1 Singlet geometries

Cartesian coordinates in Å

Benzene

C	0.000000	1.396915	0.000000
C	0.000000	-1.396915	0.000000
C	1.209764	0.698457	0.000000
C	-1.209764	0.698457	0.000000
C	-1.209764	-0.698457	0.000000
C	1.209764	-0.698457	0.000000
H	0.000000	2.484064	0.000000
H	2.151262	1.242032	0.000000
H	-2.151262	1.242032	0.000000
H	-2.151262	-1.242032	0.000000
H	2.151262	-1.242032	0.000000
H	0.000000	-2.484064	0. 000000

Naphthalene

C	0.000000	2.434012	0.708635
C	0.000000	1.245004	1.402781
C	0.000000	1.245004	-1.402781
C	0.000000	0.000000	0.716898
C	0.000000	2.434012	-0.708635
C	0.000000	0.000000	-0.716898
C	0.000000	-1.245004	1.402781
C	0.000000	-2.434012	0.708635
C	0.000000	-2.434012	-0.708635
C	0.000000	-1.245004	-1.402781
H	0.000000	3.378853	1.245785
H	0.000000	1.242353	2.490559
H	0.000000	3.378853	-1.245785
H	0.000000	-1.242353	-2.490559
H	0.000000	1.242353	-2.490559
H	0.000000	-1.242353	2.490559
H	0.000000	-3.378853	1.245785
H	0.000000	-3.378853	-1.245785

Anthracene

C	0.000000	3.661282	0.713343
C	0.000000	2.479963	1.407288
C	0.000000	2.479963	-1.407288
C	0.000000	1.224041	0.722608
C	0.000000	3.661282	-0.713343
C	0.000000	1.224041	-0.722608
C	0.000000	0.000000	1.403669
C	0.000000	-1.224041	0.722608
C	0.000000	-2.479963	1.407288
C	0.000000	-1.224041	-0.722608
C	0.000000	-2.479963	-1.407288
C	0.000000	0.000000	-1.403669
C	0.000000	-3.661282	0.713343
C	0.000000	-3.661282	-0.713343
H	0.000000	4.608042	1.246984
H	0.000000	2.477436	2.494941
H	0.000000	4.608042	-1.246984
H	0.000000	0.000000	-2.492092
H	0.000000	2.477436	-2.494941
H	0.000000	0.000000	2.492092
H	0.000000	-2.477436	2.494941
H	0.000000	-2.477436	-2.494941
H	0.000000	-4.608042	1.246984
H	0.000000	-4.608042	-1.246984

Tetracene

C	0.000000	3.711092	1.409333
C	0.000000	2.450448	0.725881
C	0.000000	1.235383	1.406384
C	0.000000	1.235383	-1.406384
C	0.000000	0.000000	0.726115
C	0.000000	2.450448	-0.725881
C	0.000000	0.000000	-0.726115
C	0.000000	-1.235383	1.406384
C	0.000000	3.711092	-1.409333
C	0.000000	-2.450448	0.725881
C	0.000000	-3.711092	1.409333
C	0.000000	-2.450448	-0.725881
C	0.000000	-1.235383	-1.406384

C	0.000000	-4.888809	0.715432
C	0.000000	-4.888809	-0.715432
C	0.000000	-3.711092	-1.409333
C	0.000000	4.888809	0.715432
C	0.000000	4.888809	-0.715432
H	0.000000	1.235190	2.494613
H	0.000000	-1.235190	-2.494613
H	0.000000	1.235190	-2.494613
H	0.000000	-1.235190	2.494613
H	0.000000	-3.708768	-2.496861
H	0.000000	-3.708768	2.496861
H	0.000000	-5.836389	1.247314
H	0.000000	-5.836389	-1.247314
H	0.000000	3.708768	2.496861
H	0.000000	3.708768	-2.496861
H	0.000000	5.836389	1.247314
H	0.000000	5.836389	-1.247314

Pentacene

C	0.000000	4.941685	1.410525
C	0.000000	3.678505	0.727639
C	0.000000	2.467629	1.407935
C	0.000000	2.467629	-1.407935
C	0.000000	1.226411	0.728500
C	0.000000	3.678505	-0.727639
C	0.000000	1.226411	-0.728500
C	0.000000	0.000000	1.408574
C	0.000000	4.941685	-1.410525
C	0.000000	-1.226411	0.728500
C	0.000000	-2.467629	1.407935
C	0.000000	-1.226411	-0.728500
C	0.000000	0.000000	-1.408574
C	0.000000	-3.678505	0.727639
C	0.000000	-4.941685	1.410525
C	0.000000	-3.678505	-0.727639
C	0.000000	-4.941685	-1.410525
C	0.000000	-2.467629	-1.407935
C	0.000000	6.117700	0.716631
C	0.000000	6.117700	-0.716631

C	0.000000	-6.117700	-0.716631
C	0.000000	-6.117700	0.716631
H	0.000000	2.467551	2.496138
H	0.000000	0.000000	-2.496666
H	0.000000	2.467551	-2.496138
H	0.000000	0.000000	2.496666
H	0.000000	-2.467551	-2.496138
H	0.000000	-2.467551	2.496138
H	0.000000	4.939471	2.498046
H	0.000000	4.939471	-2.498046
H	0.000000	7.065792	1.247576
H	0.000000	7.065792	-1.247576
H	0.000000	-4.939471	-2.498046
H	0.000000	-4.939471	2.498046
H	0.000000	-7.065792	-1.247576
H	0.000000	-7.065792	1.247576

Hexacene

C	0.000000	6.172241	1.411100
C	0.000000	4.907691	0.728779
C	0.000000	3.698818	1.408621
C	0.000000	3.698818	-1.408621
C	0.000000	2.454528	0.730015
C	0.000000	4.907691	-0.728779
C	0.000000	2.454528	-0.730015
C	0.000000	1.232441	1.409718
C	0.000000	6.172241	-1.411100
C	0.000000	0.000000	0.730594
C	0.000000	-1.232441	1.409718
C	0.000000	0.000000	-0.730594
C	0.000000	1.232441	-1.409718
C	0.000000	-2.454528	0.730015
C	0.000000	-3.698818	1.408621
C	0.000000	-2.454528	-0.730015
C	0.000000	-3.698818	-1.408621
C	0.000000	-1.232441	-1.409718
C	0.000000	7.347388	0.717297
C	0.000000	7.347388	-0.717297
C	0.000000	-4.907691	0.728779

C	0.000000	-4.907691	-0.728779
C	0.000000	-6.172241	-1.411100
C	0.000000	-6.172241	1.411100
C	0.000000	-7.347388	0.717297
C	0.000000	-7.347388	-0.717297
H	0.000000	3.698587	2.496777
H	0.000000	1.232439	-2.497709
H	0.000000	3.698587	-2.496777
H	0.000000	1.232439	2.497709
H	0.000000	-1.232439	-2.497709
H	0.000000	-1.232439	2.497709
H	0.000000	6.169798	2.498552
H	0.000000	6.169798	-2.498552
H	0.000000	8.295785	1.247528
H	0.000000	8.295785	-1.247528
H	0.000000	-3.698587	2.496777
H	0.000000	-3.698587	-2.496777
H	0.000000	-6.169798	2.498552
H	0.000000	-6.169798	-2.498552
H	0.000000	-8.295785	1.247528
H	0.000000	-8.295785	-1.247528

Decacene

C	0.000000	11.090345	1.411798
C	0.000000	9.824806	0.729719
C	0.000000	8.618058	1.409785
C	0.000000	8.618058	-1.409785
C	0.000000	7.370873	0.731625
C	0.000000	9.824806	-0.729719
C	0.000000	7.370873	-0.731625
C	0.000000	6.153434	1.411329
C	0.000000	11.090345	-1.411798
C	0.000000	4.914812	0.733006
C	0.000000	3.691406	1.412091
C	0.000000	4.914812	-0.733006
C	0.000000	6.153434	-1.411329
C	0.000000	2.457555	0.733547
C	0.000000	1.230332	1.412386
C	0.000000	2.457555	-0.733547

C	0.000000	1.230332	-1.412386
C	0.000000	3.691406	-1.412091
C	0.000000	12.264759	0.717717
C	0.000000	12.264759	-0.717717
C	0.000000	0.000000	0.733618
C	0.000000	0.000000	-0.733618
C	0.000000	-1.230332	-1.412386
C	0.000000	-1.230332	1.412386
C	0.000000	-2.457555	0.733547
C	0.000000	-2.457555	-0.733547
C	0.000000	-3.691406	1.412091
C	0.000000	-3.691406	-1.412091
C	0.000000	-4.914812	0.733006
C	0.000000	-4.914812	-0.733006
C	0.000000	-6.153434	1.411329
C	0.000000	-6.153434	-1.411329
C	0.000000	-7.370873	0.731625
C	0.000000	-7.370873	-0.731625
C	0.000000	-8.618058	-1.409785
C	0.000000	-8.618058	1.409785
C	0.000000	-9.824806	-0.729719
C	0.000000	-9.824806	0.729719
C	0.000000	-11.090345	-1.411798
C	0.000000	-11.090345	1.411798
C	0.000000	-12.264759	0.717717
C	0.000000	-12.264759	-0.717717
H	0.000000	8.618647	2.497987
H	0.000000	6.153821	-2.499396
H	0.000000	8.618647	-2.497987
H	0.000000	6.153821	2.499396
H	0.000000	3.691260	-2.500129
H	0.000000	3.691260	2.500129
H	0.000000	11.088911	2.499305
H	0.000000	11.088911	-2.499305
H	0.000000	13.213111	1.248177
H	0.000000	13.213111	-1.248177
H	0.000000	1.230087	2.500407
H	0.000000	1.230087	-2.500407
H	0.000000	-1.230087	2.500407
H	0.000000	-1.230087	-2.500407

H	0.000000	-3.691260	2.500129
H	0.000000	-3.691260	-2.500129
H	0.000000	-6.153821	2.499396
H	0.000000	-6.153821	-2.499396
H	0.000000	-8.618647	-2.497987
H	0.000000	-8.618647	2.497987
H	0.000000	-11.088911	2.499305
H	0.000000	-11.088911	-2.499305
H	0.000000	-13.213111	1.248177
H	0.000000	-13.213111	-1.248177

13acene

C	-0.000000	8.603009	0.733137
H	-0.000000	9.842593	2.499431
C	-0.000000	9.842219	1.411425
C	-0.000000	9.842219	-1.411425
C	-0.000000	11.059088	0.731706
C	-0.000000	8.603009	-0.733137
C	-0.000000	11.059088	-0.731706
C	-0.000000	12.306735	1.409867
H	-0.000000	12.307065	-2.498028
H	-0.000000	9.842593	-2.499431
C	-0.000000	13.513083	0.729876
H	-0.000000	12.307065	2.498028
C	-0.000000	14.778946	1.411935
C	-0.000000	13.513083	-0.729876
H	-0.000000	14.777225	-2.499403
C	-0.000000	12.306735	-1.409867
C	-0.000000	15.953115	0.717935
H	-0.000000	14.777225	2.499403
H	-0.000000	16.901576	1.248082
C	-0.000000	15.953115	-0.717935
H	-0.000000	16.901576	-1.248082
C	-0.000000	14.778946	-1.411935
C	-0.000000	7.380410	1.412274
H	-0.000000	7.380567	2.500234
C	-0.000000	7.380410	-1.412274
H	-0.000000	7.380567	-2.500234
C	-0.000000	6.145628	0.733924

C	-0.000000	6.145628	-0.733924
C	-0.000000	4.919804	1.412766
H	-0.000000	4.919869	2.500701
C	-0.000000	4.919804	-1.412766
H	-0.000000	4.919869	-2.500701
C	-0.000000	3.687593	-0.734347
C	-0.000000	3.687593	0.734347
C	-0.000000	2.459774	1.413016
H	-0.000000	2.459802	2.500938
C	-0.000000	1.229238	0.734531
C	-0.000000	1.229238	-0.734531
C	-0.000000	2.459774	-1.413016
H	-0.000000	2.459802	-2.500938
C	-0.000000	-0.000016	1.413093
H	-0.000000	-0.000003	2.501010
C	-0.000000	-0.000016	-1.413093
H	-0.000000	-0.000003	-2.501010
C	-0.000000	-1.229214	-0.734531
C	-0.000000	-1.229214	0.734531
C	-0.000000	-2.459808	1.413015
H	-0.000000	-2.459806	2.500937
C	-0.000000	-3.687566	0.734347
C	-0.000000	-3.687566	-0.734347
C	-0.000000	-2.459808	-1.413015
H	-0.000000	-2.459806	-2.500937
C	-0.000000	-4.919839	1.412764
H	-0.000000	-4.919868	2.500701
C	-0.000000	-6.145597	0.733928
C	-0.000000	-6.145597	-0.733928
C	-0.000000	-4.919839	-1.412764
H	-0.000000	-4.919868	-2.500701
C	0.000000	-7.380441	1.412274
H	0.000000	-7.380564	2.500236
C	0.000000	-8.602979	0.733146
C	0.000000	-8.602979	-0.733146
C	0.000000	-7.380441	-1.412274
H	0.000000	-7.380564	-2.500236
C	0.000000	-9.842242	1.411428
H	0.000000	-9.842592	2.499435
C	0.000000	-11.059064	0.731716

C	0.000000	-11.059064	-0.731716
C	0.000000	-9.842242	-1.411428
H	0.000000	-9.842592	-2.499435
C	0.000000	-12.306750	1.409872
H	0.000000	-12.307065	2.498034
C	0.000000	-13.513066	0.729887
C	0.000000	-13.513066	-0.729887
C	0.000000	-12.306750	-1.409872
H	0.000000	-12.307065	-2.498034
C	0.000000	-14.778954	1.411942
H	0.000000	-14.777221	2.499410
C	0.000000	-15.953107	0.717947
H	0.000000	-16.901575	1.248079
C	0.000000	-15.953107	-0.717947
H	0.000000	-16.901575	-1.248079
C	0.000000	-14.778954	-1.411942
H	0.000000	-14.777221	-2.499410

2 Triplet geometries

Cartesian coordinates in Å

Benzene

C	0.000000	1.442916	0.000000
C	0.000000	-1.442916	0.000000
C	0.000000	0.760980	-1.210053
C	0.000000	0.760980	1.210053
C	0.000000	-0.760980	1.210053
C	0.000000	-0.760980	-1.210053
H	0.000000	2.530990	0.000000
H	0.000000	1.287874	-2.157802
H	0.000000	1.287874	2.157802
H	0.000000	-1.287874	2.157802
H	0.000000	-1.287874	-2.157802
H	0.000000	-2.530990	0.000000

Naphthalene

C	0.000000	2.487805	0.681686
C	0.000000	1.237994	1.400915

C	0.000000	1.237994	-1.400915
C	0.000000	0.000000	0.725252
C	0.000000	2.487805	-0.681686
C	0.000000	0.000000	-0.725252
C	0.000000	-1.237994	1.400915
C	0.000000	-2.487805	0.681686
C	0.000000	-2.487805	-0.681686
C	0.000000	-1.237994	-1.400915
H	0.000000	3.419182	1.240611
H	0.000000	1.246282	2.487572
H	0.000000	3.419182	-1.240611
H	0.000000	-1.246282	-2.487572
H	0.000000	1.246282	-2.487572
H	0.000000	-1.246282	2.487572
H	0.000000	-3.419182	1.240611
H	0.000000	-3.419182	-1.240611

Anthracene

C	0.000000	3.705292	0.691689
C	0.000000	2.480114	1.395971
C	0.000000	2.480114	-1.395971
C	0.000000	1.254941	0.720486
C	0.000000	3.705292	-0.691689
C	0.000000	1.254941	-0.720486
C	0.000000	0.000000	1.406386
C	0.000000	-1.254941	0.720486
C	0.000000	-2.480114	1.395971
C	0.000000	-1.254941	-0.720486
C	0.000000	-2.480114	-1.395971
C	0.000000	0.000000	-1.406386
C	0.000000	-3.705292	0.691689
C	0.000000	-3.705292	-0.691689
H	0.000000	4.641163	1.243315
H	0.000000	2.483623	2.483370
H	0.000000	4.641163	-1.243315
H	0.000000	0.000000	-2.493811
H	0.000000	2.483623	-2.483370
H	0.000000	0.000000	2.493811
H	0.000000	-2.483623	2.483370

H	0.000000	-2.483623	-2.483370
H	0.000000	-4.641163	1.243315
H	0.000000	-4.641163	-1.243315

Tetracene

C	0.000000	3.716518	1.397489
C	0.000000	2.486929	0.717305
C	0.000000	1.230990	1.405050
C	0.000000	1.230990	-1.405050
C	0.000000	0.000000	0.730697
C	0.000000	2.486929	-0.717305
C	0.000000	0.000000	-0.730697
C	0.000000	-1.230990	1.405050
C	0.000000	3.716518	-1.397489
C	0.000000	-2.486929	0.717305
C	0.000000	-3.716518	1.397489
C	0.000000	-2.486929	-0.717305
C	0.000000	-1.230990	-1.405050
C	0.000000	-4.925844	0.698725
C	0.000000	-4.925844	-0.698725
C	0.000000	-3.716518	-1.397489
C	0.000000	4.925844	0.698725
C	0.000000	4.925844	-0.698725
H	0.000000	1.234632	2.492856
H	0.000000	-1.234632	-2.492856
H	0.000000	1.234632	-2.492856
H	0.000000	-1.234632	2.492856
H	0.000000	-3.715486	-2.485107
H	0.000000	-3.715486	2.485107
H	0.000000	-5.865918	1.243399
H	0.000000	-5.865918	-1.243399
H	0.000000	3.715486	2.485107
H	0.000000	3.715486	-2.485107
H	0.000000	5.865918	1.243399
H	0.000000	5.865918	-1.243399

Pentacene

C	0.000000	4.949869	1.400091

C	0.000000	3.713268	0.717502
C	0.000000	2.464151	1.403045
C	0.000000	2.464151	-1.403045
C	0.000000	1.244464	0.729574
C	0.000000	3.713268	-0.717502
C	0.000000	1.244464	-0.729574
C	0.000000	0.000000	1.408693
C	0.000000	4.949869	-1.400091
C	0.000000	-1.244464	0.729574
C	0.000000	-2.464151	1.403045
C	0.000000	-1.244464	-0.729574
C	0.000000	0.000000	-1.408693
C	0.000000	-3.713268	0.717502
C	0.000000	-4.949869	1.400091
C	0.000000	-3.713268	-0.717502
C	0.000000	-4.949869	-1.400091
C	0.000000	-2.464151	-1.403045
C	0.000000	6.148927	0.703646
C	0.000000	6.148927	-0.703646
C	0.000000	-6.148927	-0.703646
C	0.000000	-6.148927	0.703646
H	0.000000	2.467170	2.491172
H	0.000000	0.000000	-2.496417
H	0.000000	2.467170	-2.491172
H	0.000000	0.000000	2.496417
H	0.000000	-2.467170	-2.491172
H	0.000000	-2.467170	2.491172
H	0.000000	4.947521	2.487711
H	0.000000	4.947521	-2.487711
H	0.000000	7.091406	1.244287
H	0.000000	7.091406	-1.244287
H	0.000000	-4.947521	-2.487711
H	0.000000	-4.947521	2.487711
H	0.000000	-7.091406	-1.244287
H	0.000000	-7.091406	1.244287

Hexacene

C	0.000000	6.181528	1.402451
C	0.000000	4.938540	0.718918

C	0.000000	3.697549	1.402694
C	0.000000	3.697549	-1.402694
C	0.000000	2.479538	0.727244
C	0.000000	4.938540	-0.718918
C	0.000000	2.479538	-0.727244
C	0.000000	1.229175	1.408241
C	0.000000	6.181528	-1.402451
C	0.000000	0.000000	0.733586
C	0.000000	-1.229175	1.408241
C	0.000000	0.000000	-0.733586
C	0.000000	1.229175	-1.408241
C	0.000000	-2.479538	0.727244
C	0.000000	-3.697549	1.402694
C	0.000000	-2.479538	-0.727244
C	0.000000	-3.697549	-1.402694
C	0.000000	-1.229175	-1.408241
C	0.000000	7.373798	0.707128
C	0.000000	7.373798	-0.707128
C	0.000000	-4.938540	0.718918
C	0.000000	-4.938540	-0.718918
C	0.000000	-6.181528	-1.402451
C	0.000000	-6.181528	1.402451
C	0.000000	-7.373798	0.707128
C	0.000000	-7.373798	-0.707128
H	0.000000	3.699383	2.490912
H	0.000000	1.230993	-2.496120
H	0.000000	3.699383	-2.490912
H	0.000000	1.230993	2.496120
H	0.000000	-1.230993	-2.496120
H	0.000000	-1.230993	2.496120
H	0.000000	6.178841	2.490024
H	0.000000	6.178841	-2.490024
H	0.000000	8.317871	1.245042
H	0.000000	8.317871	-1.245042
H	0.000000	-3.699383	2.490912
H	0.000000	-3.699383	-2.490912
H	0.000000	-6.178841	2.490024
H	0.000000	-6.178841	-2.490024
H	0.000000	-8.317871	1.245042
H	0.000000	-8.317871	-1.245042

Decacene

C	0.000000	11.101540	1.408165
C	0.000000	9.843976	0.724756
C	0.000000	8.624474	1.405669
C	0.000000	8.624474	-1.405669
C	0.000000	7.392609	0.726699
C	0.000000	9.843976	-0.724756
C	0.000000	7.392609	-0.726699
C	0.000000	6.154556	1.407296
C	0.000000	11.101540	-1.408165
C	0.000000	4.936330	0.729732
C	0.000000	3.688760	1.408941
C	0.000000	4.936330	-0.729732
C	0.000000	6.154556	-1.407296
C	0.000000	2.472125	0.733442
C	0.000000	1.228457	1.410448
C	0.000000	2.472125	-0.733442
C	0.000000	1.228457	-1.410448
C	0.000000	3.688760	-1.408941
C	0.000000	12.281617	0.714063
C	0.000000	12.281617	-0.714063
C	0.000000	0.000000	0.735497
C	0.000000	0.000000	-0.735497
C	0.000000	-1.228457	-1.410448
C	0.000000	-1.228457	1.410448
C	0.000000	-2.472125	0.733442
C	0.000000	-2.472125	-0.733442
C	0.000000	-3.688760	1.408941
C	0.000000	-3.688760	-1.408941
C	0.000000	-4.936330	0.729732
C	0.000000	-4.936330	-0.729732
C	0.000000	-6.154556	1.407296
C	0.000000	-6.154556	-1.407296
C	0.000000	-7.392609	0.726699
C	0.000000	-7.392609	-0.726699
C	0.000000	-8.624474	-1.405669
C	0.000000	-8.624474	1.405669
C	0.000000	-9.843976	-0.724756
C	0.000000	-9.843976	0.724756

C	0.000000	-11.101540	-1.408165
C	0.000000	-11.101540	1.408165
C	0.000000	-12.281617	0.714063
C	0.000000	-12.281617	-0.714063
H	0.000000	8.624347	2.493875
H	0.000000	6.155010	-2.495389
H	0.000000	8.624347	-2.493875
H	0.000000	6.155010	2.495389
H	0.000000	3.689599	-2.496997
H	0.000000	3.689599	2.496997
H	0.000000	11.098941	2.495670
H	0.000000	11.098941	-2.495670
H	0.000000	13.228692	1.246751
H	0.000000	13.228692	-1.246751
H	0.000000	1.228990	2.498439
H	0.000000	1.228990	-2.498439
H	0.000000	-1.228990	2.498439
H	0.000000	-1.228990	-2.498439
H	0.000000	-3.689599	2.496997
H	0.000000	-3.689599	-2.496997
H	0.000000	-6.155010	2.495389
H	0.000000	-6.155010	-2.495389
H	0.000000	-8.624347	-2.493875
H	0.000000	-8.624347	2.493875
H	0.000000	-11.098941	2.495670
H	0.000000	-11.098941	-2.495670
H	0.000000	-13.228692	1.246751
H	0.000000	-13.228692	-1.246751

13acene

C	0.000012	-8.620545	0.730093
H	-0.000034	-9.846995	2.496824
C	-0.000030	-9.846722	1.408746
C	-0.000030	-9.846722	-1.408746
C	-0.000074	-11.074848	0.728682
C	0.000012	-8.620545	-0.730093
C	-0.000074	-11.074848	-0.728682
C	-0.000121	-12.314240	1.407586
H	-0.000123	-12.314288	-2.495787

H	-0.000034	-9.846995	-2.496824
C	-0.000167	-13.526951	0.727235
H	-0.000123	-12.314288	2.495787
C	-0.000217	-14.788776	1.410077
C	-0.000167	-13.526951	-0.727235
H	-0.000217	-14.786616	-2.497573
C	-0.000121	-12.314240	-1.407586
C	-0.000263	-15.965704	0.716055
H	-0.000217	-14.786616	2.497573
H	-0.000300	-16.913485	1.247451
C	-0.000263	-15.965704	-0.716055
H	-0.000300	-16.913485	-1.247451
C	-0.000217	-14.788776	-1.410077
C	0.000050	-7.381444	1.409387
H	0.000046	-7.381877	2.497457
C	0.000050	-7.381444	-1.409387
H	0.000046	-7.381877	-2.497457
C	0.000086	-6.163545	0.731570
C	0.000086	-6.163545	-0.731570
C	0.000117	-4.917875	1.410015
H	0.000112	-4.918705	2.498091
C	0.000117	-4.917875	-1.410015
H	0.000112	-4.918705	-2.498091
C	0.000144	-3.702220	-0.733671
C	0.000144	-3.702220	0.733671
C	0.000163	-2.457263	1.410760
H	0.000158	-2.458161	2.498828
C	0.000179	-1.235168	0.735722
C	0.000179	-1.235168	-0.735722
C	0.000163	-2.457263	-1.410760
H	0.000158	-2.458161	-2.498828
C	0.000185	0.000047	1.411163
H	0.000181	-0.000014	2.499219
C	0.000185	0.000047	-1.411163
H	0.000181	-0.000014	-2.499219
C	0.000188	1.234945	-0.735763
C	0.000188	1.234945	0.735763
C	0.000181	2.457297	1.410772
H	0.000177	2.458143	2.498841
C	0.000170	3.702137	0.733736

C	0.000170	3.702137	-0.733736
C	0.000181	2.457297	-1.410772
H	0.000177	2.458143	-2.498841
C	0.000149	4.917819	1.410032
H	0.000145	4.918690	2.498109
C	0.000122	6.163600	0.731598
C	0.000122	6.163600	-0.731598
C	0.000149	4.917819	-1.410032
H	0.000145	4.918690	-2.498109
C	0.000086	7.381358	1.409396
H	0.000084	7.381865	2.497466
C	0.000045	8.620663	0.730081
C	0.000045	8.620663	-0.730081
C	0.000086	7.381358	-1.409396
H	0.000084	7.381865	-2.497466
C	-0.000005	9.846659	1.408739
H	-0.000007	9.846994	2.496816
C	-0.000058	11.074968	0.728647
C	-0.000058	11.074968	-0.728647
C	-0.000005	9.846659	-1.408739
H	-0.000007	9.846994	-2.496816
C	-0.000118	12.314215	1.407566
H	-0.000119	12.314299	2.495766
C	-0.000180	13.527041	0.727192
C	-0.000180	13.527041	-0.727192
C	-0.000118	12.314215	-1.407566
H	-0.000119	12.314299	-2.495766
C	-0.000248	14.788786	1.410051
H	-0.000249	14.786634	2.497547
C	-0.000311	15.965765	0.716021
H	-0.000362	16.913526	1.247452
C	-0.000311	15.965765	-0.716021
H	-0.000362	16.913526	-1.247452
C	-0.000248	14.788786	-1.410051
H	-0.000249	14.786634	-2.497547

3 Measure of spin contamination

To understand the extent of spin contamination, we have computed the $\langle S^2 \rangle$ value with 6-31G basis for polyacenes. Tetracene was calculated with C atoms containing 6-31G basis and H atoms with STO-3G basis and pentacene with minimal STO-3G basis for all atoms. Since the calculation of $\langle S^2 \rangle$ value requires two electron properties it is computationally expensive.

Table 1: Calculated $\langle S^2 \rangle$ (in a.u.) values.

System	$\langle S^2 \rangle$
Benzene	0.006
Naphthalene	0.022
Anthracene	0.028
Tetracene	0.031
Pentacene	0.039

4 ST gaps calculated with SF-TDDFT

Table 2: Comparison of SF-TDDFT computed ST gaps with collinear and non-collinear kernels. The energies are given in kcal/mol.

System	Collinear (50-50)	Non-collinear (PBE0)	Non-collinear (50-50)	Expt.
Naphthalene	69.7	63.33	60.6	60.9-61.0
Anthracene	48.3	43.1	40.9	42.6-43.1
Tetracene	33.9	29.4	28.1	29.0-29.5
Pentacene	23.8	20.2	18.9	19.8

5 Effect of basis set on the SF-CCSD ST gaps

Table 3: ST gaps of different size polyacenes calculated with SF-CCSD method with different basis sets with or without FNO, compared to experimental results. The energies are given in kcal/mol.

System	6-311++G(d,p)		6-311G		6-31+G(d,p)	6-31G	Expt.
	(FNO)	(No FNO)	(FNO)	(No FNO)	(FNO)	(FNO)	
Benzene	88.5	88.0	89.0	90.2	88.8	88.7	84.3
Naphthalene	62.4	62.3	64.2	64.9	63.2	64.7	60.9, 61.0
Anthracene	44.9	n.a.	46.3	46.9	44.8	46.5	42.6, 43.1
Tetracene	30.5	n.a.	33.1	33.4	31.7	33.3	29.5, 29.3
Pentacene	n.a.	n.a.	24.3	24.5	22.7	24.5	19.8
Hexacene	n.a.	n.a.	18.4	18.0	16.5	18.6	12.4
Decacene	n.a.	n.a.	n.a.	n.a.	n.a.	8.84	n.a.