00000	-2.14463	-4.08566
H	0.00000	0.00000	-5.31371
C	0.00000	0.00000	0.00256
C	0.00000	1.22260	0.70943
C	0.00000	2.46974	-0.01034
C	0.00000	1.22075	2.12981
C	0.00000	3.67563	0.72898
C	0.00000	2.47356	2.82112
C	0.00000	3.66215	2.12423
H	0.00000	2.46939	3.90633
H	0.00000	4.60263	2.66586
C	0.00000	-1.22260	0.70943
C	0.00000	-1.22075	2.12981
C	0.00000	-2.46974	-0.01034
C	0.00000	-2.47356	2.82112
C	0.00000	-3.67563	0.72898
C	0.00000	-3.66215	2.12423
H	0.00000	-2.46939	3.90633
H	0.00000	-4.61857	0.19168
H	0.00000	-4.60263	2.66586
C	0.00000	-2.44942	-1.40394
C	0.00000	2.44942	-1.40394
C	0.00000	0.00000	2.80979
H	0.00000	-3.38854	-1.94952
H	0.00000	3.38854	-1.94952

H	0.00000	0.00000	3.89627
H	0.00000	4.61857	0.19168

singlet_open_shell_unrestricted_uthrene.xyz:

C	-0.13003	-1.21522	2.10409
C	0.13003	1.21522	2.10409
C	0.42795	3.65260	2.17578
C	0.44093	4.87038	1.51774
C	0.22439	4.93052	0.14942
C	-0.29794	3.81057	-1.98168
C	-0.59498	2.65158	-2.67419
C	-0.52340	1.41236	-2.05167
C	0.52340	-1.41236	-2.05167
C	0.59498	-2.65158	-2.67419
C	0.29794	-3.81057	-1.98168
C	-0.22439	-4.93052	0.14942
C	-0.44093	-4.87038	1.51774
C	-0.42795	-3.65260	2.17578
C	0.00000	3.75115	-0.60961
C	0.04637	2.48171	0.03897
C	-0.13373	1.28074	-0.70255
C	0.00000	0.00000	-0.02542
C	0.22429	2.44040	1.46154
C	0.00000	0.00000	1.38477
C	0.13373	-1.28074	-0.70255
C	-0.04637	-2.48171	0.03897
C	0.00000	-3.75115	-0.60961
C	-0.22429	-2.44040	1.46154
H	-0.17839	-1.17405	3.18822
H	0.17839	1.17405	3.18822
H	0.56652	3.60478	3.25113
H	0.60464	5.78502	2.07832
H	0.20863	5.88741	-0.36246
H	-0.33502	4.77678	-2.47497
H	-0.89695	2.70456	-3.71524
H	-0.82162	0.53732	-2.61011
H	0.82162	-0.53732	-2.61011
H	0.89695	-2.70456	-3.71524
H	0.33502	-4.77678	-2.47497
H	-0.20863	-5.88741	-0.36246
H	-0.60464	-5.78502	2.07832

H	-0.56652	-3.60478	3.25113
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singlet_open_shell_unrestricted_zethrene.xyz:

C	-1.64998	0.78968	0.00000
C	-1.06710	-1.62247	0.00000
C	-0.34398	-3.98443	0.00000
C	0.71132	-4.93336	0.00000
C	2.01866	-4.52538	0.00000
C	2.37800	2.06778	0.00000
C	2.69195	3.43549	0.00000
C	1.69958	4.38112	0.00000
C	-0.71132	4.93336	0.00000
C	-2.01866	4.52538	0.00000
C	-2.33273	3.15475	0.00000
C	2.33273	-3.15475	0.00000
C	1.33678	-2.19721	0.00000
C	1.64998	-0.78968	0.00000
C	0.71132	0.18530	0.00000
C	-0.03043	-2.59925	0.00000
C	-0.71132	-0.18530	0.00000
C	1.06710	1.62247	0.00000
C	0.03043	2.59925	0.00000
C	0.34398	3.98443	0.00000
C	-1.33678	2.19721	0.00000
H	-2.70442	0.53826	0.00000
H	0.46149	-5.98987	0.00000
H	2.81900	-5.25805	0.00000
H	3.19718	1.35921	0.00000
H	3.73390	3.73852	0.00000
H	1.94032	5.43974	0.00000
H	-0.46149	5.98987	0.00000
H	-2.81900	5.25805	0.00000
H	-3.37178	2.83923	0.00000
C	-2.37800	-2.06778	0.00000
C	-1.69958	-4.38112	0.00000
C	-2.69195	-3.43549	0.00000
H	-3.73390	-3.73852	0.00000
H	-3.19718	-1.35921	0.00000
H	-1.94032	-5.43974	0.00000
H	2.70442	-0.53826	0.00000
H	3.37178	-2.83923	0.00000

triplet_restricted_open_fulminene.xyz:

C	2.18248	-3.76059	0.00000
C	2.04488	-2.39622	0.00000
C	1.74482	0.53432	0.00000
C	1.62049	1.96418	0.00000
C	1.35482	4.91510	0.00000
C	1.19163	6.28375	0.00000
C	-0.09355	6.84487	0.00000
C	-1.19163	6.01973	0.00000
C	-2.18248	3.76059	0.00000
C	-2.04488	2.39622	0.00000
C	-1.74482	-0.53432	0.00000
C	-1.62049	-1.96418	0.00000
C	-1.35482	-4.91510	0.00000
C	-1.19163	-6.28375	0.00000
C	0.09355	-6.84487	0.00000
C	1.19163	-6.01973	0.00000
C	-1.04516	4.61609	0.00000
C	0.25020	4.04421	0.00000
C	-0.78823	1.77051	0.00000
C	0.38996	2.58657	0.00000
C	-0.66276	0.29718	0.00000
C	0.66276	-0.29718	0.00000
C	-0.38996	-2.58657	0.00000
C	0.78823	-1.77051	0.00000
C	-0.25020	-4.04421	0.00000
C	1.04516	-4.61609	0.00000
H	3.17130	-4.20785	0.00000
H	2.94517	-1.79457	0.00000
H	2.75046	0.13382	0.00000
H	2.53484	2.54222	0.00000
H	2.36127	4.51479	0.00000
H	2.06402	6.92889	0.00000
H	-0.21733	7.92276	0.00000
H	-2.19444	6.43658	0.00000
H	-3.17130	4.20785	0.00000
H	-2.94517	1.79457	0.00000
H	-2.75046	-0.13382	0.00000
H	-2.53484	-2.54222	0.00000
H	-2.36127	-4.51479	0.00000

H	-2.06402	-6.92889	0.00000
H	0.21733	-7.92276	0.00000
H	2.19444	-6.43658	0.00000

triplet_restricted_open_hexacene.xyz:

C	0.00000	7.34109	0.70601
C	0.00000	6.15705	1.39684
C	0.00000	4.91753	0.71261
C	0.00000	4.91753	-0.71261
C	0.00000	6.15705	-1.39684
C	0.00000	7.34109	-0.70601
C	0.00000	3.67979	1.39631
C	0.00000	3.67979	-1.39631
C	0.00000	2.47415	-0.72276
C	0.00000	2.47415	0.72276
C	0.00000	1.22021	1.40436
H	0.00000	1.22299	2.49056
C	0.00000	0.00000	0.73294
C	0.00000	0.00000	-0.73294
C	0.00000	1.22021	-1.40436
H	0.00000	3.68287	2.48304
H	0.00000	8.28387	1.24309
H	0.00000	6.15355	2.48287
H	0.00000	6.15355	-2.48287
H	0.00000	8.28387	-1.24309
H	0.00000	3.68287	-2.48304
H	0.00000	1.22299	-2.49056
C	0.00000	-1.22021	-1.40436
C	0.00000	-1.22021	1.40436
C	0.00000	-2.47415	0.72276
C	0.00000	-2.47415	-0.72276
H	0.00000	-1.22299	2.49056
H	0.00000	-1.22299	-2.49056
C	0.00000	-3.67979	-1.39631
C	0.00000	-3.67979	1.39631
C	0.00000	-4.91753	0.71261
C	0.00000	-4.91753	-0.71261
H	0.00000	-3.68287	-2.48304
H	0.00000	-3.68287	2.48304
C	0.00000	-6.15705	-1.39684
C	0.00000	-6.15705	1.39684

C	0.00000	-7.34109	-0.70601
H	0.00000	-8.28387	-1.24309
C	0.00000	-7.34109	0.70601
H	0.00000	-8.28387	1.24309
H	0.00000	-6.15355	-2.48287
H	0.00000	-6.15355	2.48287

triplet_restricted_open_triangulene.xyz:

C	1.20525	3.54410	0.00000
C	1.23578	2.12971	0.00000
C	0.00000	1.41757	0.00000
C	-1.23578	2.12971	0.00000
C	-1.20525	3.54410	0.00000
C	0.00000	4.22796	0.00000
H	2.14438	4.08806	0.00000
H	-2.14438	4.08806	0.00000
H	0.00000	5.31317	0.00000
C	0.00000	0.00000	0.00000
C	1.22765	-0.70879	0.00000
C	2.46227	0.00536	0.00000
C	1.22649	-2.13507	0.00000
C	3.67191	-0.72828	0.00000
C	2.46666	-2.81582	0.00000
C	3.66152	-2.11398	0.00000
H	2.46818	-3.90111	0.00000
H	4.60134	-2.65659	0.00000
C	-1.22765	-0.70879	0.00000
C	-1.22649	-2.13507	0.00000
C	-2.46227	0.00536	0.00000
C	-2.46666	-2.81582	0.00000
C	-3.67191	-0.72828	0.00000
C	-3.66152	-2.11398	0.00000
H	-2.46818	-3.90111	0.00000
H	-4.61255	-0.18695	0.00000
H	-4.60134	-2.65659	0.00000
C	-2.43969	1.40856	0.00000
C	2.43969	1.40856	0.00000
C	0.00000	-2.81711	0.00000
H	-3.38028	1.95161	0.00000
H	3.38028	1.95161	0.00000
H	0.00000	-3.90321	0.00000

H	4.61255	-0.18695	0.00000
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triplet_restricted_open_uthrene.xyz:

C	-0.11608	-1.21047	2.11220
C	0.11608	1.21047	2.11220
C	0.37543	3.65205	2.16367
C	0.36821	4.87651	1.50118
C	0.14388	4.93047	0.14242
C	-0.37407	3.79704	-1.98572
C	-0.65562	2.63723	-2.66920
C	-0.56351	1.39552	-2.03931
C	0.56351	-1.39552	-2.03931
C	0.65562	-2.63723	-2.66920
C	0.37407	-3.79704	-1.98572
C	-0.14388	-4.93047	0.14242
C	-0.36821	-4.87651	1.50118
C	-0.37543	-3.65205	2.16367
C	-0.06671	3.74720	-0.60915
C	0.00000	2.48556	0.04256
C	-0.16787	1.27361	-0.69875
C	0.00000	0.00000	-0.02372
C	0.18881	2.45076	1.46018
C	0.00000	0.00000	1.40407
C	0.16787	-1.27361	-0.69875
C	0.00000	-2.48556	0.04256
C	0.06671	-3.74720	-0.60915
C	-0.18881	-2.45076	1.46018
H	-0.16373	-1.17807	3.19642
H	0.16373	1.17807	3.19642
H	0.51678	3.61212	3.23910
H	0.52144	5.79275	2.06205
H	0.11038	5.88546	-0.37248
H	-0.42596	4.76151	-2.48110
H	-0.95880	2.67973	-3.71037
H	-0.84843	0.51402	-2.59522
H	0.84843	-0.51402	-2.59522
H	0.95880	-2.67973	-3.71037
H	0.42596	-4.76151	-2.48110
H	-0.11038	-5.88546	-0.37248
H	-0.52144	-5.79275	2.06205
H	-0.51678	-3.61212	3.23910

triplet_restricted_open_zethrene.xyz:

C	-1.66868	0.83304	0.00000
C	-1.04883	-1.58976	0.00000
C	-0.36202	-3.96014	0.00000
C	0.68117	-4.92090	0.00000
C	2.01292	-4.52872	0.00000
C	2.38830	2.02421	0.00000
C	2.70790	3.37311	0.00000
C	1.71474	4.33759	0.00000
C	-0.68117	4.92090	0.00000
C	-2.01292	4.52872	0.00000
C	-2.35117	3.19059	0.00000
C	2.35117	-3.19059	0.00000
C	1.34588	-2.18065	0.00000
C	1.66868	-0.83304	0.00000
C	0.68117	0.18376	0.00000
C	-0.03228	-2.57315	0.00000
C	-0.68117	-0.18376	0.00000
C	1.04883	1.58976	0.00000
C	0.03228	2.57315	0.00000
C	0.36202	3.96014	0.00000
C	-1.34588	2.18065	0.00000
H	-2.71817	0.56893	0.00000
H	0.41991	-5.97410	0.00000
H	2.79410	-5.28198	0.00000
H	3.19611	1.30479	0.00000
H	3.75088	3.67286	0.00000
H	1.97013	5.39258	0.00000
H	-0.41991	5.97410	0.00000
H	-2.79410	5.28198	0.00000
H	-3.39264	2.88533	0.00000
C	-2.38830	-2.02421	0.00000
C	-1.71474	-4.33759	0.00000
C	-2.70790	-3.37311	0.00000
H	-3.75088	-3.67286	0.00000
H	-3.19611	-1.30479	0.00000
H	-1.97013	-5.39258	0.00000
H	2.71817	-0.56893	0.00000
H	3.39264	-2.88533	0.00000

triplet_unrestricted_fulminene.xyz:

C	2.18474	-3.76370	0.00000
C	2.04702	-2.39779	0.00000
C	1.74456	0.53113	0.00000
C	1.62042	1.96692	0.00000
C	1.35440	4.91633	0.00000
C	1.19194	6.28536	0.00000
C	-0.09297	6.84732	0.00000
C	-1.19194	6.02248	0.00000
C	-2.18474	3.76370	0.00000
C	-2.04702	2.39779	0.00000
C	-1.74456	-0.53113	0.00000
C	-1.62042	-1.96692	0.00000
C	-1.35440	-4.91633	0.00000
C	-1.19194	-6.28536	0.00000
C	0.09297	-6.84732	0.00000
C	1.19194	-6.02248	0.00000
C	-1.04628	4.61910	0.00000
C	0.24904	4.04602	0.00000
C	-0.79053	1.77205	0.00000
C	0.38855	2.58883	0.00000
C	-0.66486	0.29778	0.00000
C	0.66486	-0.29778	0.00000
C	-0.38855	-2.58883	0.00000
C	0.79053	-1.77205	0.00000
C	-0.24904	-4.04602	0.00000
C	1.04628	-4.61910	0.00000
H	3.17343	-4.21135	0.00000
H	2.94767	-1.79652	0.00000
H	2.75049	0.13136	0.00000
H	2.53526	2.54432	0.00000
H	2.36071	4.51555	0.00000
H	2.06491	6.92975	0.00000
H	-0.21646	7.92525	0.00000
H	-2.19441	6.44023	0.00000
H	-3.17343	4.21135	0.00000
H	-2.94767	1.79652	0.00000
H	-2.75049	-0.13136	0.00000
H	-2.53526	-2.54432	0.00000
H	-2.36071	-4.51555	0.00000
H	-2.06491	-6.92975	0.00000

H	0.21646	-7.92525	0.00000
H	2.19441	-6.44023	0.00000

triplet_unrestricted_hexacene.xyz:

C	0.00000	7.34386	0.70567
C	0.00000	6.15914	1.39634
C	0.00000	4.92032	0.71222
C	0.00000	4.92032	-0.71222
C	0.00000	6.15914	-1.39634
C	0.00000	7.34386	-0.70567
C	0.00000	3.68116	1.39642
C	0.00000	3.68116	-1.39642
C	0.00000	2.47559	-0.72350
C	0.00000	2.47559	0.72350
C	0.00000	1.22164	1.40614
H	0.00000	1.22498	2.49249
C	0.00000	0.00000	0.73466
C	0.00000	0.00000	-0.73466
C	0.00000	1.22164	-1.40614
H	0.00000	3.68416	2.48321
H	0.00000	8.28651	1.24300
H	0.00000	6.15540	2.48240
H	0.00000	6.15540	-2.48240
H	0.00000	8.28651	-1.24300
H	0.00000	3.68416	-2.48321
H	0.00000	1.22498	-2.49249
C	0.00000	-1.22164	-1.40614
C	0.00000	-1.22164	1.40614
C	0.00000	-2.47559	0.72350
C	0.00000	-2.47559	-0.72350
H	0.00000	-1.22498	2.49249
H	0.00000	-1.22498	-2.49249
C	0.00000	-3.68116	-1.39642
C	0.00000	-3.68116	1.39642
C	0.00000	-4.92032	0.71222
C	0.00000	-4.92032	-0.71222
H	0.00000	-3.68416	-2.48321
H	0.00000	-3.68416	2.48321
C	0.00000	-6.15914	-1.39634
C	0.00000	-6.15914	1.39634
C	0.00000	-7.34386	-0.70567

H	0.00000	-8.28651	-1.24300
C	0.00000	-7.34386	0.70567
H	0.00000	-8.28651	1.24300
H	0.00000	-6.15540	-2.48240
H	0.00000	-6.15540	2.48240

triplet_unrestricted_triangulene.xyz:

C	1.20629	3.54759	0.00000
C	1.23620	2.13181	0.00000
C	0.00000	1.41911	0.00000
C	-1.23620	2.13181	0.00000
C	-1.20629	3.54759	0.00000
C	0.00000	4.23291	0.00000
H	2.14573	4.09124	0.00000
H	-2.14573	4.09124	0.00000
H	0.00000	5.31815	0.00000
C	0.00000	0.00000	0.00000
C	1.22899	-0.70956	0.00000
C	2.46430	0.00468	0.00000
C	1.22810	-2.13649	0.00000
C	3.67544	-0.72912	0.00000
C	2.46916	-2.81847	0.00000
C	3.66581	-2.11646	0.00000
H	2.47025	-3.90388	0.00000
H	4.60565	-2.65907	0.00000
C	-1.22899	-0.70956	0.00000
C	-1.22810	-2.13649	0.00000
C	-2.46430	0.00468	0.00000
C	-2.46916	-2.81847	0.00000
C	-3.67544	-0.72912	0.00000
C	-3.66581	-2.11646	0.00000
H	-2.47025	-3.90388	0.00000
H	-4.61598	-0.18736	0.00000
H	-4.60565	-2.65907	0.00000
C	-2.44163	1.40968	0.00000
C	2.44163	1.40968	0.00000
C	0.00000	-2.81935	0.00000
H	-3.38236	1.95281	0.00000
H	3.38236	1.95281	0.00000
H	0.00000	-3.90562	0.00000
H	4.61598	-0.18736	0.00000

triplet_unrestricted_uthrene.xyz:

C	-0.11766	-1.21175	2.11362
C	0.11766	1.21175	2.11362
C	0.37752	3.65593	2.16626
C	0.37021	4.87801	1.50442
C	0.14524	4.93132	0.14148
C	-0.37220	3.79739	-1.98652
C	-0.65505	2.63542	-2.67209
C	-0.56413	1.39549	-2.04307
C	0.56413	-1.39549	-2.04307
C	0.65505	-2.63542	-2.67209
C	0.37220	-3.79739	-1.98652
C	-0.14524	-4.93132	0.14148
C	-0.37021	-4.87801	1.50442
C	-0.37752	-3.65593	2.16626
C	-0.06592	3.74752	-0.60976
C	0.00000	2.48471	0.04288
C	-0.16702	1.27329	-0.69824
C	0.00000	0.00000	-0.02488
C	0.18943	2.45008	1.46077
C	0.00000	0.00000	1.40607
C	0.16702	-1.27329	-0.69824
C	0.00000	-2.48471	0.04288
C	0.06592	-3.74752	-0.60976
C	-0.18943	-2.45008	1.46077
H	-0.16625	-1.17999	3.19799
H	0.16625	1.17999	3.19799
H	0.52059	3.61490	3.24143
H	0.52383	5.79507	2.06372
H	0.11221	5.88631	-0.37330
H	-0.42369	4.76169	-2.48216
H	-0.95948	2.67954	-3.71276
H	-0.85171	0.51366	-2.59693
H	0.85171	-0.51366	-2.59693
H	0.95948	-2.67954	-3.71276
H	0.42369	-4.76169	-2.48216
H	-0.11221	-5.88631	-0.37330
H	-0.52383	-5.79507	2.06372
H	-0.52059	-3.61490	3.24143

triplet_unrestricted_zethrene.xyz:

C	-1.67044	0.83397	0.00000
C	-1.04698	-1.58956	0.00000
C	-0.36258	-3.96127	0.00000
C	0.67974	-4.92312	0.00000
C	2.01428	-4.53170	0.00000
C	2.38889	2.02333	0.00000
C	2.71011	3.37252	0.00000
C	1.71699	4.33808	0.00000
C	-0.67974	4.92312	0.00000
C	-2.01428	4.53170	0.00000
C	-2.35359	3.19306	0.00000
C	2.35359	-3.19306	0.00000
C	1.34726	-2.18162	0.00000
C	1.67044	-0.83397	0.00000
C	0.67974	0.18427	0.00000
C	-0.03119	-2.57329	0.00000
C	-0.67974	-0.18427	0.00000
C	1.04698	1.58956	0.00000
C	0.03119	2.57329	0.00000
C	0.36258	3.96127	0.00000
C	-1.34726	2.18162	0.00000
H	-2.72003	0.56965	0.00000
H	0.41722	-5.97616	0.00000
H	2.79490	-5.28557	0.00000
H	3.19597	1.30297	0.00000
H	3.75338	3.67131	0.00000
H	1.97306	5.39297	0.00000
H	-0.41722	5.97616	0.00000
H	-2.79490	5.28557	0.00000
H	-3.39531	2.88824	0.00000
C	-2.38889	-2.02333	0.00000
C	-1.71699	-4.33808	0.00000
C	-2.71011	-3.37252	0.00000
H	-3.75338	-3.67131	0.00000
H	-3.19597	-1.30297	0.00000
H	-1.97306	-5.39297	0.00000
H	2.72003	-0.56965	0.00000
H	3.39531	-2.88824	0.00000
