All calculations were performed with unrestricted spin and 6-31g(d,p) level of theory using the different functions. e.g. u**cam**-**b3lyp/**6-31g(d,p)

Function	**S2** **Before annihilation**	**S2** **After annihilation**
LSDA	0	0
BPV86	0	0
B3LYP	0.86	1.06
CAM-B3LYP	1.86	6.42
B3PW91	0.95	1.38
MPW1PW91	1.27	3.05
PBEPBE	0	0
HSEH1PBE	0	0
HCTH	0	0
TPSSTPSS	0	0
WB97XD	1.81	6.10

- The coordinates of **15** obtained using above functions are given in PDF_2

Coordinates of decaphyrin **15**, obtained using different functions.

*To reduce the computational cost, the all meso-substituents of the ring **15** were removed.

(1) Function and Basis set-ub3lyp/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673

C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086
C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(2) Function and Basis set-ucam-b3lyp/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(3) Function and Basis set- ubvp86/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(4) Function and Basis set- ub3pw91/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(5) Function and Basis set-ulsda/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(6) Function and Basis set-umpw1pw91/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(7) Function and Basis set-upbepbe/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(8) Function and Basis set-uhseh1pbe/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(9) Function and Basis set-uhcth/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(10) Function and Basis set- utpsstpss/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058

(11) Function and Basis set- uwb97xd/6-31g(d,p)

Atom	X	Y	Z
S	0.39162	-1.85159	3.71017
S	-2.86981	-2.37923	3.12655
S	4.63286	-0.64061	3.32882
S	-6.8011	-2.07653	0.02533
S	7.32104	0.65814	2.62672
C	-0.32982	-1.75885	2.1059
C	0.64034	-1.39293	1.17109
H	0.42167	-1.27518	0.11673
C	1.91276	-1.19074	1.71789
H	2.77617	-0.90943	1.12552
C	1.98097	-1.39539	3.09588
C	-1.71195	-2.01107	1.85896
C	-4.21556	-2.48417	1.97271
C	-3.72275	-2.25263	0.6767
H	-4.33703	-2.30981	-0.21086
C	-2.35408	-1.99285	0.61718
H	-1.82937	-1.80374	-0.31187
C	3.11138	-1.26785	3.95234
C	3.24066	-1.56536	5.31006
H	2.42444	-1.96965	5.89867
C	4.50879	-1.3057	5.83115
H	4.78124	-1.48135	6.86398
C	5.43002	-0.78234	4.90472
C	-5.52709	-2.75772	2.45178
C	-6.70443	-2.67014	1.69177
C	-8.01704	-2.99233	2.13195
H	-8.19867	-3.37391	3.1289
C	-9.01115	-2.77358	1.20142
H	-10.05999	-2.95714	1.39505
C	-8.56315	-2.26533	-0.04551
C	6.77834	-0.41814	5.17816
C	7.68613	0.18329	4.29499
C	9.03334	0.54064	4.58106
H	9.47528	0.34307	5.54955
C	9.70122	1.15697	3.54524
H	10.7243	1.50271	3.61661
C	8.93758	1.33443	2.36122
C	-9.36265	-1.95349	-1.16602
S	-0.39162	1.85159	-3.71017
S	2.86981	2.37923	-3.12655
S	-4.63286	0.64061	-3.32882
S	6.8011	2.07653	-0.02533
S	-7.32104	-0.65814	-2.62672
C	0.32982	1.75885	-2.1059
C	-0.64034	1.39293	-1.17109
H	-0.42167	1.27518	-0.11673
C	-1.91276	1.19074	-1.71789
H	-2.77617	0.90943	-1.12552
C	-1.98097	1.39539	-3.09588
C	1.71195	2.01107	-1.85896
C	4.21556	2.48417	-1.97271
C	3.72275	2.25263	-0.6767
H	4.33703	2.30981	0.21086

C	2.35408	1.99285	-0.61718
H	1.82937	1.80374	0.31187
C	-3.11138	1.26785	-3.95234
C	-3.24066	1.56536	-5.31006
H	-2.42444	1.96965	-5.89867
C	-4.50879	1.3057	-5.83115
H	-4.78124	1.48135	-6.86398
C	-5.43002	0.78234	-4.90472
C	5.52709	2.75772	-2.45178
C	6.70443	2.67014	-1.69177
C	8.01704	2.99233	-2.13195
H	8.19867	3.37391	-3.1289
C	9.01115	2.77358	-1.20142
H	10.05999	2.95714	-1.39505
C	8.56315	2.26533	0.04551
C	-6.77834	0.41814	-5.17816
C	-7.68613	-0.18329	-4.29499
C	-9.03334	-0.54064	-4.58106
H	-9.47528	-0.34307	-5.54955
C	-9.70122	-1.15697	-3.54524
H	-10.7243	-1.50271	-3.61661
C	-8.93758	-1.33443	-2.36122
C	9.36265	1.95349	1.16602
H	5.63357	3.03709	-3.47917
H	-7.12825	0.61492	-6.17
H	-10.39807	-2.21651	-1.1058
H	-5.63357	-3.03709	3.47917
H	7.12825	-0.61492	6.17
H	10.39807	2.21651	1.1058