Supporting Information

A theoretical study of electronic structure and charge transport property for thieno[2, 3-*b*]benzothiophene based derivatives

Lijuan Wang, Tao Li, Yuxin Shen, and Yan Song*

School of Materials Science and Engineering, Harbin Institute of Technology at Weihai, 2West Wenhua Road, Weihai, 264209, China

* Corresponding author's email address: sy@hitwh.edu.cn

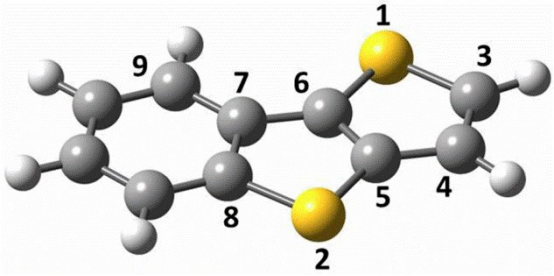

Fig. S1. Optimized ground state geometry structures of TBT. The atom indices are labeled on the molecular structures.

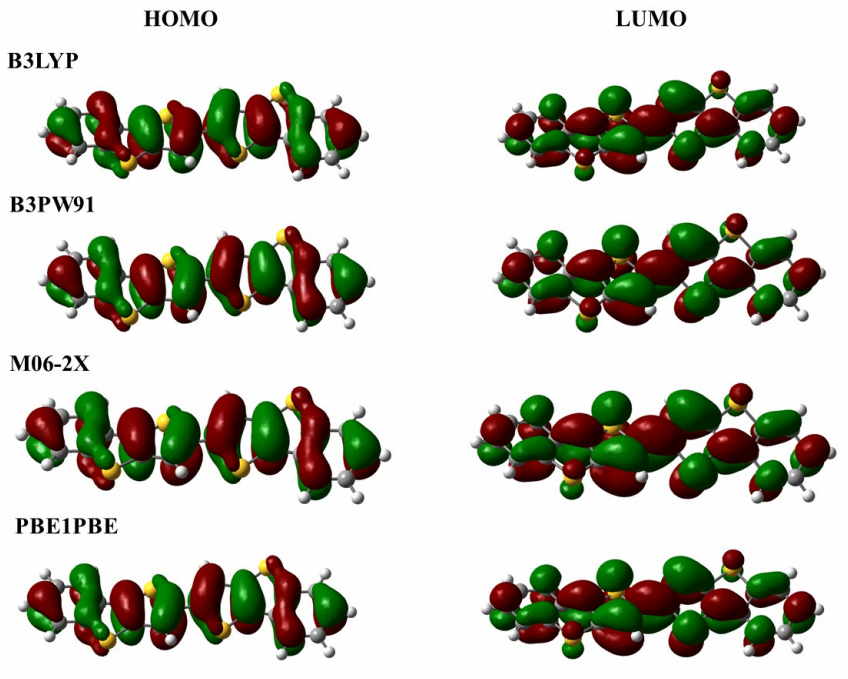

Fig. S2. The frontier orbitals obtained with B3LYP/6-31G**, B3PW91/6-31G**, M06-2X/6-31G** and PBE1PBE/6-31G** basis sets for compound 1.

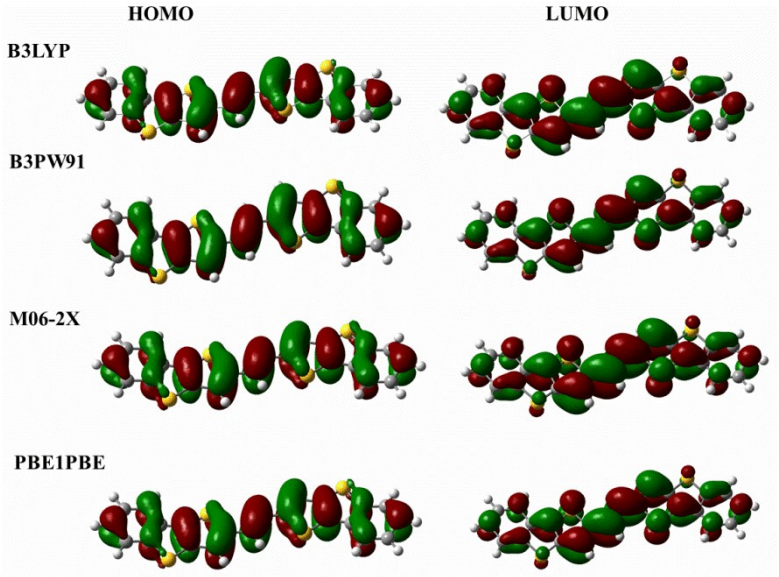

Fig. S3. The frontier orbitals obtained with B3LYP/6-31G**, B3PW91/6-31G**, M06-2X/6-31G** and PBE1PBE/6-31G** basis sets for compound 2.

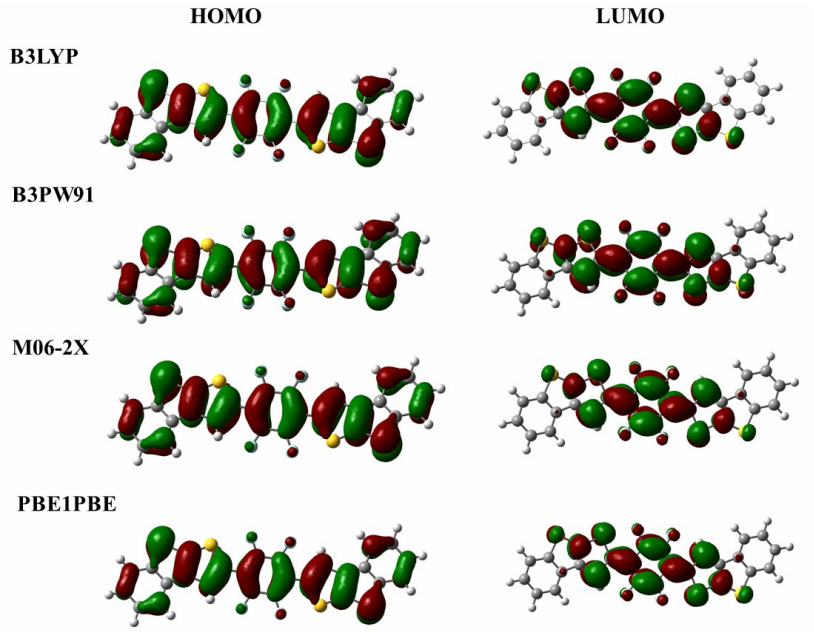

Fig. S4. The frontier orbitals obtained with B3LYP/6-31G**, B3PW91/6-31G**, M06-2X/6-31G** and PBE1PBE/6-31G** basis sets for compound 4.

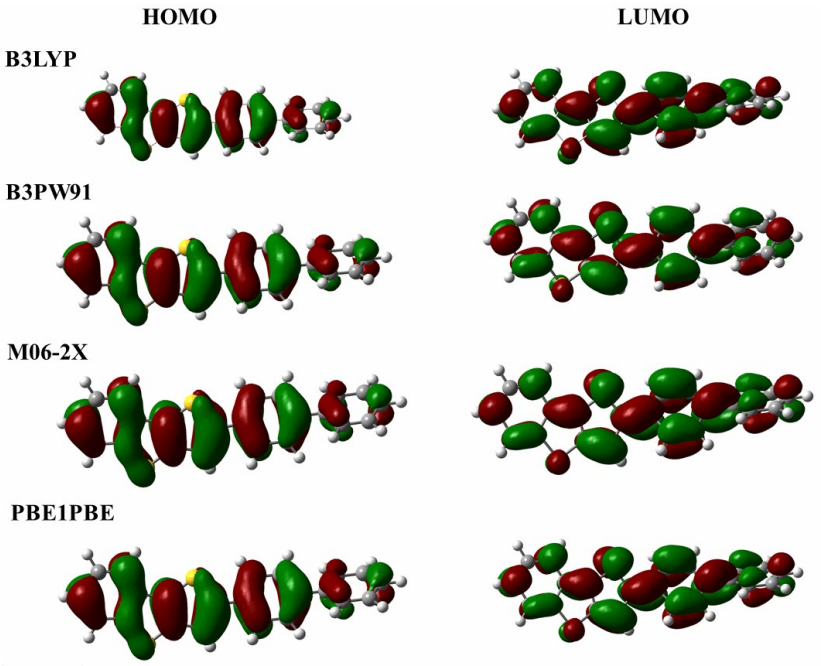

Fig. S5. The frontier orbitals obtained with B3LYP/6-31G**, B3PW91/6-31G**, M06-2X/6-31G** and PBE1PBE/6-31G** basis sets for compound 6.

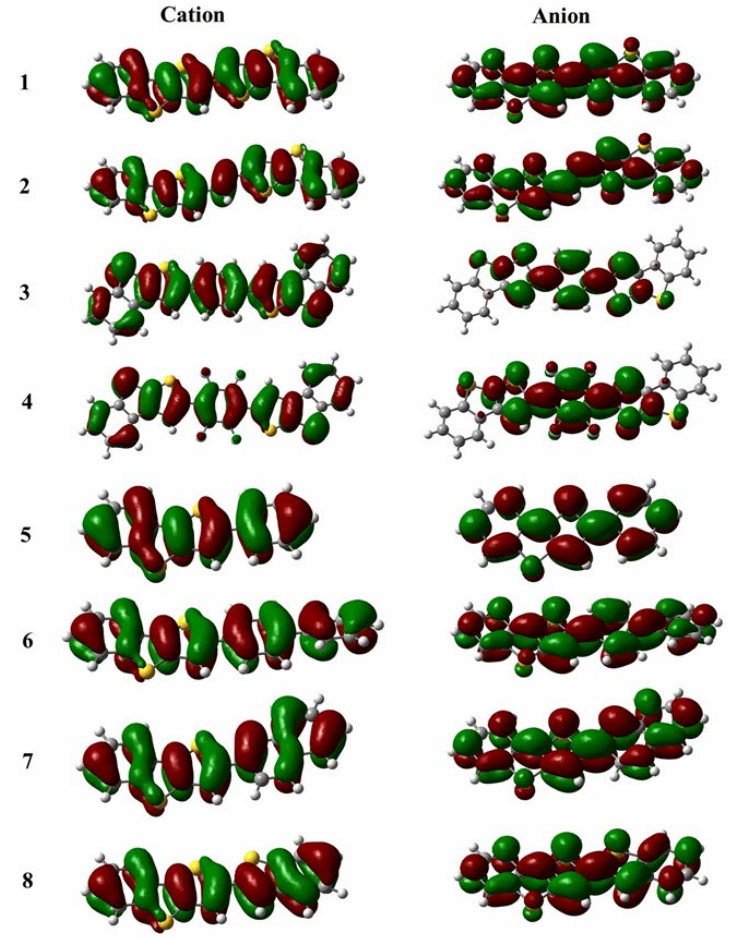

Fig. S6. The SOMO orbitals for the cation and anion of compounds 1 to 8 based on B3LYP/6-31G** basis set

Table S1. Selected Optimized bond parameters of TBT in the neutral and ionic states (the unit of bond lengths is angstroms, the bond angles and dihedral angles is degrees)

TBT	Bond Parameters	Neutral	Cationic	Anionic
	R(C7-C6)	1.44	1.41	1.40
	R(C5-S2)	1.76	1.72	1.78
	R(C5-C6)	1.38	1.44	1.42
	R(C6-S1)	1.74	1.74	1.78
	θ(C9-C7-C8)	119.0	119.5	116.8
	θ(C6-C5-S2)	112.1	112.7	110.0
	θ(S1-C3-C4)	113.0	114.8	111.5
	θ(C7-C6-C5)	114.6	113.8	116.4
	θ(C7-C6-C5-S2)	0.0	0.0	0.0
	θ(C7-C8-S2-C5)	0.0	0.0	0.0

Table S2. Selected Optimized bond parameters of compound 3 in the neutral and ionic states (the unit of bond lengths is angstroms, the bond angles and dihedral angles is degrees)

3	Bond Parameters	Neutral	Cationic	Anionic
	R(S1-C2)	1.78	1.78	1.81
	R(C2-C3)	1.46	1.43	1.43
	R(C2-C6)	1.37	1.40	1.40
	R(C6-C7)	1.43	1.40	1.42
	θ(C6-C2-C3)	128.6	128.4	130.4
	θ(C6-C2-S1)	111.0	110.8	109.6
	θ(C2-C3-C4)	120.5	121.0	121.5
	θ(C2-C3-C5)	122.0	121.9	123.2
	θ(C4-C3-C5)	117.6	117.1	115.4
	θ(C6-C2-C3-C4)	26.3	0.6	1.4
	θ(S1-C2-C3-C5)	27.4	0.6	1.5

Table S3. Selected Optimized bond parameters of compound 5 in the neutral and ionic states (the unit of bond lengths is angstroms, the bond angles and dihedral angles is degrees)

5	Bond Parameters	Neutral	Cationic	Anionic
	R(S1-C2)	1.77	1.78	1.81
	R(C2-C3)	1.47	1.44	1.43
	R(C2-C6)	1.38	1.41	1.42
	R(C6-C7)	1.42	1.39	1.39
	R(C7-C8)	1.38	1.43	1.40
	θ(S1-C2-C6)	111.3	111.4	109.5
	θ(C6-C2-C3)	128.0	127.8	129.3
	θ(C2-C3-C5)	120.2	120.4	121.5
	θ(C6-C7-C8)	114.3	113.8	116.0
	θ(S1-C2-C3-C4)	28.4	0.1	0.0
	θ(S1-C2-C3-C5)	151.9	179.9	180.0

Table S4. Selected Optimized bond parameters of compound 7 in the neutral and ionic states (the unit of bond lengths is angstroms, the bond angles and dihedral angles is degrees)

7	Bond Parameters	Neutral	Cationic	Anionic
	R(S1-C2)	1.77	1.78	1.80
	R(C2-C3)	1.47	1.43	1.43
	R(C2-C6)	1.38	1.40	1.41
	R(C3-C4)	1.39	1.41	1.42
	R(C6-C7)	1.42	1.39	1.40
	R(C7-C8)	1.38	1.42	1.40
	θ(S1-C2-C6)	111.3	111.2	109.7
	θ(C6-C2-C3)	127.9	127.6	129.8
	θ(C2-C3-C4)	122.0	120.9	123.4
	θ(C4-C3-C5)	118.4	118.2	116.2
	θ(S1-C2-C3-C4)	26.2	0.0	0.0
	θ(S1-C2-C3-C5)	153.9	180.0	180.0

Table S5. Selected Optimized bond parameters of compound 8 in the neutral and ionic states (the unit of bond lengths is angstroms, the bond angles and dihedral angles is degrees)

8	Bond Parameters	Neutral	Cationic	Anionic
	R(S1-C2)	1.77	1.78	1.80
	R(C2-C3)	1.45	1.42	1.41
	R(C2-C6)	1.38	1.41	1.42
	R(C6-C7)	1.42	1.39	1.39
	R(C7-C8)	1.39	1.42	1.40
	R(C3-C5)	1.37	1.40	1.40
	θ(S1-C2-C6)	111.6	111.6	110.0
	θ(C2-C3-S4)	121.0	122.6	121.4
	θ(C2-C3-C5)	127.3	125.9	128.9
	θ(S4-C3-C5)	111.7	111.5	109.7
	θ(S1-C2-C3-S4)	29.9	0.0	0.0
	θ(S1-C2-C3-C5)	151.2	180.0	180.0

Table S6 The HOMO, LUMO energies and energy gaps based on B3LYP/6-31G**, B3PW91/6-31G**, M06-2X/6-31G** and PBE1PBE/6-31G** basis sets compared with experimental results (All energies are in unit of eV)

Compd. 1	**B3LYP**	**B3PW91**	**M06-2X**	**PBE1PBE**	**Expt.**
$\mathbf{E_{HOMO}}$**(eV)**	-5.29	-5.43	-6.56	-5.56	-5.46
$\mathbf{E_{LUMO}}$**(eV)**	-1.87	-1.95	-1.01	-1.77	-2.31
$\mathbf{E_{gap}}$**(eV)**	3.42	3.48	5.55	3.79	3.15
Compd. 2					
$\mathbf{E_{HOMO}}$**(eV)**	-5.11	-5.23	-6.34	-5.36	-5.53
$\mathbf{E_{LUMO}}$**(eV)**	-2.10	-2.20	-1.31	-2.03	-2.81
$\mathbf{E_{gap}}$**(eV)**	3.01	3.03	5.03	3.33	2.72
Compd. 4					
$\mathbf{E_{HOMO}}$**(eV)**	-5.43	-5.55	-6.68	-5.68	-5.34
$\mathbf{E_{LUMO}}$**(eV)**	-2.00	-2.07	-1.20	-1.90	-2.31
$\mathbf{E_{gap}}$**(eV)**	3.43	3.48	5.48	3.78	3.03
Compd. 6					
$\mathbf{E_{HOMO}}$**(eV)**	-5.40	-5.54	-6.67	-5.67	-5.53
$\mathbf{E_{LUMO}}$**(eV)**	-1.56	-1.64	-0.70	-1.46	-2.09
$\mathbf{E_{gap}}$**(eV)**	3.84	3.90	5.97	4.21	3.44

Cartesian coordinates of compound TBT for the neutral geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-2.08362100	-1.54709900	-0.00007700	S	2.08453500	-1.54821500	-0.00020600
S	0.07947600	2.06278200	-0.00003500	S	-0.07905600	2.06353900	-0.00001700
C	-3.23963800	-0.23574000	0.00014700	C	3.24079600	-0.23675200	0.00012000
C	-2.64950800	0.99786800	0.00002600	C	2.65065800	0.99958000	-0.00002100
H	-3.20247700	1.92905000	0.00005200	H	3.20433800	1.93065200	0.00002400
C	-1.22896500	0.88832600	-0.00002300	C	1.22918400	0.88948900	-0.00003300
C	-0.75995800	-0.41401800	-0.00001600	C	0.76128200	-0.41492500	-0.00003300
C	0.67164100	-0.53515200	0.00001000	C	-0.67120600	-0.53580100	0.00002800
C	1.49686900	-1.67191900	0.00001800	C	-1.49778800	-1.67348500	0.00003700
H	1.05344400	-2.66337400	0.00001100	H	-1.05522700	-2.66549700	0.00000400
C	2.87724300	-1.51702900	0.00003000	C	-2.88014100	-1.51832000	0.00009100
H	3.51569300	-2.39512600	0.00003800	H	-3.51905200	-2.39628800	0.00010100
C	3.45689300	-0.23787300	0.00003000	C	-3.45993800	-0.23699700	0.00013000
H	4.53770300	-0.13566400	0.00003700	H	-4.54082900	-0.13393700	0.00016700
C	2.66054200	0.90420300	0.00001100	C	-2.66141400	0.90585600	0.00010700
H	3.10989000	1.89247600	0.00000200	H	-3.11072300	1.89441600	0.00012500
C	1.27295900	0.75227000	0.00000100	C	-1.27212200	0.75313800	0.00005600
H	-4.29640300	-0.46391600	0.00026400	H	4.29796800	-0.46522600	0.00024900

Cartesian coordinates of compound TBT for the cationic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-2.04406500	-1.58240100	-0.00003300	S	-2.04397300	-1.58313200	-0.00006000
S	0.04006300	2.08342000	-0.00004200	S	0.03766600	2.08168700	-0.00004800
C	-3.19732900	-0.25906600	0.00012300	C	-3.19949900	-0.25902100	0.00015700
C	-2.63274700	0.99936800	0.00002100	C	-2.63544600	0.99965200	0.00001700
H	-3.21114800	1.91444300	0.00002600	H	-3.21321400	1.91538700	0.00002000
C	-1.22986900	0.91610800	-0.00000800	C	-1.23067800	0.91573800	-0.00001200
C	-0.73948100	-0.43695900	0.00000700	C	-0.74083400	-0.43871900	0.00000600
C	0.66478000	-0.53309500	0.00000500	C	0.66583100	-0.53394100	0.00000900
C	1.50076300	-1.68021300	0.00000500	C	1.50324200	-1.67973700	0.00000700
H	1.06139300	-2.67271600	0.00000500	H	1.06654700	-2.67354700	0.00000200
C	2.87813600	-1.51400200	0.00000800	C	2.88288900	-1.51166900	0.00001700
H	3.52900900	-2.38089800	0.00001000	H	3.53441900	-2.37837900	0.00001900
C	3.43392100	-0.22647300	0.00000600	C	3.43749100	-0.22360700	0.00002100
H	4.51277500	-0.10856500	0.00000400	H	4.51631600	-0.10396000	0.00002300
C	2.62379300	0.93299800	0.00000000	C	2.62415700	0.93541000	0.00001300
H	3.08090400	1.91680800	-0.00000900	H	3.07989400	1.92016000	0.00000500
C	1.25570300	0.76947400	-0.00000200	C	1.25518900	0.76904300	0.00000500
H	-4.25493500	-0.49420200	0.00017900	H	-4.25711400	-0.49542500	0.00023000

Cartesian coordinates of compound TBT for the anionic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	2.09291500	-1.56857000	-0.00003800	S	2.08577700	-1.56929600	-0.00003200
S	-0.08237000	2.07987900	0.00001700	S	-0.07991700	2.08003500	0.00001700
C	3.28038300	-0.23622100	-0.00004000	C	3.27754000	-0.24325000	-0.00003600
C	2.65098700	1.00841500	-0.00002200	C	2.65311000	1.00882700	-0.00002300
H	3.20118200	1.94471600	-0.00002000	H	3.20766200	1.94208300	-0.00002300
C	1.25742800	0.90704800	-0.00000500	C	1.25747000	0.90912800	-0.00001000
C	0.74521300	-0.41200800	-0.00001000	C	0.74742700	-0.41044300	-0.00001200
C	-0.65201000	-0.53743400	0.00000400	C	-0.65222100	-0.53439800	0.00000200
C	-1.51139000	-1.68306800	0.00000400	C	-1.50686800	-1.68435800	0.00000300
H	-1.07563900	-2.67900300	-0.00000900	H	-1.06947800	-2.67935000	-0.00000900
C	-2.89253000	-1.51592900	0.00002100	C	-2.89213600	-1.51832300	0.00001900
H	-3.52731200	-2.40234500	0.00002100	H	-3.52704500	-2.40376600	0.00001900
C	-3.49198500	-0.24829200	0.00003800	C	-3.49099600	-0.24828500	0.00003500
H	-4.57358900	-0.14427100	0.00005200	H	-4.57266000	-0.14511600	0.00004500
C	-2.66424900	0.90626800	0.00003700	C	-2.66383400	0.91025900	0.00003600
H	-3.10757800	1.89999400	0.00004900	H	-3.10930800	1.90268400	0.00004900
C	-1.29227700	0.75467900	0.00002000	C	-1.28895100	0.75795000	0.00002100
H	4.33679400	-0.46079500	-0.00004700	H	4.33382000	-0.47100900	-0.00005800

Frequency coordinates of compound TBT for the optimized neutral geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-2.08362100	-1.54709900	-0.00007700	S	2.08453500	-1.54821500	-0.00020600
S	0.07947600	2.06278200	-0.00003500	S	-0.07905600	2.06353900	-0.00001700
C	-3.23963800	-0.23574000	0.00014700	C	3.24079600	-0.23675200	0.00012000
C	-2.64950800	0.99786800	0.00002600	C	2.65065800	0.99958000	-0.00002100
H	-3.20247700	1.92905000	0.00005200	H	3.20433800	1.93065200	0.00002400
C	-1.22896500	0.88832600	-0.00002300	C	1.22918400	0.88948900	-0.00003300
C	-0.75995800	-0.41401800	-0.00001600	C	0.76128200	-0.41492500	-0.00003300
C	0.67164100	-0.53515200	0.00001000	C	-0.67120600	-0.53580100	0.00002800
C	1.49686900	-1.67191900	0.00001800	C	-1.49778800	-1.67348500	0.00003700
H	1.05344400	-2.66337400	0.00001100	H	-1.05522700	-2.66549700	0.00000400
C	2.87724300	-1.51702900	0.00003000	C	-2.88014100	-1.51832000	0.00009100
H	3.51569300	-2.39512600	0.00003800	H	-3.51905200	-2.39628800	0.00010100
C	3.45689300	-0.23787300	0.00003000	C	-3.45993800	-0.23699700	0.00013000
H	4.53770300	-0.13566400	0.00003700	H	-4.54082900	-0.13393700	0.00016700
C	2.66054200	0.90420300	0.00001100	C	-2.66141400	0.90585600	0.00010700
H	3.10989000	1.89247600	0.00000200	H	-3.11072300	1.89441600	0.00012500
C	1.27295900	0.75227000	0.00000000	C	-1.27212200	0.75313800	0.00005600
H	-4.29640300	-0.46391600	0.00026400	H	4.29796800	-0.46522600	0.00024900

Frequency coordinates of compound TBT for the optimized cationic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-2.04406500	-1.58240100	-0.00003300	S	-2.04397300	-1.58313200	-0.00006000
S	0.04006300	2.08342000	-0.00004200	S	0.03766600	2.08168700	-0.00004800
C	-3.19732900	-0.25906600	0.00012300	C	-3.19949900	-0.25902100	0.00015700
C	-2.63274700	0.99936800	0.00002100	C	-2.63544600	0.99965200	0.00001700
H	-3.21114800	1.91444300	0.00002600	H	-3.21321400	1.91538700	0.00002000
C	-1.22986900	0.91610800	-0.00000800	C	-1.23067800	0.91573800	-0.00001200
C	-0.73948100	-0.43695900	0.00000700	C	-0.74083400	-0.43871900	0.00000600
C	0.66478000	-0.53309500	0.00000500	C	0.66583100	-0.53394100	0.00000900
C	1.50076300	-1.68021300	0.00000500	C	1.50324200	-1.67973700	0.00000700
H	1.06139300	-2.67271600	0.00000500	H	1.06654700	-2.67354700	0.00000200
C	2.87813600	-1.51400200	0.00000800	C	2.88288900	-1.51166900	0.00001700
H	3.52900900	-2.38089800	0.00001000	H	3.53441900	-2.37837900	0.00001900
C	3.43392100	-0.22647300	0.00000600	C	3.43749100	-0.22360700	0.00002100
H	4.51277500	-0.10856500	0.00000400	H	4.51631600	-0.10396000	0.00002300
C	2.62379300	0.93299800	0.00000000	C	2.62415700	0.93541000	0.00001300
H	3.08090400	1.91680800	-0.00000900	H	3.07989400	1.92016000	0.00000500
C	1.25570300	0.76947400	-0.00000200	C	1.25518900	0.76904300	0.00000500
H	-4.25493500	-0.49420200	0.00017900	H	-4.25711400	-0.49542600	0.00023000

Frequency coordinates of compound TBT for the optimized anionic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	2.09291500	-1.56857000	-0.00003800	S	2.08577700	-1.56929600	-0.00003200
S	-0.08237000	2.07987900	0.00001700	S	-0.07991700	2.08003500	0.00001700
C	3.28038300	-0.23622100	-0.00004000	C	3.27754000	-0.24325000	-0.00003600
C	2.65098700	1.00841500	-0.00002200	C	2.65311000	1.00882700	-0.00002300
H	3.20118200	1.94471600	-0.00002000	H	3.20766200	1.94208300	-0.00002300
C	1.25742800	0.90704800	-0.00000500	C	1.25747000	0.90912800	-0.00001000
C	0.74521300	-0.41200800	-0.00001000	C	0.74742700	-0.41044300	-0.00001200
C	-0.65201000	-0.53743400	0.00000400	C	-0.65222100	-0.53439800	0.00000200
C	-1.51139000	-1.68306800	0.00000400	C	-1.50686800	-1.68435800	0.00000300
H	-1.07563900	-2.67900300	-0.00000900	H	-1.06947800	-2.67935000	-0.00000900
C	-2.89253000	-1.51592900	0.00002100	C	-2.89213600	-1.51832300	0.00001900
H	-3.52731200	-2.40234500	0.00002100	H	-3.52704500	-2.40376600	0.00001900
C	-3.49198500	-0.24829200	0.00003800	C	-3.49099600	-0.24828500	0.00003500
H	-4.57358900	-0.14427100	0.00005200	H	-4.57266000	-0.14511600	0.00004500
C	-2.66424900	0.90626800	0.00003700	C	-2.66383400	0.91025900	0.00003600
H	-3.10757800	1.89999400	0.00004900	H	-3.10930800	1.90268400	0.00004900
C	-1.29227700	0.75467900	0.00002000	C	-1.28895100	0.75795000	0.00002100
H	4.33679400	-0.46079500	-0.00004700	H	4.33382000	-0.47100900	-0.00005800

Cartesian coordinates of compound 1 for the neutral geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	1.78317100	-1.29728500	-0.21890800	S	1.78222500	1.28937400	-0.25186900
S	4.23773600	2.07519100	0.34792200	S	4.24069900	-2.06560200	0.39736300
C	0.71751200	0.08954400	0.05949200	C	0.71853700	-0.08961200	0.06358600
C	1.43756700	1.25188500	0.24791700	C	1.43913600	-1.24854400	0.27972200
H	0.97316300	2.20958800	0.44941200	H	0.97553600	-2.20099700	0.50712300
C	2.83539900	1.02823900	0.17970300	C	2.83806300	-1.02522000	0.20302400
C	3.19391700	-0.28952700	-0.05357200	C	3.19403600	0.28821600	-0.06371100
C	4.60763200	-0.52513900	-0.10843400	C	4.60855400	0.52336300	-0.12418700
C	5.33399000	-1.70929700	-0.32158500	C	5.33539900	1.70307700	-0.36707700
H	4.80851500	-2.64682600	-0.47796200	H	4.81061000	2.63682100	-0.54745700
C	6.72205000	-1.66892800	-0.32989800	C	6.72533300	1.66350500	-0.37356600
H	7.28433600	-2.58290200	-0.49427800	H	7.28732100	2.57345900	-0.56054700
C	7.40734800	-0.45964700	-0.12818500	C	7.41184400	0.45829300	-0.14065900
H	8.49279700	-0.44707000	-0.13804900	H	8.49741300	0.44550000	-0.14931300
C	6.71045600	0.72691500	0.08535500	C	6.71367000	-0.72377800	0.10244500
H	7.24214400	1.66035800	0.24163300	H	7.24611200	-1.65276100	0.28249200
C	5.31555300	0.69095900	0.09490500	C	5.31703500	-0.68809400	0.11015400
S	-1.78317100	1.29729100	-0.21884400	S	-1.78224900	-1.28941600	-0.25178100

S	-4.23774000	-2.07518800	0.34794700	S	-4.24067300	2.06560800	0.39739300
C	-0.71751100	-0.08954400	0.05950700	C	-0.71854000	0.08953300	0.06360400
C	-1.43756700	-1.25188000	0.24795900	C	-1.43912000	1.24848700	0.27980400
H	-0.97316500	-2.20958200	0.44945300	H	-0.97545500	2.20091300	0.50720200
C	-2.83540300	-1.02823200	0.17975900	C	-2.83804200	1.02518900	0.20314600
C	-3.19391800	0.28953300	-0.05351600	C	-3.19405500	-0.28825400	-0.06359300
C	-4.60763200	0.52513900	-0.10842000	C	-4.60856100	-0.52335600	-0.12415600
C	-5.33398900	1.70929400	-0.32157200	C	-5.33543100	-1.70305900	-0.36705300
H	-4.80851400	2.64683000	-0.47793000	H	-4.81065300	-2.63682700	-0.54739200
C	-6.72204800	1.66892000	-0.32992200	C	-6.72535500	-1.66343300	-0.37360400
H	-7.28433000	2.58289400	-0.49430300	H	-7.28737400	-2.57336300	-0.56059200
C	-7.40734400	0.45963600	-0.12823900	C	-7.41184000	-0.45821100	-0.14074800
H	-8.49279300	0.44705700	-0.13812800	H	-8.49740700	-0.44539000	-0.14945000
C	-6.71045400	-0.72692400	0.08530800	C	-6.71365000	0.72384300	0.10237400
H	-7.24214400	-1.66037500	0.24156900	H	-7.24609000	1.65284400	0.28239000
C	-5.31555300	-0.69096400	0.09488900	C	-5.31701900	0.68811800	0.11013700

Cartesian coordinates of compound 1 for the cationic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-1.29344600	-0.56167000	1.72058300	S	-1.29386100	-0.56127000	1.72060100
S	-4.56087800	1.08673000	-0.38277100	S	-4.56231900	1.08696600	-0.38155200
C	-0.68346200	0.05642600	0.16623400	C	-0.68416900	0.05663100	0.16643200
C	-1.71424200	0.62617300	-0.60236900	C	-1.71537600	0.62718200	-0.60306900
H	-1.54959200	1.05894300	-1.58194200	H	-1.55143300	1.06012600	-1.58283300
C	-2.94632200	0.56482000	0.04073600	C	-2.94819100	0.56553200	0.04123600
C	-2.89875600	-0.05042400	1.31472100	C	-2.89883700	-0.05043800	1.31591900
C	-4.15026800	-0.11753500	1.97809100	C	-4.15145300	-0.11764200	1.97971900
C	-4.48662200	-0.65179400	3.24145100	C	-4.48885100	-0.65205500	3.24375200
H	-3.71968700	-1.10095800	3.86466800	H	-3.72294000	-1.10143700	3.86838400
C	-5.80157200	-0.59375900	3.66920100	C	-5.80542300	-0.59423200	3.67171800
H	-6.07380000	-1.00009200	4.63708700	H	-6.07783500	-1.00065400	4.63975100
C	-6.79275400	-0.01031000	2.85729600	C	-6.79725700	-0.01040600	2.85860000
H	-7.81820800	0.02567200	3.21053500	H	-7.82315200	0.02557400	3.21105700
C	-6.48748000	0.52513500	1.60419500	C	-6.49035000	0.52525800	1.60465400
H	-7.26337100	0.97121400	0.99135200	H	-7.26636500	0.97127800	0.99141700
C	-5.16832300	0.47006800	1.16799400	C	-5.16950900	0.47025700	1.16862800
S	1.29344600	0.56167000	-1.72058300	S	1.29386100	0.56127000	-1.72060100
S	4.56087800	-1.08673000	0.38277100	S	4.56231900	-1.08696600	0.38155200
C	0.68346200	-0.05642600	-0.16623400	C	0.68416900	-0.05663100	-0.16643200
C	1.71424200	-0.62617300	0.60236900	C	1.71537600	-0.62718200	0.60306900
H	1.54959200	-1.05894300	1.58194200	H	1.55143300	-1.06012600	1.58283300
C	2.94632200	-0.56482000	-0.04073600	C	2.94819100	-0.56553200	-0.04123600
C	2.89875600	0.05042400	-1.31472100	C	2.89883700	0.05043800	-1.31591900

C	4.15026800	0.11753500	-1.97809100	C	4.15145300	0.11764200	-1.97971900
C	4.48662200	0.65179400	-3.24145100	C	4.48885100	0.65205500	-3.24375200
H	3.71968700	1.10095800	-3.86466800	H	3.72294000	1.10143700	-3.86838400
C	5.80157200	0.59375900	-3.66920100	C	5.80542300	0.59423200	-3.67171800
H	6.07380000	1.00009200	-4.63708700	H	6.07783500	1.00065400	-4.63975100
C	6.79275400	0.01031000	-2.85729600	C	6.79725700	0.01040600	-2.85860000
H	7.81820800	-0.02567200	-3.21053500	H	7.82315200	-0.02557400	-3.21105700
C	6.48748000	-0.52513500	-1.60419500	C	6.49035000	-0.52525800	-1.60465400
H	7.26337100	-0.97121400	-0.99135200	H	7.26636500	-0.97127800	-0.99141700
C	5.16832300	-0.47006800	-1.16799400	C	5.16950900	-0.47025700	-1.16862800

Cartesian coordinates of compound 1 for the anionic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-1.30381000	-0.56422300	1.72990600	S	-1.30463600	-0.56227100	1.72738800
S	-4.60033000	1.07907000	-0.34958400	S	-4.60097100	1.08073900	-0.35084600
C	-0.68190300	0.05894700	0.16027900	C	-0.68294400	0.05961500	0.15989300
C	-1.73496500	0.62523300	-0.59119600	C	-1.73419400	0.62785700	-0.59563500
H	-1.58246800	1.06063000	-1.57112800	H	-1.58132200	1.06294100	-1.57579100
C	-2.96226000	0.55359700	0.07161600	C	-2.96419600	0.55645000	0.06840600
C	-2.94146600	-0.05053600	1.33324800	C	-2.93997100	-0.04838200	1.33019400
C	-4.19075800	-0.11838600	1.99704400	C	-4.18981500	-0.11704700	1.99547800
C	-4.55051800	-0.64726400	3.25897300	C	-4.54722100	-0.64728300	3.25892600
H	-3.78772800	-1.09809200	3.88774400	H	-3.78387600	-1.09772700	3.88743000
C	-5.87254100	-0.58799100	3.68678100	C	-5.87123800	-0.58937200	3.68891700
H	-6.13479400	-0.99845800	4.65936900	H	-6.13278900	-1.00007800	4.66141200
C	-6.87250000	-0.01040000	2.89038300	C	-6.87321500	-0.01129200	2.89135100
H	-7.89971300	0.02682700	3.24147600	H	-7.90044900	0.02495300	3.24261800
C	-6.54395500	0.52160100	1.63477200	C	-6.54506200	0.52214300	1.63350100
H	-7.31118600	0.97160600	1.00982000	H	-7.31366600	0.97141300	1.00962600
C	-5.22728100	0.46655800	1.19998400	C	-5.22669900	0.46808700	1.19766600
S	1.30381000	0.56422300	-1.72990600	S	1.30463600	0.56227100	-1.72738800
S	4.60033000	-1.07907000	0.34958400	S	4.60097100	-1.08073900	0.35084600
C	0.68190300	-0.05894700	-0.16027900	C	0.68294400	-0.05961500	-0.15989300
C	1.73496500	-0.62523300	0.59119600	C	1.73419400	-0.62785700	0.59563500
H	1.58246800	-1.06063000	1.57112800	H	1.58132200	-1.06294100	1.57579100
C	2.96226000	-0.55359700	-0.07161600	C	2.96419600	-0.55645000	-0.06840600
C	2.94146600	0.05053600	-1.33324800	C	2.93997100	0.04838200	-1.33019400
C	4.19075800	0.11838600	-1.99704400	C	4.18981500	0.11704700	-1.99547800
C	4.55051800	0.64726400	-3.25897300	C	4.54722100	0.64728300	-3.25892600
H	3.78772800	1.09809200	-3.88774400	H	3.78387600	1.09772700	-3.88743000
C	5.87254100	0.58799100	-3.68678100	C	5.87123800	0.58937200	-3.68891700
H	6.13479400	0.99845800	-4.65936900	H	6.13278900	1.00007800	-4.66141200
C	6.87250000	0.01040000	-2.89038300	C	6.87321500	0.01129200	-2.89135100

H	7.89971300	-0.02682700	-3.24147600	H	7.90044900	-0.02495300	-3.24261800
C	6.54395500	-0.52160100	-1.63477200	C	6.54506200	-0.52214300	-1.63350100
H	7.31118600	-0.97160600	-1.00982000	H	7.31366600	-0.97141300	-1.00962600
C	5.22728100	-0.46655800	-1.19998400	C	5.22669900	-0.46808700	-1.19766600

Frequency coordinates of compound 1 for the optimized neutral geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	1.78317100	-1.29728500	-0.21890800	S	1.78222500	1.28937400	-0.25186900
S	4.23773600	2.07519100	0.34792200	S	4.24069900	-2.06560200	0.39736300
C	0.71751200	0.08954400	0.05949200	C	0.71853700	-0.08961200	0.06358600
C	1.43756700	1.25188500	0.24791700	C	1.43913600	-1.24854400	0.27972200
H	0.97316300	2.20958800	0.44941200	H	0.97553600	-2.20099700	0.50712300
C	2.83539900	1.02823900	0.17970300	C	2.83806300	-1.02522000	0.20302400
C	3.19391700	-0.28952700	-0.05357200	C	3.19403600	0.28821600	-0.06371100
C	4.60763200	-0.52513900	-0.10843400	C	4.60855400	0.52336300	-0.12418700
C	5.33399000	-1.70929700	-0.32158500	C	5.33539900	1.70307700	-0.36707700
H	4.80851500	-2.64682600	-0.47796200	H	4.81061000	2.63682100	-0.54745700
C	6.72205000	-1.66892800	-0.32989800	C	6.72533300	1.66350500	-0.37356600
H	7.28433600	-2.58290200	-0.49427800	H	7.28732100	2.57345900	-0.56054700
C	7.40734800	-0.45964700	-0.12818500	C	7.41184400	0.45829300	-0.14065900
H	8.49279700	-0.44707000	-0.13804900	H	8.49741300	0.44550000	-0.14931300
C	6.71045600	0.72691500	0.08535500	C	6.71367000	-0.72377800	0.10244500
H	7.24214400	1.66035800	0.24163300	H	7.24611200	-1.65276100	0.28249200
C	5.31555300	0.69095900	0.09490500	C	5.31703500	-0.68809400	0.11015400
S	-1.78317100	1.29729100	-0.21884400	S	-1.78224900	-1.28941600	-0.25178100
S	-4.23774000	-2.07518800	0.34794700	S	-4.24067300	2.06560800	0.39739300
C	-0.71751100	-0.08954400	0.05950700	C	-0.71854000	0.08953300	0.06360400
C	-1.43756700	-1.25188000	0.24795900	C	-1.43912000	1.24848700	0.27980400
H	-0.97316500	-2.20958200	0.44945300	H	-0.97545500	2.20091300	0.50720200
C	-2.83540300	-1.02823200	0.17975900	C	-2.83804200	1.02518900	0.20314600
C	-3.19391800	0.28953300	-0.05351600	C	-3.19405500	-0.28825400	-0.06359300
C	-4.60763200	0.52513900	-0.10842000	C	-4.60856100	-0.52335600	-0.12415600
C	-5.33398900	1.70929400	-0.32157200	C	-5.33543100	-1.70305900	-0.36705300
H	-4.80851400	2.64683000	-0.47793000	H	-4.81065300	-2.63682700	-0.54739200
C	-6.72204800	1.66892000	-0.32992200	C	-6.72535500	-1.66343300	-0.37360400
H	-7.28433000	2.58289400	-0.49430300	H	-7.28737400	-2.57336300	-0.56059200
C	-7.40734400	0.45963600	-0.12823900	C	-7.41184000	-0.45821100	-0.14074800
H	-8.49279300	0.44705700	-0.13812800	H	-8.49740700	-0.44539000	-0.14945000
C	-6.71045400	-0.72692400	0.08530800	C	-6.71365000	0.72384300	0.10237400
H	-7.24214400	-1.66037500	0.24156900	H	-7.24609000	1.65284400	0.28239000
C	-5.31555300	-0.69096400	0.09488900	C	-5.31701900	0.68811800	0.11013700

Frequency coordinates of compound 1 for the optimized cationic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-1.29344600	-0.56167000	1.72058300	S	-1.29386100	-0.56127000	1.72060100
S	-4.56087800	1.08673000	-0.38277100	S	-4.56231900	1.08696600	-0.38155200
C	-0.68346200	0.05642600	0.16623400	C	-0.68416900	0.05663100	0.16643200
C	-1.71424200	0.62617300	-0.60236900	C	-1.71537600	0.62718200	-0.60306900
H	-1.54959200	1.05894300	-1.58194200	H	-1.55143300	1.06012600	-1.58283300
C	-2.94632200	0.56482000	0.04073600	C	-2.94819100	0.56553200	0.04123600
C	-2.89875600	-0.05042400	1.31472100	C	-2.89883700	-0.05043800	1.31591900
C	-4.15026800	-0.11753500	1.97809100	C	-4.15145300	-0.11764200	1.97971900
C	-4.48662200	-0.65179400	3.24145100	C	-4.48885100	-0.65205500	3.24375200
H	-3.71968700	-1.10095800	3.86466800	H	-3.72294000	-1.10143700	3.86838400
C	-5.80157200	-0.59375900	3.66920100	C	-5.80542300	-0.59423200	3.67171800
H	-6.07380000	-1.00009200	4.63708700	H	-6.07783500	-1.00065400	4.63975100
C	-6.79275400	-0.01031000	2.85729600	C	-6.79725700	-0.01040600	2.85860000
H	-7.81820800	0.02567200	3.21053500	H	-7.82315200	0.02557400	3.21105700
C	-6.48748000	0.52513500	1.60419500	C	-6.49035000	0.52525800	1.60465400
H	-7.26337100	0.97121400	0.99135200	H	-7.26636500	0.97127800	0.99141700
C	-5.16832300	0.47006800	1.16799400	C	-5.16950900	0.47025700	1.16862800
S	1.29344600	0.56167000	-1.72058300	S	1.29386100	0.56127000	-1.72060100
S	4.56087800	-1.08673000	0.38277100	S	4.56231900	-1.08696600	0.38155200
C	0.68346200	-0.05642600	-0.16623400	C	0.68416900	-0.05663100	-0.16643200
C	1.71424200	-0.62617300	0.60236900	C	1.71537600	-0.62718200	0.60306900
H	1.54959200	-1.05894300	1.58194200	H	1.55143300	-1.06012600	1.58283300
C	2.94632200	-0.56482000	-0.04073600	C	2.94819100	-0.56553200	-0.04123600
C	2.89875600	0.05042400	-1.31472100	C	2.89883700	0.05043800	-1.31591900
C	4.15026800	0.11753500	-1.97809100	C	4.15145300	0.11764200	-1.97971900
C	4.48662200	0.65179400	-3.24145100	C	4.48885100	0.65205500	-3.24375200
H	3.71968700	1.10095800	-3.86466800	H	3.72294000	1.10143700	-3.86838400
C	5.80157200	0.59375900	-3.66920100	C	5.80542300	0.59423200	-3.67171800
H	6.07380000	1.00009200	-4.63708700	H	6.07783500	1.00065400	-4.63975100
C	6.79275400	0.01031000	-2.85729600	C	6.79725700	0.01040600	-2.85860000
H	7.81820800	-0.02567200	-3.21053500	H	7.82315200	-0.02557400	-3.21105700
C	6.48748000	-0.52513500	-1.60419500	C	6.49035000	-0.52525800	-1.60465400
H	7.26337100	-0.97121400	-0.99135200	H	7.26636500	-0.97127800	-0.99141700
C	5.16832300	-0.47006800	-1.16799400	C	5.16950900	-0.47025700	-1.16862800

Frequency coordinates of compound 1 for the optimized anionic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-1.30381000	-0.56422300	1.72990600	S	-1.30463600	-0.56227100	1.72738800
S	-4.60033000	1.07907000	-0.34958400	S	-4.60097100	1.08073900	-0.35084600
C	-0.68190300	0.05894700	0.16027900	C	-0.68294400	0.05961500	0.15989300

C	-1.73496500	0.62523300	-0.59119600	C	-1.73419400	0.62785700	-0.59563500
H	-1.58246800	1.06063000	-1.57112800	H	-1.58132200	1.06294100	-1.57579100
C	-2.96226000	0.55359700	0.07161600	C	-2.96419600	0.55645000	0.06840600
C	-2.94146600	-0.05053600	1.33324800	C	-2.93997100	-0.04838200	1.33019400
C	-4.19075800	-0.11838600	1.99704400	C	-4.18981500	-0.11704700	1.99547800
C	-4.55051800	-0.64726400	3.25897300	C	-4.54722100	-0.64728300	3.25892600
H	-3.78772800	-1.09809200	3.88774400	H	-3.78387600	-1.09772700	3.88743000
C	-5.87254100	-0.58799100	3.68678100	C	-5.87123800	-0.58937200	3.68891700
H	-6.13479400	-0.99845800	4.65936900	H	-6.13278900	-1.00007800	4.66141200
C	-6.87250000	-0.01040000	2.89038300	C	-6.87321500	-0.01129200	2.89135100
H	-7.89971300	0.02682700	3.24147600	H	-7.90044900	0.02495300	3.24261800
C	-6.54395500	0.52160100	1.63477200	C	-6.54506200	0.52214300	1.63350100
H	-7.31118600	0.97160600	1.00982000	H	-7.31366600	0.97141300	1.00962600
C	-5.22728100	0.46655800	1.19998400	C	-5.22669900	0.46808700	1.19766600
S	1.30381000	0.56422300	-1.72990600	S	1.30463600	0.56227100	-1.72738800
S	4.60033000	-1.07907000	0.34958400	S	4.60097100	-1.08073900	0.35084600
C	0.68190300	-0.05894700	-0.16027900	C	0.68294400	-0.05961500	-0.15989300
C	1.73496500	-0.62523300	0.59119600	C	1.73419400	-0.62785700	0.59563500
H	1.58246800	-1.06063000	1.57112800	H	1.58132200	-1.06294100	1.57579100
C	2.96226000	-0.55359700	-0.07161600	C	2.96419600	-0.55645000	-0.06840600
C	2.94146600	0.05053600	-1.33324800	C	2.93997100	0.04838200	-1.33019400
C	4.19075800	0.11838600	-1.99704400	C	4.18981500	0.11704700	-1.99547800
C	4.55051800	0.64726400	-3.25897300	C	4.54722100	0.64728300	-3.25892600
H	3.78772800	1.09809200	-3.88774400	H	3.78387600	1.09772700	-3.88743000
C	5.87254100	0.58799100	-3.68678100	C	5.87123800	0.58937200	-3.68891700
H	6.13479400	0.99845800	-4.65936900	H	6.13278900	1.00007800	-4.66141200
C	6.87250000	0.01040000	-2.89038300	C	6.87321500	0.01129200	-2.89135100
H	7.89971300	-0.02682700	-3.24147600	H	7.90044900	-0.02495300	-3.24261800
C	6.54395500	-0.52160100	-1.63477200	C	6.54506200	-0.52214300	-1.63350100
H	7.31118600	-0.97160600	-1.00982000	H	7.31366600	-0.97141300	-1.00962600
C	5.22728100	-0.46655800	-1.19998400	C	5.22669900	-0.46808700	-1.19766600

Cartesian coordinates of compound 2 for the neutral geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	4.60792400	3.26126800	1.92693000	S	4.61115900	3.26148400	1.92793200
S	2.95468600	-0.16201100	0.11235100	S	2.95663100	-0.16239500	0.11496300
C	5.96178200	2.20516500	1.48744200	C	5.96442800	2.20635400	1.48844400
C	7.31424800	2.46944500	1.70601500	C	7.31850400	2.47195600	1.70645600
H	7.62863600	3.39085400	2.18620300	H	7.63305100	3.39384900	2.18613500
C	8.25347300	1.52675400	1.29536300	C	8.25988100	1.52910200	1.29555100
H	9.30937000	1.71870100	1.45869100	H	9.31575400	1.72241900	1.45824400
C	7.84952400	0.33361200	0.67380900	C	7.85597700	0.33361600	0.67408200
H	8.59790800	-0.38797600	0.36115500	H	8.60470600	-0.38776800	0.36134300

C	6.50468300	0.06632400	0.45442700	C	6.50934000	0.06532100	0.45554300
H	6.19704500	-0.85742100	-0.02674100	H	6.20315500	-0.85940300	-0.02497900
C	5.53687200	1.00190200	0.85965800	C	5.54010600	1.00139700	0.86092200
C	4.10748900	0.97625900	0.75475600	C	4.10994600	0.97524000	0.75646300
C	3.46910800	2.09328200	1.27071900	C	3.47268100	2.09406200	1.27301000
C	2.05834600	2.05886000	1.16212500	C	2.06038100	2.06022900	1.16437500
H	1.38754200	2.83688200	1.50660300	H	1.38957300	2.83871800	1.50851800
C	1.60622500	0.90094300	0.55495400	C	1.60878500	0.90046800	0.55625700
C	0.23099000	0.56395600	0.29701600	C	0.23166000	0.56418300	0.29779900
H	-0.48063800	1.31901900	0.62826300	H	-0.47880300	1.32004000	0.62999100
S	-4.60792400	-3.26126800	-1.92693000	S	-4.61115900	-3.26148400	-1.92793200
S	-2.95468600	0.16201100	-0.11235100	S	-2.95663100	0.16239500	-0.11496300
C	-5.96178200	-2.20516500	-1.48744200	C	-5.96442800	-2.20635400	-1.48844400
C	-7.31424800	-2.46944500	-1.70601500	C	-7.31850400	-2.47195600	-1.70645600
H	-7.62863600	-3.39085400	-2.18620300	H	-7.63305100	-3.39384900	-2.18613500
C	-8.25347300	-1.52675400	-1.29536300	C	-8.25988100	-1.52910200	-1.29555100
H	-9.30937000	-1.71870100	-1.45869100	H	-9.31575400	-1.72241900	-1.45824400
C	-7.84952400	-0.33361200	-0.67380900	C	-7.85597700	-0.33361600	-0.67408200
H	-8.59790800	0.38797600	-0.36115500	H	-8.60470600	0.38776800	-0.36134300
C	-6.50468300	-0.06632400	-0.45442700	C	-6.50934000	-0.06532100	-0.45554300
H	-6.19704500	0.85742100	0.02674100	H	-6.20315500	0.85940300	0.02497900
C	-5.53687200	-1.00190200	-0.85965800	C	-5.54010600	-1.00139700	-0.86092200
C	-4.10748900	-0.97625900	-0.75475600	C	-4.10994600	-0.97524000	-0.75646300
C	-3.46910800	-2.09328200	-1.27071900	C	-3.47268100	-2.09406200	-1.27301000
C	-2.05834600	-2.05886000	-1.16212500	C	-2.06038100	-2.06022900	-1.16437500
H	-1.38754200	-2.83688200	-1.50660300	H	-1.38957300	-2.83871800	-1.50851800
C	-1.60622500	-0.90094300	-0.55495400	C	-1.60878500	-0.90046800	-0.55625700
C	-0.23099000	-0.56395600	-0.29701600	C	-0.23166000	-0.56418300	-0.29779900
H	0.48063800	-1.31901900	-0.62826300	H	0.47880300	-1.32004000	-0.62999100

Cartesian coordinates of compound 2 for the cationic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	4.56683300	3.26853500	1.92816300	S	4.56975000	3.26874100	1.92887500
S	2.93866700	-0.17538800	0.10484600	S	2.94007600	-0.17536700	0.10662000
C	5.91323400	2.20233600	1.48295300	C	5.91559300	2.20301900	1.48371500
C	7.26322900	2.46316300	1.69946700	C	7.26706700	2.46496000	1.69998000
H	7.58681600	3.38107200	2.17843100	H	7.59062200	3.38335700	2.17866900
C	8.19561800	1.51231000	1.28418700	C	8.20130700	1.51418700	1.28457600
H	9.25171800	1.70218700	1.44626700	H	9.25742800	1.70514900	1.44630700
C	7.79549500	0.31495800	0.66094000	C	7.80123300	0.31518600	0.66128800
H	8.54648500	-0.40314400	0.35015900	H	8.55250600	-0.40286200	0.35034300
C	6.45475300	0.04892200	0.44265700	C	6.45892600	0.04830900	0.44349200
H	6.14333100	-0.87335100	-0.03782000	H	6.14906900	-0.87484300	-0.03668800

C	5.49012200	0.99411300	0.85289200	C	5.49300800	0.99365000	0.85378300
C	4.07414600	0.96677700	0.74812800	C	4.07593300	0.96599000	0.74914100
C	3.42965800	2.10799700	1.27583700	C	3.43253400	2.10876400	1.27741700
C	2.04288800	2.07054300	1.16715400	C	2.04442300	2.07201100	1.16894900
H	1.36571600	2.84429300	1.50910600	H	1.36742700	2.84625700	1.51082800
C	1.58462200	0.89192800	0.54913300	C	1.58645000	0.89207200	0.55021800
C	0.23661700	0.57605700	0.30329700	C	0.23695800	0.57642300	0.30379600
H	-0.47844100	1.32782400	0.63224200	H	-0.47750500	1.32881800	0.63309000
S	-4.56683300	-3.26853500	-1.92816300	S	-4.56975000	-3.26874100	-1.92887500
S	-2.93866700	0.17538800	-0.10484600	S	-2.94007600	0.17536700	-0.10662000
C	-5.91323400	-2.20233600	-1.48295300	C	-5.91559300	-2.20301900	-1.48371500
C	-7.26322900	-2.46316300	-1.69946700	C	-7.26706700	-2.46496000	-1.69998000
H	-7.58681600	-3.38107200	-2.17843100	H	-7.59062200	-3.38335700	-2.17866900
C	-8.19561800	-1.51231000	-1.28418700	C	-8.20130700	-1.51418700	-1.28457600
H	-9.25171800	-1.70218700	-1.44626700	H	-9.25742800	-1.70514900	-1.44630700
C	-7.79549500	-0.31495800	-0.66094000	C	-7.80123300	-0.31518600	-0.66128800
H	-8.54648500	0.40314400	-0.35015900	H	-8.55250600	0.40286200	-0.35034300
C	-6.45475300	-0.04892200	-0.44265700	C	-6.45892600	-0.04830900	-0.44349200
H	-6.14333100	0.87335100	0.03782000	H	-6.14906900	0.87484300	0.03668800
C	-5.49012200	-0.99411300	-0.85289200	C	-5.49300800	-0.99365000	-0.85378300
C	-4.07414600	-0.96677700	-0.74812800	C	-4.07593300	-0.96599000	-0.74914100
C	-3.42965800	-2.10799700	-1.27583700	C	-3.43253400	-2.10876400	-1.27741700
C	-2.04288800	-2.07054300	-1.16715400	C	-2.04442300	-2.07201100	-1.16894900
H	-1.36571600	-2.84429300	-1.50910600	H	-1.36742700	-2.84625700	-1.51082800
C	-1.58462200	-0.89192800	-0.54913300	C	-1.58645000	-0.89207200	-0.55021800
C	-0.23661700	-0.57605700	-0.30329700	C	-0.23695800	-0.57642300	-0.30379600
H	0.47844100	-1.32782400	-0.63224200	H	0.47750500	-1.32881800	-0.63309000

Cartesian coordinates of compound 2 for the anionic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.62133200	3.26908400	1.93194500	S	4.62292400	3.27126500	1.93360400
S	2.94755000	-0.16009100	0.11332100	S	2.94618600	-0.15647400	0.11640500
C	5.98133900	2.21075000	1.49145300	C	5.98118900	2.21254500	1.49283800
C	7.32890900	2.46916800	1.70657900	C	7.33076900	2.47063600	1.70690700
H	7.64241200	3.39216500	2.18739700	H	7.64618200	3.39338300	2.18714100
C	8.27826600	1.52484800	1.29576900	C	8.28108800	1.52421800	1.29466600
H	9.33513200	1.71552600	1.45835400	H	9.33820700	1.71479300	1.45599300
C	7.86166100	0.33696400	0.67624200	C	7.86284000	0.33432200	0.67484700
H	8.60543700	-0.39069900	0.36025400	H	8.60582300	-0.39373900	0.35824700
C	6.51431700	0.07102400	0.45754700	C	6.51267300	0.06926500	0.45760100
H	6.20632700	-0.85303100	-0.02365400	H	6.20409000	-0.85497700	-0.02305300
C	5.53502300	1.00589800	0.86165300	C	5.53416400	1.00662500	0.86310700
C	4.11964600	0.98194900	0.75883900	C	4.11784400	0.98413500	0.76134800

C	3.46463600	2.10189000	1.27521300	C	3.46551100	2.10645300	1.27867700
C	2.06905700	2.08627800	1.17686500	C	2.06760800	2.09141200	1.18012700
H	1.40803600	2.87092700	1.52518100	H	1.40628800	2.87629800	1.52799900
C	1.57956800	0.91622800	0.56101200	C	1.57981800	0.91899000	0.56326000
C	0.23815900	0.57863400	0.30472700	C	0.23623300	0.57990200	0.30566400
H	-0.48489500	1.32588200	0.63103200	H	-0.48783800	1.32618400	0.63182600
S	-4.62133200	-3.26908400	-1.93194500	S	-4.62292400	-3.27126500	-1.93360400
S	-2.94755000	0.16009100	-0.11332100	S	-2.94618600	0.15647400	-0.11640500
C	-5.98133900	-2.21075000	-1.49145300	C	-5.98118900	-2.21254500	-1.49283800
C	-7.32890900	-2.46916800	-1.70657900	C	-7.33076900	-2.47063600	-1.70690700
H	-7.64241200	-3.39216500	-2.18739700	H	-7.64618200	-3.39338300	-2.18714100
C	-8.27826600	-1.52484800	-1.29576900	C	-8.28108800	-1.52421800	-1.29466600
H	-9.33513200	-1.71552600	-1.45835400	H	-9.33820700	-1.71479300	-1.45599300
C	-7.86166100	-0.33696400	-0.67624200	C	-7.86284000	-0.33432200	-0.67484700
H	-8.60543700	0.39069900	-0.36025400	H	-8.60582300	0.39373900	-0.35824700
C	-6.51431700	-0.07102400	-0.45754700	C	-6.51267300	-0.06926500	-0.45760100
H	-6.20632700	0.85303100	0.02365400	H	-6.20409000	0.85497700	0.02305300
C	-5.53502300	-1.00589800	-0.86165300	C	-5.53416400	-1.00662500	-0.86310700
C	-4.11964600	-0.98194900	-0.75883900	C	-4.11784400	-0.98413500	-0.76134800
C	-3.46463600	-2.10189000	-1.27521300	C	-3.46551100	-2.10645300	-1.27867700
C	-2.06905700	-2.08627800	-1.17686500	C	-2.06760800	-2.09141200	-1.18012700
H	-1.40803600	-2.87092700	-1.52518100	H	-1.40628800	-2.87629800	-1.52799900
C	-1.57956800	-0.91622800	-0.56101200	C	-1.57981800	-0.91899000	-0.56326000
C	-0.23815900	-0.57863400	-0.30472700	C	-0.23623300	-0.57990200	-0.30566400
H	0.48489500	-1.32588200	-0.63103200	H	0.48783800	-1.32618400	-0.63182600

Frequency coordinates of compound 2 for the optimized neutral geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	4.60792400	3.26126800	1.92693000	S	4.61115900	3.26148400	1.92793200
S	2.95468600	-0.16201100	0.11235100	S	2.95663100	-0.16239500	0.11496300
C	5.96178200	2.20516500	1.48744200	C	5.96442800	2.20635400	1.48844400
C	7.31424800	2.46944500	1.70601500	C	7.31850400	2.47195600	1.70645600
H	7.62863600	3.39085400	2.18620300	H	7.63305100	3.39384900	2.18613500
C	8.25347300	1.52675400	1.29536300	C	8.25988100	1.52910200	1.29555100
H	9.30937000	1.71870100	1.45869100	H	9.31575400	1.72241900	1.45824400
C	7.84952400	0.33361200	0.67380900	C	7.85597700	0.33361600	0.67408200
H	8.59790800	-0.38797600	0.36115500	H	8.60470600	-0.38776800	0.36134300
C	6.50468300	0.06632400	0.45442700	C	6.50934000	0.06532100	0.45554300
H	6.19704500	-0.85742100	-0.02674100	H	6.20315500	-0.85940300	-0.02497900
C	5.53687200	1.00190200	0.85965800	C	5.54010600	1.00139700	0.86092200
C	4.10748900	0.97625900	0.75475600	C	4.10994600	0.97524000	0.75646300
C	3.46910800	2.09328200	1.27071900	C	3.47268100	2.09406200	1.27301000
C	2.05834600	2.05886000	1.16212500	C	2.06038100	2.06022900	1.16437500

H	1.38754200	2.83688200	1.50660300	H	1.38957300	2.83871800	1.50851800
C	1.60622500	0.90094300	0.55495400	C	1.60878500	0.90046800	0.55625700
C	0.23099000	0.56395600	0.29701600	C	0.23166000	0.56418300	0.29779900
H	-0.48063800	1.31901900	0.62826300	H	-0.47880300	1.32004000	0.62999100
S	-4.60792400	-3.26126800	-1.92693000	S	-4.61115900	-3.26148400	-1.92793200
S	-2.95468600	0.16201100	-0.11235100	S	-2.95663100	0.16239500	-0.11496300
C	-5.96178200	-2.20516500	-1.48744200	C	-5.96442800	-2.20635400	-1.48844400
C	-7.31424800	-2.46944500	-1.70601500	C	-7.31850400	-2.47195600	-1.70645600
H	-7.62863600	-3.39085400	-2.18620300	H	-7.63305100	-3.39384900	-2.18613500
C	-8.25347300	-1.52675400	-1.29536300	C	-8.25988100	-1.52910200	-1.29555100
H	-9.30937000	-1.71870100	-1.45869100	H	-9.31575400	-1.72241900	-1.45824400
C	-7.84952400	-0.33361200	-0.67380900	C	-7.85597700	-0.33361600	-0.67408200
H	-8.59790800	0.38797600	-0.36115500	H	-8.60470600	0.38776800	-0.36134300
C	-6.50468300	-0.06632400	-0.45442700	C	-6.50934000	-0.06532100	-0.45554300
H	-6.19704500	0.85742100	0.02674100	H	-6.20315500	0.85940300	0.02497900
C	-5.53687200	-1.00190200	-0.85965800	C	-5.54010600	-1.00139700	-0.86092200
C	-4.10748900	-0.97625900	-0.75475600	C	-4.10994600	-0.97524000	-0.75646300
C	-3.46910800	-2.09328200	-1.27071900	C	-3.47268100	-2.09406200	-1.27301000
C	-2.05834600	-2.05886000	-1.16212500	C	-2.06038100	-2.06022900	-1.16437500
H	-1.38754200	-2.83688200	-1.50660300	H	-1.38957300	-2.83871800	-1.50851800
C	-1.60622500	-0.90094300	-0.55495400	C	-1.60878500	-0.90046800	-0.55625700
C	-0.23099000	-0.56395600	-0.29701600	C	-0.23166000	-0.56418300	-0.29779900
H	0.48063800	-1.31901900	-0.62826300	H	0.47880300	-1.32004000	-0.62999100

Frequency coordinates of compound 2 for the optimized cationic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	4.56683300	3.26853500	1.92816300	S	4.56975000	3.26874100	1.92887500
S	2.93866700	-0.17538800	0.10484600	S	2.94007600	-0.17536700	0.10662000
C	5.91323400	2.20233600	1.48295300	C	5.91559300	2.20301900	1.48371500
C	7.26322900	2.46316300	1.69946700	C	7.26706700	2.46496000	1.69998000
H	7.58681600	3.38107200	2.17843100	H	7.59062200	3.38335700	2.17866900
C	8.19561800	1.51231000	1.28418700	C	8.20130700	1.51418700	1.28457600
H	9.25171800	1.70218700	1.44626700	H	9.25742800	1.70514900	1.44630700
C	7.79549500	0.31495800	0.66094000	C	7.80123300	0.31518600	0.66128800
H	8.54648500	-0.40314400	0.35015900	H	8.55250600	-0.40286200	0.35034300
C	6.45475300	0.04892200	0.44265700	C	6.45892600	0.04830900	0.44349200
H	6.14333100	-0.87335100	-0.03782000	H	6.14906900	-0.87484300	-0.03668800
C	5.49012200	0.99411300	0.85289200	C	5.49300800	0.99365000	0.85378300
C	4.07414600	0.96677700	0.74812800	C	4.07593300	0.96599000	0.74914100
C	3.42965800	2.10799700	1.27583700	C	3.43253400	2.10876400	1.27741700
C	2.04288800	2.07054300	1.16715400	C	2.04442300	2.07201100	1.16894900
H	1.36571600	2.84429300	1.50910600	H	1.36742700	2.84625700	1.51082800

C	1.58462200	0.89192800	0.54913300	C	1.58645000	0.89207200	0.55021800
C	0.23661700	0.57605700	0.30329700	C	0.23695800	0.57642300	0.30379600
H	-0.47844100	1.32782400	0.63224200	H	-0.47750500	1.32881800	0.63309000
S	-4.56683300	-3.26853500	-1.92816300	S	-4.56975000	-3.26874100	-1.92887500
S	-2.93866700	0.17538800	-0.10484600	S	-2.94007600	0.17536700	-0.10662000
C	-5.91323400	-2.20233600	-1.48295300	C	-5.91559300	-2.20301900	-1.48371500
C	-7.26322900	-2.46316300	-1.69946700	C	-7.26706700	-2.46496000	-1.69998000
H	-7.58681600	-3.38107200	-2.17843100	H	-7.59062200	-3.38335700	-2.17866900
C	-8.19561800	-1.51231000	-1.28418700	C	-8.20130700	-1.51418700	-1.28457600
H	-9.25171800	-1.70218700	-1.44626700	H	-9.25742800	-1.70514900	-1.44630700
C	-7.79549500	-0.31495800	-0.66094000	C	-7.80123300	-0.31518600	-0.66128800
H	-8.54648500	0.40314400	-0.35015900	H	-8.55250600	0.40286200	-0.35034300
C	-6.45475300	-0.04892200	-0.44265700	C	-6.45892600	-0.04830900	-0.44349200
H	-6.14333100	0.87335100	0.03782000	H	-6.14906900	0.87484300	0.03668800
C	-5.49012200	-0.99411300	-0.85289200	C	-5.49300800	-0.99365000	-0.85378300
C	-4.07414600	-0.96677700	-0.74812800	C	-4.07593300	-0.96599000	-0.74914100
C	-3.42965800	-2.10799700	-1.27583700	C	-3.43253400	-2.10876400	-1.27741700
C	-2.04288800	-2.07054300	-1.16715400	C	-2.04442300	-2.07201100	-1.16894900
H	-1.36571600	-2.84429300	-1.50910600	H	-1.36742700	-2.84625700	-1.51082800
C	-1.58462200	-0.89192800	-0.54913300	C	-1.58645000	-0.89207200	-0.55021800
C	-0.23661700	-0.57605700	-0.30329700	C	-0.23695800	-0.57642300	-0.30379600
H	0.47844100	-1.32782400	-0.63224200	H	0.47750500	-1.32881800	-0.63309000

Frequency coordinates of compound 2 for the optimized anionic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	4.62133200	3.26908400	1.93194500	S	4.62292400	3.27126500	1.93360400
S	2.94755000	-0.16009100	0.11332100	S	2.94618600	-0.15647400	0.11640500
C	5.98133900	2.21075000	1.49145300	C	5.98118900	2.21254500	1.49283800
C	7.32890900	2.46916800	1.70657900	C	7.33076900	2.47063600	1.70690700
H	7.64241200	3.39216500	2.18739700	H	7.64618200	3.39338300	2.18714100
C	8.27826600	1.52484800	1.29576900	C	8.28108800	1.52421800	1.29466600
H	9.33513200	1.71552600	1.45835400	H	9.33820700	1.71479300	1.45599300
C	7.86166100	0.33696400	0.67624200	C	7.86284000	0.33432200	0.67484700
H	8.60543700	-0.39069900	0.36025400	H	8.60582300	-0.39373900	0.35824700
C	6.51431700	0.07102400	0.45754700	C	6.51267300	0.06926500	0.45760100
H	6.20632700	-0.85303100	-0.02365400	H	6.20409000	-0.85497700	-0.02305300
C	5.53502300	1.00589800	0.86165300	C	5.53416400	1.00662500	0.86310700
C	4.11964600	0.98194900	0.75883900	C	4.11784400	0.98413500	0.76134800
C	3.46463600	2.10189000	1.27521300	C	3.46551100	2.10645300	1.27867700
C	2.06905700	2.08627800	1.17686500	C	2.06760800	2.09141200	1.18012700
H	1.40803600	2.87092700	1.52518100	H	1.40628800	2.87629800	1.52799900
C	1.57956800	0.91622800	0.56101200	C	1.57981800	0.91899000	0.56326000
C	0.23815900	0.57863400	0.30472700	C	0.23623300	0.57990200	0.30566400

H	-0.48489500	1.32588200	0.63103200	H	-0.48783800	1.32618400	0.63182600
S	-4.62133200	-3.26908400	-1.93194500	S	-4.62292400	-3.27126500	-1.93360400
S	-2.94755000	0.16009100	-0.11332100	S	-2.94618600	0.15647400	-0.11640500
C	-5.98133900	-2.21075000	-1.49145300	C	-5.98118900	-2.21254500	-1.49283800
C	-7.32890900	-2.46916800	-1.70657900	C	-7.33076900	-2.47063600	-1.70690700
H	-7.64241200	-3.39216500	-2.18739700	H	-7.64618200	-3.39338300	-2.18714100
C	-8.27826600	-1.52484800	-1.29576900	C	-8.28108800	-1.52421800	-1.29466600
H	-9.33513200	-1.71552600	-1.45835400	H	-9.33820700	-1.71479300	-1.45599300
C	-7.86166100	-0.33696400	-0.67624200	C	-7.86284000	-0.33432200	-0.67484700
H	-8.60543700	0.39069900	-0.36025400	H	-8.60582300	0.39373900	-0.35824700
C	-6.51431700	-0.07102400	-0.45754700	C	-6.51267300	-0.06926500	-0.45760100
H	-6.20632700	0.85303100	0.02365400	H	-6.20409000	0.85497700	0.02305300
C	-5.53502300	-1.00589800	-0.86165300	C	-5.53416400	-1.00662500	-0.86310700
C	-4.11964600	-0.98194900	-0.75883900	C	-4.11784400	-0.98413500	-0.76134800
C	-3.46463600	-2.10189000	-1.27521300	C	-3.46551100	-2.10645300	-1.27867700
C	-2.06905700	-2.08627800	-1.17686500	C	-2.06760800	-2.09141200	-1.18012700
H	-1.40803600	-2.87092700	-1.52518100	H	-1.40628800	-2.87629800	-1.52799900
C	-1.57956800	-0.91622800	-0.56101200	C	-1.57981800	-0.91899000	-0.56326000
C	-0.23815900	-0.57863400	-0.30472700	C	-0.23623300	-0.57990200	-0.30566400
H	0.48489500	-1.32588200	-0.63103200	H	0.48783800	-1.32618400	-0.63182600

Cartesian coordinates of compound 3 for the neutral geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	1.02728500	3.10621000	6.25733100	S	1.04373200	3.11117600	6.25601300
S	0.24326100	2.50115700	3.23079600	S	0.25947400	2.50554600	3.22983200
C	1.75834700	1.71201600	7.08199300	C	1.76510700	1.71529500	7.08414600
C	2.19662700	1.68605300	8.40636700	C	2.20139000	1.68965100	8.41096700
H	2.11041800	2.56370800	9.03933700	H	2.11933700	2.56911200	9.04235200
C	2.74784300	0.50573800	8.89908100	C	2.74566800	0.50615500	8.90856100
H	3.09407300	0.46625500	9.92726600	H	3.08968400	0.46745100	9.93764600
C	2.85939200	-0.62911000	8.08089500	C	2.85226600	-0.63284800	8.09212200
H	3.29216400	-1.53988500	8.48334700	H	3.27897100	-1.54535000	8.49747000
C	2.42228500	-0.60008300	6.76162500	C	2.41702500	-0.60374400	6.77033100
H	2.51157400	-1.48179900	6.13376900	H	2.50262300	-1.48804900	6.14536800
C	1.86256700	0.57666200	6.23960400	C	1.86439600	0.57619100	6.24420500
C	1.34391900	0.85129900	4.91690900	C	1.34961600	0.85132500	4.91964300
C	0.87353800	2.14985600	4.80361800	C	0.88638600	2.15363800	4.80384900
C	1.18424300	0.11634000	3.70360400	C	1.18696600	0.11479800	3.70660300
H	1.45678700	-0.92590100	3.58617900	H	1.45379400	-0.92921500	3.59013700
C	0.60556800	0.84609100	2.69401500	C	0.61287400	0.84912000	2.69532400
C	0.29577100	0.42758400	1.32536200	C	0.30029100	0.42999300	1.32565700
C	1.03388000	-0.60005400	0.70869600	C	1.05278500	-0.58162400	0.69807900
C	0.74291900	-1.01908300	-0.58233200	C	0.75721000	-1.00353400	-0.59334700

S	-1.02728500	-3.10621000	-6.25733100	S	-1.04373200	-3.11117600	-6.25601300
S	-0.24326100	-2.50115700	-3.23079600	S	-0.25947400	-2.50554600	-3.22983200
C	-1.75834700	-1.71201600	-7.08199300	C	-1.76510700	-1.71529500	-7.08414600
C	-2.19662700	-1.68605300	-8.40636700	C	-2.20139000	-1.68965100	-8.41096700
H	-2.11041800	-2.56370800	-9.03933700	H	-2.11933700	-2.56911200	-9.04235200
C	-2.74784300	-0.50573800	-8.89908100	C	-2.74566800	-0.50615500	-8.90856100
H	-3.09407300	-0.46625500	-9.92726600	H	-3.08968400	-0.46745100	-9.93764600
C	-2.85939200	0.62911000	-8.08089500	C	-2.85226600	0.63284800	-8.09212200
H	-3.29216400	1.53988500	-8.48334700	H	-3.27897100	1.54535000	-8.49747000
C	-2.42228500	0.60008300	-6.76162500	C	-2.41702500	0.60374400	-6.77033100
H	-2.51157400	1.48179900	-6.13376900	H	-2.50262300	1.48804900	-6.14536800
C	-1.86256700	-0.57666200	-6.23960400	C	-1.86439600	-0.57619100	-6.24420500
C	-1.34391900	-0.85129900	-4.91690900	C	-1.34961600	-0.85132500	-4.91964300
C	-0.87353800	-2.14985600	-4.80361800	C	-0.88638600	-2.15363800	-4.80384900
C	-1.18424300	-0.11634000	-3.70360400	C	-1.18696600	-0.11479800	-3.70660300
H	-1.45678700	0.92590100	-3.58617900	H	-1.45379400	0.92921500	-3.59013700
C	-0.60556800	-0.84609100	-2.69401500	C	-0.61287400	-0.84912000	-2.69532400
C	-0.29577100	-0.42758400	-1.32536200	C	-0.30029100	-0.42999300	-1.32565700
C	-1.03388000	0.60005400	-0.70869600	C	-1.05278500	0.58162400	-0.69807900
C	-0.74291900	1.01908300	0.58233200	C	-0.75721000	1.00353400	0.59334700
H	1.35430200	-1.79388500	-1.03568200	H	1.38021100	-1.76520300	-1.05326900
H	1.86643900	-1.05157200	1.23849500	H	1.89925900	-1.01983400	1.21727200
H	-1.35430200	1.79388500	1.03568200	H	-1.38021100	1.76520300	1.05326900
H	-1.86643900	1.05157200	-1.23849500	H	-1.89925900	1.01983400	-1.21727200

Cartesian coordinates of compound 3 for the cationic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	0.75069700	2.98333000	6.29692300	S	0.74949400	2.98192400	6.30105800
S	-0.00727400	2.40574400	3.29341300	S	-0.00625700	2.40462500	3.29709200
C	1.64934500	1.65367600	7.08485400	C	1.64910500	1.65389900	7.08924300
C	2.09981900	1.65579200	8.40075800	C	2.09858100	1.65674800	8.40706800
H	1.92465400	2.50237600	9.05614700	H	1.92128900	2.50294200	9.06281400
C	2.78867100	0.52992800	8.85825600	C	2.78965400	0.53132100	8.86640800
H	3.14987100	0.50825100	9.88113100	H	3.14952900	0.51055100	9.88994900
C	3.01733000	-0.56576200	8.01611800	C	3.02152700	-0.56512700	8.02356700
H	3.55484600	-1.42915400	8.39361000	H	3.56035600	-1.42765900	8.40170500
C	2.56255400	-0.55954400	6.70016000	C	2.56745000	-0.55929600	6.70566200
H	2.74323100	-1.41244300	6.05325900	H	2.75097400	-1.41251300	6.05970600
C	1.86851700	0.55860000	6.21708500	C	1.87130700	0.55835200	6.22136600
C	1.30138400	0.80671600	4.90790400	C	1.30430100	0.80585900	4.91115500
C	0.68099700	2.06999200	4.83795200	C	0.68201500	2.06939900	4.84176100
C	1.21148600	0.11285400	3.69166900	C	1.21522600	0.11163900	3.69426200
H	1.62572700	-0.87507700	3.53555900	H	1.63046700	-0.87586200	3.53727000

C	0.53641600	0.81765800	2.69249600	C	0.53833700	0.81805500	2.69528900
C	0.26558800	0.41254300	1.34292300	C	0.26674300	0.41277000	1.34443400
C	0.68511500	-0.85830300	0.86103300	C	0.68232200	-0.86021400	0.86262400
C	0.42878200	-1.25317400	-0.43073000	C	0.42488300	-1.25538100	-0.43061300
S	-0.75069700	-2.98333000	-6.29692300	S	-0.74949400	-2.98192400	-6.30105800
S	0.00727400	-2.40574400	-3.29341300	S	0.00625700	-2.40462500	-3.29709200
C	-1.64934500	-1.65367600	-7.08485400	C	-1.64910500	-1.65389900	-7.08924300
C	-2.09981900	-1.65579200	-8.40075800	C	-2.09858100	-1.65674800	-8.40706800
H	-1.92465400	-2.50237600	-9.05614700	H	-1.92128900	-2.50294200	-9.06281400
C	-2.78867100	-0.52992800	-8.85825600	C	-2.78965400	-0.53132100	-8.86640800
H	-3.14987100	-0.50825100	-9.88113100	H	-3.14952900	-0.51055100	-9.88994900
C	-3.01733000	0.56576200	-8.01611800	C	-3.02152700	0.56512700	-8.02356700
H	-3.55484600	1.42915400	-8.39361000	H	-3.56035600	1.42765900	-8.40170500
C	-2.56255400	0.55954400	-6.70016000	C	-2.56745000	0.55929600	-6.70566200
H	-2.74323100	1.41244300	-6.05325900	H	-2.75097400	1.41251300	-6.05970600
C	-1.86851700	-0.55860000	-6.21708500	C	-1.87130700	-0.55835200	-6.22136600
C	-1.30138400	-0.80671600	-4.90790400	C	-1.30430100	-0.80585900	-4.91115500
C	-0.68099700	-2.06999200	-4.83795200	C	-0.68201500	-2.06939900	-4.84176100
C	-1.21148600	-0.11285400	-3.69166900	C	-1.21522600	-0.11163900	-3.69426200
H	-1.62572700	0.87507700	-3.53555900	H	-1.63046700	0.87586200	-3.53727000
C	-0.53641600	-0.81765800	-2.69249600	C	-0.53833700	-0.81805500	-2.69528900
C	-0.26558800	-0.41254300	-1.34292300	C	-0.26674300	-0.41277000	-1.34443400
C	-0.68511500	0.85830300	-0.86103300	C	-0.68232200	0.86021400	-0.86262400
C	-0.42878200	1.25317400	0.43073000	C	-0.42488300	1.25538100	0.43061300
H	0.76846900	-2.23335400	-0.74981800	H	0.76161000	-2.23728700	-0.74771600
H	1.21639600	-1.53778000	1.51680400	H	1.21085100	-1.54240300	1.51798800
H	-0.76846900	2.23335400	0.74981800	H	-0.76161000	2.23728700	0.74771600
H	-1.21639600	1.53778000	-1.51680400	H	-1.21085100	1.54240300	-1.51798800

Cartesian coordinates of compound 3 for the anionic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	0.75927000	3.00162100	6.38074500	S	0.76412700	3.00191300	6.37774300
S	-0.00784800	2.40310700	3.32999100	S	0.00302800	2.40302100	3.32948100
C	1.65508200	1.67837200	7.14809900	C	1.65672600	1.67926800	7.14897200
C	2.12071000	1.65521100	8.46298300	C	2.11840400	1.65779400	8.46698700
H	1.94819800	2.49848300	9.12597200	H	1.94403600	2.50164600	9.12892700
C	2.81175600	0.53061800	8.91159800	C	2.80854400	0.53187200	8.92001900
H	3.18035600	0.49893600	9.93320700	H	3.17341900	0.50130700	9.94301500
C	3.03254800	-0.55693500	8.05207200	C	3.03224800	-0.55857900	8.06094500
H	3.57282000	-1.42738000	8.41461700	H	3.57107900	-1.42877500	8.42624700
C	2.56697400	-0.53239500	6.74136900	C	2.57023000	-0.53497900	6.74703500
H	2.74048900	-1.37721300	6.08075000	H	2.74571200	-1.38066700	6.08796600
C	1.86733800	0.58750500	6.26171200	C	1.87179300	0.58638900	6.26446100

C	1.29830000	0.83043400	4.95324900	C	1.30629200	0.82871200	4.95429100
C	0.68438800	2.07377500	4.89347100	C	0.69372100	2.07316300	4.89227900
C	1.22343300	0.11192200	3.73049900	C	1.23030200	0.10846300	3.72967900
H	1.65064300	-0.87233300	3.58504500	H	1.65344700	-0.87752300	3.58411000
C	0.55031200	0.79519400	2.71361000	C	0.55620200	0.79709700	2.71467600
C	0.27271400	0.40953300	1.36575400	C	0.27577100	0.41056100	1.36522000
C	0.67118300	-0.86611700	0.85714800	C	0.68054900	-0.86307800	0.85601500
C	0.41207400	-1.25218600	-0.43697100	C	0.41752700	-1.25084100	-0.44076200
S	-0.75927000	-3.00162100	-6.38074500	S	-0.76412700	-3.00191300	-6.37774300
S	0.00784800	-2.40310700	-3.32999100	S	-0.00302800	-2.40302100	-3.32948100
C	-1.65508200	-1.67837200	-7.14809900	C	-1.65672600	-1.67926800	-7.14897200
C	-2.12071000	-1.65521100	-8.46298300	C	-2.11840400	-1.65779400	-8.46698700
H	-1.94819800	-2.49848300	-9.12597200	H	-1.94403600	-2.50164600	-9.12892700
C	-2.81175600	-0.53061800	-8.91159800	C	-2.80854400	-0.53187200	-8.92001900
H	-3.18035600	-0.49893600	-9.93320700	H	-3.17341900	-0.50130700	-9.94301500
C	-3.03254800	0.55693500	-8.05207200	C	-3.03224800	0.55857900	-8.06094500
H	-3.57282000	1.42738000	-8.41461700	H	-3.57107900	1.42877500	-8.42624700
C	-2.56697400	0.53239500	-6.74136900	C	-2.57023000	0.53497900	-6.74703500
H	-2.74048900	1.37721300	-6.08075000	H	-2.74571200	1.38066700	-6.08796600
C	-1.86733800	-0.58750500	-6.26171200	C	-1.87179300	-0.58638900	-6.26446100
C	-1.29830000	-0.83043400	-4.95324900	C	-1.30629200	-0.82871200	-4.95429100
C	-0.68438800	-2.07377500	-4.89347100	C	-0.69372100	-2.07316300	-4.89227900
C	-1.22343300	-0.11192200	-3.73049900	C	-1.23030200	-0.10846300	-3.72967900
H	-1.65064300	0.87233300	-3.58504500	H	-1.65344700	0.87752300	-3.58411000
C	-0.55031200	-0.79519400	-2.71361000	C	-0.55620200	-0.79709700	-2.71467600
C	-0.27271400	-0.40953300	-1.36575400	C	-0.27577100	-0.41056100	-1.36522000
C	-0.67118300	0.86611700	-0.85714800	C	-0.68054900	0.86307800	-0.85601500
C	-0.41207400	1.25218600	0.43697100	C	-0.41752700	1.25084100	0.44076200
H	0.74011600	-2.23896100	-0.75694100	H	0.75205400	-2.23513600	-0.76085700
H	1.19233200	-1.55940700	1.51160700	H	1.20978600	-1.55428500	1.50573500
H	-0.74011600	2.23896100	0.75694100	H	-0.75205400	2.23513600	0.76085700
H	-1.19233200	1.55940700	-1.51160700	H	-1.20978600	1.55428500	-1.50573500

Frequency coordinates of compound 3 for the optimized neutral geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	1.02728500	3.10621000	6.25733100	S	1.04373200	3.11117600	6.25601300
S	0.24326100	2.50115700	3.23079600	S	0.25947400	2.50554600	3.22983200
C	1.75834700	1.71201600	7.08199300	C	1.76510700	1.71529500	7.08414600
C	2.19662700	1.68605300	8.40636700	C	2.20139000	1.68965100	8.41096700
H	2.11041800	2.56370800	9.03933700	H	2.11933700	2.56911200	9.04235200
C	2.74784300	0.50573800	8.89908100	C	2.74566800	0.50615500	8.90856100
H	3.09407300	0.46625500	9.92726600	H	3.08968400	0.46745100	9.93764600
C	2.85939200	-0.62911000	8.08089500	C	2.85226600	-0.63284800	8.09212200

H	3.29216400	-1.53988500	8.48334700	H	3.27897100	-1.54535000	8.49747000
C	2.42228500	-0.60008300	6.76162500	C	2.41702500	-0.60374400	6.77033100
H	2.51157400	-1.48179900	6.13376900	H	2.50262300	-1.48804900	6.14536800
C	1.86256700	0.57666200	6.23960400	C	1.86439600	0.57619100	6.24420500
C	1.34391900	0.85129900	4.91690900	C	1.34961600	0.85132500	4.91964300
C	0.87353800	2.14985600	4.80361800	C	0.88638600	2.15363800	4.80384900
C	1.18424300	0.11634000	3.70360400	C	1.18696600	0.11479800	3.70660300
H	1.45678700	-0.92590100	3.58617900	H	1.45379400	-0.92921500	3.59013700
C	0.60556800	0.84609100	2.69401500	C	0.61287400	0.84912000	2.69532400
C	0.29577100	0.42758400	1.32536200	C	0.30029100	0.42999300	1.32565700
C	1.03388000	-0.60005400	0.70869600	C	1.05278500	-0.58162400	0.69807900
C	0.74291900	-1.01908300	-0.58233200	C	0.75721000	-1.00353400	-0.59334700
S	-1.02728500	-3.10621000	-6.25733100	S	-1.04373200	-3.11117600	-6.25601300
S	-0.24326100	-2.50115700	-3.23079600	S	-0.25947400	-2.50554600	-3.22983200
C	-1.75834700	-1.71201600	-7.08199300	C	-1.76510700	-1.71529500	-7.08414600
C	-2.19662700	-1.68605300	-8.40636700	C	-2.20139000	-1.68965100	-8.41096700
H	-2.11041800	-2.56370800	-9.03933700	H	-2.11933700	-2.56911200	-9.04235200
C	-2.74784300	-0.50573800	-8.89908100	C	-2.74566800	-0.50615500	-8.90856100
H	-3.09407300	-0.46625500	-9.92726600	H	-3.08968400	-0.46745100	-9.93764600
C	-2.85939200	0.62911000	-8.08089500	C	-2.85226600	0.63284800	-8.09212200
H	-3.29216400	1.53988500	-8.48334700	H	-3.27897100	1.54535000	-8.49747000
C	-2.42228500	0.60008300	-6.76162500	C	-2.41702500	0.60374400	-6.77033100
H	-2.51157400	1.48179900	-6.13376900	H	-2.50262300	1.48804900	-6.14536800
C	-1.86256700	-0.57666200	-6.23960400	C	-1.86439600	-0.57619100	-6.24420500
C	-1.34391900	-0.85129900	-4.91690900	C	-1.34961600	-0.85132500	-4.91964300
C	-0.87353800	-2.14985600	-4.80361800	C	-0.88638600	-2.15363800	-4.80384900
C	-1.18424300	-0.11634000	-3.70360400	C	-1.18696600	-0.11479800	-3.70660300
H	-1.45678700	0.92590100	-3.58617900	H	-1.45379400	0.92921500	-3.59013700
C	-0.60556800	-0.84609100	-2.69401500	C	-0.61287400	-0.84912000	-2.69532400
C	-0.29577100	-0.42758400	-1.32536200	C	-0.30029100	-0.42999300	-1.32565700
C	-1.03388000	0.60005400	-0.70869600	C	-1.05278500	0.58162400	-0.69807900
C	-0.74291900	1.01908300	0.58233200	C	-0.75721000	1.00353400	0.59334700
H	1.35430200	-1.79388500	-1.03568200	H	1.38021100	-1.76520300	-1.05326900
H	1.86643900	-1.05157200	1.23849500	H	1.89925900	-1.01983400	1.21727200
H	-1.35430200	1.79388500	1.03568200	H	-1.38021100	1.76520300	1.05326900
H	-1.86643900	1.05157200	-1.23849500	H	-1.89925900	1.01983400	-1.21727200

Frequency coordinates of compound 3 for the optimized cationic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	0.75069700	2.98333000	6.29692300	S	0.74949400	2.98192400	6.30105800
S	-0.00727400	2.40574400	3.29341300	S	-0.00625700	2.40462500	3.29709200
C	1.64934500	1.65367600	7.08485400	C	1.64910500	1.65389900	7.08924300
C	2.09981900	1.65579200	8.40075800	C	2.09858100	1.65674800	8.40706800

H	1.92465400	2.50237600	9.05614700	H	1.92128900	2.50294200	9.06281400
C	2.78867100	0.52992800	8.85825600	C	2.78965400	0.53132100	8.86640800
H	3.14987100	0.50825100	9.88113100	H	3.14952900	0.51055100	9.88994900
C	3.01733000	-0.56576200	8.01611800	C	3.02152700	-0.56512700	8.02356700
H	3.55484600	-1.42915400	8.39361000	H	3.56035600	-1.42765900	8.40170500
C	2.56255400	-0.55954400	6.70016000	C	2.56745000	-0.55929600	6.70566200
H	2.74323100	-1.41244300	6.05325900	H	2.75097400	-1.41251300	6.05970600
C	1.86851700	0.55860000	6.21708500	C	1.87130700	0.55835200	6.22136600
C	1.30138400	0.80671600	4.90790400	C	1.30430100	0.80585900	4.91115500
C	0.68099700	2.06999200	4.83795200	C	0.68201500	2.06939900	4.84176100
C	1.21148600	0.11285400	3.69166900	C	1.21522600	0.11163900	3.69426200
H	1.62572700	-0.87507700	3.53555900	H	1.63046700	-0.87586200	3.53727000
C	0.53641600	0.81765800	2.69249600	C	0.53833700	0.81805500	2.69528900
C	0.26558800	0.41254300	1.34292300	C	0.26674300	0.41277000	1.34443400
C	0.68511500	-0.85830300	0.86103300	C	0.68232200	-0.86021400	0.86262400
C	0.42878200	-1.25317400	-0.43073000	C	0.42488300	-1.25538100	-0.43061300
S	-0.75069700	-2.98333000	-6.29692300	S	-0.74949400	-2.98192400	-6.30105800
S	0.00727400	-2.40574400	-3.29341300	S	0.00625700	-2.40462500	-3.29709200
C	-1.64934500	-1.65367600	-7.08485400	C	-1.64910500	-1.65389900	-7.08924300
C	-2.09981900	-1.65579200	-8.40075800	C	-2.09858100	-1.65674800	-8.40706800
H	-1.92465400	-2.50237600	-9.05614700	H	-1.92128900	-2.50294200	-9.06281400
C	-2.78867100	-0.52992800	-8.85825600	C	-2.78965400	-0.53132100	-8.86640800
H	-3.14987100	-0.50825100	-9.88113100	H	-3.14952900	-0.51055100	-9.88994900
C	-3.01733000	0.56576200	-8.01611800	C	-3.02152700	0.56512700	-8.02356700
H	-3.55484600	1.42915400	-8.39361000	H	-3.56035600	1.42765900	-8.40170500
C	-2.56255400	0.55954400	-6.70016000	C	-2.56745000	0.55929600	-6.70566200
H	-2.74323100	1.41244300	-6.05325900	H	-2.75097400	1.41251300	-6.05970600
C	-1.86851700	-0.55860000	-6.21708500	C	-1.87130700	-0.55835200	-6.22136600
C	-1.30138400	-0.80671600	-4.90790400	C	-1.30430100	-0.80585900	-4.91115500
C	-0.68099700	-2.06999200	-4.83795200	C	-0.68201500	-2.06939900	-4.84176100
C	-1.21148600	-0.11285400	-3.69166900	C	-1.21522600	-0.11163900	-3.69426200
H	-1.62572700	0.87507700	-3.53555900	H	-1.63046700	0.87586200	-3.53727000
C	-0.53641600	-0.81765800	-2.69249600	C	-0.53833700	-0.81805500	-2.69528900
C	-0.26558800	-0.41254300	-1.34292300	C	-0.26674300	-0.41277000	-1.34443400
C	-0.68511500	0.85830300	-0.86103300	C	-0.68232200	0.86021400	-0.86262400
C	-0.42878200	1.25317400	0.43073000	C	-0.42488300	1.25538100	0.43061300
H	0.76846900	-2.23335400	-0.74981800	H	0.76161000	-2.23728700	-0.74771600
H	1.21639600	-1.53778000	1.51680400	H	1.21085100	-1.54240300	1.51798800
H	-0.76846900	2.23335400	0.74981800	H	-0.76161000	2.23728700	0.74771600
H	-1.21639600	1.53778000	-1.51680400	H	-1.21085100	1.54240300	-1.51798800

Frequency coordinates of compound 3 for the optimized anionic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	0.75927000	3.00162100	6.38074500	S	0.76412700	3.00191300	6.37774300
S	-0.00784800	2.40310700	3.32999100	S	0.00302800	2.40302100	3.32948100
C	1.65508200	1.67837200	7.14809900	C	1.65672600	1.67926800	7.14897200
C	2.12071000	1.65521100	8.46298300	C	2.11840400	1.65779400	8.46698700
H	1.94819800	2.49848300	9.12597200	H	1.94403600	2.50164600	9.12892700
C	2.81175600	0.53061800	8.91159800	C	2.80854400	0.53187200	8.92001900
H	3.18035600	0.49893600	9.93320700	H	3.17341900	0.50130700	9.94301500
C	3.03254800	-0.55693500	8.05207200	C	3.03224800	-0.55857900	8.06094500
H	3.57282000	-1.42738000	8.41461700	H	3.57107900	-1.42877500	8.42624700
C	2.56697400	-0.53239500	6.74136900	C	2.57023000	-0.53497900	6.74703500
H	2.74048900	-1.37721300	6.08075000	H	2.74571200	-1.38066700	6.08796600
C	1.86733800	0.58750500	6.26171200	C	1.87179300	0.58638900	6.26446100
C	1.29830000	0.83043400	4.95324900	C	1.30629200	0.82871200	4.95429100
C	0.68438800	2.07377500	4.89347100	C	0.69372100	2.07316300	4.89227900
C	1.22343300	0.11192200	3.73049900	C	1.23030200	0.10846300	3.72967900
H	1.65064300	-0.87233300	3.58504500	H	1.65344700	-0.87752300	3.58411000
C	0.55031200	0.79519400	2.71361000	C	0.55620200	0.79709700	2.71467600
C	0.27271400	0.40953300	1.36575400	C	0.27577100	0.41056100	1.36522000
C	0.67118300	-0.86611700	0.85714800	C	0.68054900	-0.86307800	0.85601500
C	0.41207400	-1.25218600	-0.43697100	C	0.41752700	-1.25084100	-0.44076200
S	-0.75927000	-3.00162100	-6.38074500	S	-0.76412700	-3.00191300	-6.37774300
S	0.00784800	-2.40310700	-3.32999100	S	-0.00302800	-2.40302100	-3.32948100
C	-1.65508200	-1.67837200	-7.14809900	C	-1.65672600	-1.67926800	-7.14897200
C	-2.12071000	-1.65521100	-8.46298300	C	-2.11840400	-1.65779400	-8.46698700
H	-1.94819800	-2.49848300	-9.12597200	H	-1.94403600	-2.50164600	-9.12892700
C	-2.81175600	-0.53061800	-8.91159800	C	-2.80854400	-0.53187200	-8.92001900
H	-3.18035600	-0.49893600	-9.93320700	H	-3.17341900	-0.50130700	-9.94301500
C	-3.03254800	0.55693500	-8.05207200	C	-3.03224800	0.55857900	-8.06094500
H	-3.57282000	1.42738000	-8.41461700	H	-3.57107900	1.42877500	-8.42624700
C	-2.56697400	0.53239500	-6.74136900	C	-2.57023000	0.53497900	-6.74703500
H	-2.74048900	1.37721300	-6.08075000	H	-2.74571200	1.38066700	-6.08796600
C	-1.86733800	-0.58750500	-6.26171200	C	-1.87179300	-0.58638900	-6.26446100
C	-1.29830000	-0.83043400	-4.95324900	C	-1.30629200	-0.82871200	-4.95429100
C	-0.68438800	-2.07377500	-4.89347100	C	-0.69372100	-2.07316300	-4.89227900
C	-1.22343300	-0.11192200	-3.73049900	C	-1.23030200	-0.10846300	-3.72967900
H	-1.65064300	0.87233300	-3.58504500	H	-1.65344700	0.87752300	-3.58411000
C	-0.55031200	-0.79519400	-2.71361000	C	-0.55620200	-0.79709700	-2.71467600
C	-0.27271400	-0.40953300	-1.36575400	C	-0.27577100	-0.41056100	-1.36522000
C	-0.67118300	0.86611700	-0.85714800	C	-0.68054900	0.86307800	-0.85601500
C	-0.41207400	1.25218600	0.43697100	C	-0.41752700	1.25084100	0.44076200
H	0.74011600	-2.23896100	-0.75694100	H	0.75205400	-2.23513600	-0.76085700

H	1.19233200	-1.55940700	1.51160700	H	1.20978600	-1.55428500	1.50573500
H	-0.74011600	2.23896100	0.75694100	H	-0.75205400	2.23513600	0.76085700
H	-1.19233200	1.55940700	-1.51160700	H	-1.20978600	1.55428500	-1.50573500

Cartesian coordinates of compound 4 for the neutral geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	2.59396800	3.09252000	5.84406900	S	2.68663900	3.05729200	5.82476200
S	1.62107800	2.50577000	2.87960200	S	1.68480500	2.48519600	2.86821100
F	0.83016500	2.55990000	0.29443200	F	0.59604900	2.61935900	0.36025300
F	-0.02206800	1.80602100	-2.02302300	F	-0.27268000	1.85778200	-1.95989600
C	2.37099400	1.71312600	6.94473000	C	2.40928800	1.69911500	6.93829900
C	2.70552800	1.68890800	8.29877500	C	2.74295900	1.67578800	8.29425000
H	3.14394500	2.55704700	8.78083900	H	3.21531200	2.53076800	8.76814800
C	2.46318000	0.52182700	9.01957200	C	2.45467300	0.52548900	9.02824900
H	2.71654500	0.48354600	10.07450400	H	2.70651600	0.48855700	10.08370200
C	1.89657200	-0.60073700	8.39677300	C	1.84381900	-0.58194000	8.41601700
H	1.71549000	-1.50099700	8.97585700	H	1.62735900	-1.46844700	9.00429800
C	1.56459300	-0.57312500	7.04691100	C	1.51338100	-0.55501900	7.06392800
H	1.12624700	-1.44498700	6.57032900	H	1.04182400	-1.41484100	6.59702500
C	1.79835700	0.59017800	6.29789800	C	1.79314800	0.59164000	6.30263700
C	1.54318700	0.86314600	4.89898600	C	1.55017600	0.86019400	4.90010000
C	1.92045700	2.14787400	4.54038800	C	1.97905100	2.12720100	4.52947200
C	1.00032000	0.13961000	3.80261000	C	0.97939600	0.14858000	3.80971800
H	0.64733800	-0.87769200	3.87358000	H	0.58901300	-0.85510600	3.88960200
C	0.96330300	0.86470500	2.62766100	C	0.96965200	0.86830200	2.62852600
C	0.48316500	0.43526200	1.31635500	C	0.48677700	0.43864100	1.31707300
C	0.42657400	1.27812200	0.19125600	C	0.31315700	1.30528900	0.22144900
C	-0.02900300	0.87181300	-1.05365600	C	-0.14676000	0.89623500	-1.02067200
S	-2.59396800	-3.09252000	-5.84406900	S	-2.68663900	-3.05729200	-5.82476200
S	-1.62107800	-2.50577000	-2.87960200	S	-1.68480500	-2.48519600	-2.86821100
F	-0.83016500	-2.55990000	-0.29443200	F	-0.59604900	-2.61935900	-0.36025300
F	0.02206800	-1.80602100	2.02302300	F	0.27268000	-1.85778200	1.95989600
C	-2.37099400	-1.71312600	-6.94473000	C	-2.40928800	-1.69911500	-6.93829900
C	-2.70552800	-1.68890800	-8.29877500	C	-2.74295900	-1.67578800	-8.29425000
H	-3.14394500	-2.55704700	-8.78083900	H	-3.21531200	-2.53076800	-8.76814800
C	-2.46318000	-0.52182700	-9.01957200	C	-2.45467300	-0.52548900	-9.02824900
H	-2.71654500	-0.48354600	10.07450400	H	-2.70651600	-0.48855700	10.08370200
C	-1.89657200	0.60073700	-8.39677300	C	-1.84381900	0.58194000	-8.41601700
H	-1.71549000	1.50099700	-8.97585700	H	-1.62735900	1.46844700	-9.00429800
C	-1.56459300	0.57312500	-7.04691100	C	-1.51338100	0.55501900	-7.06392800
H	-1.12624700	1.44498700	-6.57032900	H	-1.04182400	1.41484100	-6.59702500
C	-1.79835700	-0.59017800	-6.29789800	C	-1.79314800	-0.59164000	-6.30263700
C	-1.54318700	-0.86314600	-4.89898600	C	-1.55017600	-0.86019400	-4.90010000

C	-1.92045700	-2.14787400	-4.54038800	C	-1.97905100	-2.12720100	-4.52947200
C	-1.00032000	-0.13961000	-3.80261000	C	-0.97939600	-0.14858000	-3.80971800
H	-0.64733800	0.87769200	-3.87358000	H	-0.58901300	0.85510600	-3.88960200
C	-0.96330300	-0.86470500	-2.62766100	C	-0.96965200	-0.86830200	-2.62852600
C	-0.48316500	-0.43526200	-1.31635500	C	-0.48677700	-0.43864100	-1.31707300
C	-0.42657400	-1.27812200	-0.19125600	C	-0.31315700	-1.30528900	-0.22144900
C	0.02900300	-0.87181300	1.05365600	C	0.14676000	-0.89623500	1.02067200

Cartesian coordinates of compound 4 for the cationic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	2.53492000	3.09092500	5.80365800	S	2.53886500	3.09088000	5.81023900
S	1.58919700	2.51968300	2.85990000	S	1.59190600	2.52186800	2.86764500
F	0.93045700	2.52929600	0.26780100	F	0.92483300	2.53276800	0.26897100
F	0.08512500	1.77269900	-2.05392400	F	0.07818300	1.77345200	-2.05489000
C	2.34025400	1.70282300	6.91562600	C	2.34318000	1.70348000	6.92254000
C	2.68067300	1.69738400	8.26328800	C	2.68515500	1.69858900	8.27118300
H	3.10383800	2.57344900	8.74322800	H	3.11001400	2.57434600	8.75075700
C	2.46087900	0.52225400	8.98850700	C	2.46449300	0.52315200	8.99858000
H	2.71857200	0.49345600	10.04203500	H	2.72336000	0.49499400	10.05200600
C	1.91521400	-0.61114800	8.37427200	C	1.91630400	-0.61100300	8.38487300
H	1.75370500	-1.51176600	8.95698000	H	1.75406000	-1.51123600	8.96830600
C	1.57701100	-0.59598900	7.02273800	C	1.57665200	-0.59588700	7.03191500
H	1.15399600	-1.47826100	6.55256600	H	1.15212400	-1.47868400	6.56375200
C	1.78784300	0.57020100	6.27444200	C	1.78865000	0.57039900	6.28230000
C	1.52452900	0.83833700	4.87589200	C	1.52501300	0.83872800	4.88290100
C	1.88514700	2.15367500	4.51578100	C	1.88772400	2.15511600	4.52290700
C	1.00307600	0.12366900	3.79142000	C	1.00292900	0.12435700	3.79844000
H	0.66712300	-0.89973800	3.85247100	H	0.66652700	-0.89915800	3.86195400
C	0.95570800	0.86547300	2.60238800	C	0.95704500	0.86837200	2.60797500
C	0.48244100	0.43656800	1.31605200	C	0.48390300	0.43896400	1.32057200
C	0.47665400	1.27161400	0.16825100	C	0.47320300	1.27067800	0.16917600
C	0.02571700	0.86750700	-1.06914600	C	0.02225800	0.86547000	-1.06746800
S	-2.53492000	-3.09092500	-5.80365800	S	-2.53886500	-3.09088000	-5.81023900
S	-1.58919700	-2.51968300	-2.85990000	S	-1.59190600	-2.52186800	-2.86764500
F	-0.93045700	-2.52929600	-0.26780100	F	-0.92483300	-2.53276800	-0.26897100
F	-0.08512500	-1.77269900	2.05392400	F	-0.07818300	-1.77345200	2.05489000
C	-2.34025400	-1.70282300	-6.91562600	C	-2.34318000	-1.70348000	-6.92254000
C	-2.68067300	-1.69738400	-8.26328800	C	-2.68515500	-1.69858900	-8.27118300
H	-3.10383800	-2.57344900	-8.74322800	H	-3.11001400	-2.57434600	-8.75075700
C	-2.46087900	-0.52225400	-8.98850700	C	-2.46449300	-0.52315200	-8.99858000
H	-2.71857200	-0.49345600	10.04203500	H	-2.72336000	-0.49499400	10.05200600
C	-1.91521400	0.61114800	-8.37427200	C	-1.91630400	0.61100300	-8.38487300
H	-1.75370500	1.51176600	-8.95698000	H	-1.75406000	1.51123600	-8.96830600

C	-1.57701100	0.59598900	-7.02273800	C	-1.57665200	0.59588700	-7.03191500
H	-1.15399600	1.47826100	-6.55256600	H	-1.15212400	1.47868400	-6.56375200
C	-1.78784300	-0.57020100	-6.27444200	C	-1.78865000	-0.57039900	-6.28230000
C	-1.52452900	-0.83833700	-4.87589200	C	-1.52501300	-0.83872800	-4.88290100
C	-1.88514700	-2.15367500	-4.51578100	C	-1.88772400	-2.15511600	-4.52290700
C	-1.00307600	-0.12366900	-3.79142000	C	-1.00292900	-0.12435700	-3.79844000
H	-0.66712300	0.89973800	-3.85247100	H	-0.66652700	0.89915800	-3.86195400
C	-0.95570800	-0.86547300	-2.60238800	C	-0.95704500	-0.86837200	-2.60797500
C	-0.48244100	-0.43656800	-1.31605200	C	-0.48390300	-0.43896400	-1.32057200
C	-0.47665400	-1.27161400	-0.16825100	C	-0.47320300	-1.27067800	-0.16917600
C	-0.02571700	-0.86750700	1.06914600	C	-0.02225800	-0.86547000	1.06746800

Cartesian coordinates of compound 4 for the anionic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	2.56430900	3.11555000	5.88509800	S	2.56948600	3.11421200	5.89042900
S	1.60045700	2.52384600	2.89630000	S	1.60448800	2.52319400	2.90536700
F	0.93278300	2.54266200	0.26832700	F	0.92022800	2.54884100	0.27338900
F	0.08888100	1.78882700	-2.05516300	F	0.07471100	1.79283700	-2.05454100
C	2.36462400	1.73005700	6.97415600	C	2.36832400	1.73064600	6.98111300
C	2.69641800	1.69463600	8.32867500	C	2.70213200	1.69716900	8.33683600
H	3.12068800	2.56686300	8.81803500	H	3.12859200	2.56927300	8.82475100
C	2.47355400	0.51860900	9.04330100	C	2.47779200	0.52105100	9.05484800
H	2.72694500	0.47587500	10.09895800	H	2.73259600	0.47984100	10.11024400
C	1.92530000	-0.60645200	8.40771900	C	1.92601400	-0.60594400	8.42068100
H	1.75707200	-1.51648200	8.97723000	H	1.75676800	-1.51479100	8.99177500
C	1.59503300	-0.56910500	7.05688200	C	1.59406500	-0.56988500	7.06826000
H	1.17078600	-1.44226400	6.56943800	H	1.16797100	-1.44354200	6.58319600
C	1.80875300	0.60248900	6.31220800	C	1.80983300	0.60184100	6.32163900
C	1.54581400	0.87074200	4.91420700	C	1.54687200	0.86926900	4.92309100
C	1.90283700	2.16393500	4.56850700	C	1.90672000	2.16231600	4.57636100
C	1.01387200	0.13041800	3.82558300	C	1.01257800	0.12913500	3.83367900
H	0.68041600	-0.89296400	3.89724800	H	0.67739700	-0.89387800	3.90827900
C	0.95735400	0.85195300	2.62828200	C	0.95863000	0.85452000	2.63515800
C	0.48954700	0.44152800	1.33900200	C	0.49079100	0.44348000	1.34403400
C	0.47415500	1.26431100	0.17272800	C	0.46750800	1.26412000	0.17536800
C	0.02603300	0.86353500	-1.06039600	C	0.01931200	0.86273600	-1.05781500
S	-2.56430900	-3.11555000	-5.88509800	S	-2.56948600	-3.11421200	-5.89042900
S	-1.60045700	-2.52384600	-2.89630000	S	-1.60448800	-2.52319400	-2.90536700
F	-0.93278300	-2.54266200	-0.26832700	F	-0.92022800	-2.54884100	-0.27338900
F	-0.08888100	-1.78882700	2.05516300	F	-0.07471100	-1.79283700	2.05454100
C	-2.36462400	-1.73005700	-6.97415600	C	-2.36832400	-1.73064600	-6.98111300
C	-2.69641800	-1.69463600	-8.32867500	C	-2.70213200	-1.69716900	-8.33683600
H	-3.12068800	-2.56686300	-8.81803500	H	-3.12859200	-2.56927300	-8.82475100

C	-2.47355400	-0.51860900	-9.04330100	C	-2.47779200	-0.52105100	-9.05484800
H	-2.72694500	-0.47587500	10.09895800	H	-2.73259600	-0.47984100	10.11024400
C	-1.92530000	0.60645200	-8.40771900	C	-1.92601400	0.60594400	-8.42068100
H	-1.75707200	1.51648200	-8.97723000	H	-1.75676800	1.51479100	-8.99177500
C	-1.59503300	0.56910500	-7.05688200	C	-1.59406500	0.56988500	-7.06826000
H	-1.17078600	1.44226400	-6.56943800	H	-1.16797100	1.44354200	-6.58319600
C	-1.80875300	-0.60248900	-6.31220800	C	-1.80983300	-0.60184100	-6.32163900
C	-1.54581400	-0.87074200	-4.91420700	C	-1.54687200	-0.86926900	-4.92309100
C	-1.90283700	-2.16393500	-4.56850700	C	-1.90672000	-2.16231600	-4.57636100
C	-1.01387200	-0.13041800	-3.82558300	C	-1.01257800	-0.12913500	-3.83367900
H	-0.68041600	0.89296400	-3.89724800	H	-0.67739700	0.89387800	-3.90827900
C	-0.95735400	-0.85195300	-2.62828200	C	-0.95863000	-0.85452000	-2.63515800
C	-0.48954700	-0.44152800	-1.33900200	C	-0.49079100	-0.44348000	-1.34403400
C	-0.47415500	-1.26431100	-0.17272800	C	-0.46750800	-1.26412000	-0.17536800
C	-0.02603300	-0.86353500	1.06039600	C	-0.01931200	-0.86273600	1.05781500

Frequency coordinates of compound 4 for the optimized neutral geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	2.59396800	3.09252000	5.84406900	S	2.68663900	3.05729200	5.82476200
S	1.62107800	2.50577000	2.87960200	S	1.68480500	2.48519600	2.86821100
F	0.83016500	2.55990000	0.29443200	F	0.59604900	2.61935900	0.36025300
F	-0.02206800	1.80602100	-2.02302300	F	-0.27268000	1.85778200	-1.95989600
C	2.37099400	1.71312600	6.94473000	C	2.40928800	1.69911500	6.93829900
C	2.70552800	1.68890800	8.29877500	C	2.74295900	1.67578800	8.29425000
H	3.14394500	2.55704700	8.78083900	H	3.21531200	2.53076800	8.76814800
C	2.46318000	0.52182700	9.01957200	C	2.45467300	0.52548900	9.02824900
H	2.71654500	0.48354600	10.07450400	H	2.70651600	0.48855700	10.08370200
C	1.89657200	-0.60073700	8.39677300	C	1.84381900	-0.58194000	8.41601700
H	1.71549000	-1.50099700	8.97585700	H	1.62735900	-1.46844700	9.00429800
C	1.56459300	-0.57312500	7.04691100	C	1.51338100	-0.55501900	7.06392800
H	1.12624700	-1.44498700	6.57032900	H	1.04182400	-1.41484100	6.59702500
C	1.79835700	0.59017800	6.29789800	C	1.79314800	0.59164000	6.30263700
C	1.54318700	0.86314600	4.89898600	C	1.55017600	0.86019400	4.90010000
C	1.92045700	2.14787400	4.54038800	C	1.97905100	2.12720100	4.52947200
C	1.00032000	0.13961000	3.80261000	C	0.97939600	0.14858000	3.80971800
H	0.64733800	-0.87769200	3.87358000	H	0.58901300	-0.85510600	3.88960200
C	0.96330300	0.86470500	2.62766100	C	0.96965200	0.86830200	2.62852600
C	0.48316500	0.43526200	1.31635500	C	0.48677700	0.43864100	1.31707300
C	0.42657400	1.27812200	0.19125600	C	0.31315700	1.30528900	0.22144900
C	-0.02900300	0.87181300	-1.05365600	C	-0.14676000	0.89623500	-1.02067200
S	-2.59396800	-3.09252000	-5.84406900	S	-2.68663900	-3.05729200	-5.82476200
S	-1.62107800	-2.50577000	-2.87960200	S	-1.68480500	-2.48519600	-2.86821100
F	-0.83016500	-2.55990000	-0.29443200	F	-0.59604900	-2.61935900	-0.36025300

F	0.02206800	-1.80602100	2.02302300	F	0.27268000	-1.85778200	1.95989600
C	-2.37099400	-1.71312600	-6.94473000	C	-2.40928800	-1.69911500	-6.93829900
C	-2.70552800	-1.68890800	-8.29877500	C	-2.74295900	-1.67578800	-8.29425000
H	-3.14394500	-2.55704700	-8.78083900	H	-3.21531200	-2.53076800	-8.76814800
C	-2.46318000	-0.52182700	-9.01957200	C	-2.45467300	-0.52548900	-9.02824900
H	-2.71654500	-0.48354600	-10.07450400	H	-2.70651600	-0.48855700	10.08370200
C	-1.89657200	0.60073700	-8.39677300	C	-1.84381900	0.58194000	-8.41601700
H	-1.71549000	1.50099700	-8.97585700	H	-1.62735900	1.46844700	-9.00429800
C	-1.56459300	0.57312500	-7.04691100	C	-1.51338100	0.55501900	-7.06392800
H	-1.12624700	1.44498700	-6.57032900	H	-1.04182400	1.41484100	-6.59702500
C	-1.79835700	-0.59017800	-6.29789800	C	-1.79314800	-0.59164000	-6.30263700
C	-1.54318700	-0.86314600	-4.89898600	C	-1.55017600	-0.86019400	-4.90010000
C	-1.92045700	-2.14787400	-4.54038800	C	-1.97905100	-2.12720100	-4.52947200
C	-1.00032000	-0.13961000	-3.80261000	C	-0.97939600	-0.14858000	-3.80971800
H	-0.64733800	0.87769200	-3.87358000	H	-0.58901300	0.85510600	-3.88960200
C	-0.96330300	-0.86470500	-2.62766100	C	-0.96965200	-0.86830200	-2.62852600
C	-0.48316500	-0.43526200	-1.31635500	C	-0.48677700	-0.43864100	-1.31707300
C	-0.42657400	-1.27812200	-0.19125600	C	-0.31315700	-1.30528900	-0.22144900
C	0.02900300	-0.87181300	1.05365600	C	0.14676000	-0.89623500	1.02067200

Frequency coordinates of compound 4 for the optimized cationic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	2.53492000	3.09092500	5.80365800	S	2.53886500	3.09088000	5.81023900
S	1.58919700	2.51968300	2.85990000	S	1.59190600	2.52186800	2.86764500
F	0.93045700	2.52929600	0.26780100	F	0.92483300	2.53276800	0.26897100
F	0.08512500	1.77269900	-2.05392400	F	0.07818300	1.77345200	-2.05489000
C	2.34025400	1.70282300	6.91562600	C	2.34318000	1.70348000	6.92254000
C	2.68067300	1.69738400	8.26328800	C	2.68515500	1.69858900	8.27118300
H	3.10383800	2.57344900	8.74322800	H	3.11001400	2.57434600	8.75075700
C	2.46087900	0.52225400	8.98850700	C	2.46449300	0.52315200	8.99858000
H	2.71857200	0.49345600	10.04203500	H	2.72336000	0.49499400	10.05200600
C	1.91521400	-0.61114800	8.37427200	C	1.91630400	-0.61100300	8.38487300
H	1.75370500	-1.51176600	8.95698000	H	1.75406000	-1.51123600	8.96830600
C	1.57701100	-0.59598900	7.02273800	C	1.57665200	-0.59588700	7.03191500
H	1.15399600	-1.47826100	6.55256600	H	1.15212400	-1.47868400	6.56375200
C	1.78784300	0.57020100	6.27444200	C	1.78865000	0.57039900	6.28230000
C	1.52452900	0.83833700	4.87589200	C	1.52501300	0.83872800	4.88290100
C	1.88514700	2.15367500	4.51578100	C	1.88772400	2.15511600	4.52290700
C	1.00307600	0.12366900	3.79142000	C	1.00292900	0.12435700	3.79844000
H	0.66712300	-0.89973800	3.85247100	H	0.66652700	-0.89915800	3.86195400
C	0.95570800	0.86547300	2.60238800	C	0.95704500	0.86837200	2.60797500
C	0.48244100	0.43656800	1.31605200	C	0.48390300	0.43896400	1.32057200
C	0.47665400	1.27161400	0.16825100	C	0.47320300	1.27067800	0.16917600

C	0.02571700	0.86750700	-1.06914600	C	0.02225800	0.86547000	-1.06746800
S	-2.53492000	-3.09092500	-5.80365800	S	-2.53886500	-3.09088000	-5.81023900
S	-1.58919700	-2.51968300	-2.85990000	S	-1.59190600	-2.52186800	-2.86764500
F	-0.93045700	-2.52929600	-0.26780100	F	-0.92483300	-2.53276800	-0.26897100
F	-0.08512500	-1.77269900	2.05392400	F	-0.07818300	-1.77345200	2.05489000
C	-2.34025400	-1.70282300	-6.91562600	C	-2.34318000	-1.70348000	-6.92254000
C	-2.68067300	-1.69738400	-8.26328800	C	-2.68515500	-1.69858900	-8.27118300
H	-3.10383800	-2.57344900	-8.74322800	H	-3.11001400	-2.57434600	-8.75075700
C	-2.46087900	-0.52225400	-8.98850700	C	-2.46449300	-0.52315200	-8.99858000
H	-2.71857200	-0.49345600	-10.04203500	H	-2.72336000	-0.49499400	10.05200600
C	-1.91521400	0.61114800	-8.37427200	C	-1.91630400	0.61100300	-8.38487300
H	-1.75370500	1.51176600	-8.95698000	H	-1.75406000	1.51123600	-8.96830600
C	-1.57701100	0.59598900	-7.02273800	C	-1.57665200	0.59588700	-7.03191500
H	-1.15399600	1.47826100	-6.55256600	H	-1.15212400	1.47868400	-6.56375200
C	-1.78784300	-0.57020100	-6.27444200	C	-1.78865000	-0.57039900	-6.28230000
C	-1.52452900	-0.83833700	-4.87589200	C	-1.52501300	-0.83872800	-4.88290100
C	-1.88514700	-2.15367500	-4.51578100	C	-1.88772400	-2.15511600	-4.52290700
C	-1.00307600	-0.12366900	-3.79142000	C	-1.00292900	-0.12435700	-3.79844000
H	-0.66712300	0.89973800	-3.85247100	H	-0.66652700	0.89915800	-3.86195400
C	-0.95570800	-0.86547300	-2.60238800	C	-0.95704500	-0.86837200	-2.60797500
C	-0.48244100	-0.43656800	-1.31605200	C	-0.48390300	-0.43896400	-1.32057200
C	-0.47665400	-1.27161400	-0.16825100	C	-0.47320300	-1.27067800	-0.16917600
C	-0.02571700	-0.86750700	1.06914600	C	-0.02225800	-0.86547000	1.06746800

Frequency coordinates of compound 4 for the optimized anionic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	2.56430900	3.11555000	5.88509800	S	2.56948600	3.11421200	5.89042900
S	1.60045700	2.52384600	2.89630000	S	1.60448800	2.52319400	2.90536700
F	0.93278300	2.54266200	0.26832700	F	0.92022800	2.54884100	0.27338900
F	0.08888100	1.78882700	-2.05516300	F	0.07471100	1.79283700	-2.05454100
C	2.36462400	1.73005700	6.97415600	C	2.36832400	1.73064600	6.98111300
C	2.69641800	1.69463600	8.32867500	C	2.70213200	1.69716900	8.33683600
H	3.12068800	2.56686300	8.81803500	H	3.12859200	2.56927300	8.82475100
C	2.47355400	0.51860900	9.04330100	C	2.47779200	0.52105100	9.05484800
H	2.72694500	0.47587500	10.09895800	H	2.73259600	0.47984100	10.11024400
C	1.92530000	-0.60645200	8.40771900	C	1.92601400	-0.60594400	8.42068100
H	1.75707200	-1.51648200	8.97723000	H	1.75676800	-1.51479100	8.99177500
C	1.59503300	-0.56910500	7.05688200	C	1.59406500	-0.56988500	7.06826000
H	1.17078600	-1.44226400	6.56943800	H	1.16797100	-1.44354200	6.58319600
C	1.80875300	0.60248900	6.31220800	C	1.80983300	0.60184100	6.32163900
C	1.54581400	0.87074200	4.91420700	C	1.54687200	0.86926900	4.92309100
C	1.90283700	2.16393500	4.56850700	C	1.90672000	2.16231600	4.57636100
C	1.01387200	0.13041800	3.82558300	C	1.01257800	0.12913500	3.83367900

H	0.68041600	-0.89296400	3.89724800	H	0.67739700	-0.89387800	3.90827900
C	0.95735400	0.85195300	2.62828200	C	0.95863000	0.85452000	2.63515800
C	0.48954700	0.44152800	1.33900200	C	0.49079100	0.44348000	1.34403400
C	0.47415500	1.26431100	0.17272800	C	0.46750800	1.26412000	0.17536800
C	0.02603300	0.86353500	-1.06039600	C	0.01931200	0.86273600	-1.05781500
S	-2.56430900	-3.11555000	-5.88509800	S	-2.56948600	-3.11421200	-5.89042900
S	-1.60045700	-2.52384600	-2.89630000	S	-1.60448800	-2.52319400	-2.90536700
F	-0.93278300	-2.54266200	-0.26832700	F	-0.92022800	-2.54884100	-0.27338900
F	-0.08888100	-1.78882700	2.05516300	F	-0.07471100	-1.79283700	2.05454100
C	-2.36462400	-1.73005700	-6.97415600	C	-2.36832400	-1.73064600	-6.98111300
C	-2.69641800	-1.69463600	-8.32867500	C	-2.70213200	-1.69716900	-8.33683600
H	-3.12068800	-2.56686300	-8.81803500	H	-3.12859200	-2.56927300	-8.82475100
C	-2.47355400	-0.51860900	-9.04330100	C	-2.47779200	-0.52105100	-9.05484800
H	-2.72694500	-0.47587500	-10.09895800	H	-2.73259600	-0.47984100	-10.11024400
C	-1.92530000	0.60645200	-8.40771900	C	-1.92601400	0.60594400	-8.42068100
H	-1.75707200	1.51648200	-8.97723000	H	-1.75676800	1.51479100	-8.99177500
C	-1.59503300	0.56910500	-7.05688200	C	-1.59406500	0.56988500	-7.06826000
H	-1.17078600	1.44226400	-6.56943800	H	-1.16797100	1.44354200	-6.58319600
C	-1.80875300	-0.60248900	-6.31220800	C	-1.80983300	-0.60184100	-6.32163900
C	-1.54581400	-0.87074200	-4.91420700	C	-1.54687200	-0.86926900	-4.92309100
C	-1.90283700	-2.16393500	-4.56850700	C	-1.90672000	-2.16231600	-4.57636100
C	-1.01387200	-0.13041800	-3.82558300	C	-1.01257800	-0.12913500	-3.83367900
H	-0.68041600	0.89296400	-3.89724800	H	-0.67739700	0.89387800	-3.90827900
C	-0.95735400	-0.85195300	-2.62828200	C	-0.95863000	-0.85452000	-2.63515800
C	-0.48954700	-0.44152800	-1.33900200	C	-0.49079100	-0.44348000	-1.34403400
C	-0.47415500	-1.26431100	-0.17272800	C	-0.46750800	-1.26412000	-0.17536800
C	-0.02603300	-0.86353500	1.06039600	C	-0.01931200	-0.86273600	1.05781500

Cartesian coordinates of compound 5 for the neutral geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	2.10219800	2.07841200	-0.20841500	S	2.10289300	2.07695500	-0.22038600
S	-0.41646200	-1.27354000	0.13885900	S	-0.41645900	-1.27272000	0.14689700
C	3.15487100	0.65953400	-0.06399400	C	3.15526300	0.65983800	-0.06833100
C	4.55034500	0.66771400	-0.06675400	C	4.55245400	0.66871100	-0.07298700
H	5.09904700	1.59955200	-0.16233300	H	5.10104600	1.60016000	-0.17529000
C	5.22555200	-0.54413200	0.05474700	C	5.22997600	-0.54301800	0.05570900
H	6.31112700	-0.55325600	0.05385300	H	6.31566500	-0.55116000	0.05363400
C	4.51784300	-1.75091200	0.17748600	C	4.52212700	-1.75104000	0.18740300
H	5.06298700	-2.68514100	0.27076800	H	5.06782000	-2.68449200	0.28643200
C	3.12896800	-1.76334800	0.18120000	C	3.13142800	-1.76374500	0.19239800
H	2.58607200	-2.69918700	0.27643900	H	2.59005200	-2.69989500	0.29445600
C	2.42442300	-0.55363300	0.06037700	C	2.42536100	-0.55407400	0.06440500
C	1.01415600	-0.28777200	0.03623900	C	1.01414700	-0.28854300	0.03929000

C	-1.45791500	0.14830500	-0.01772100	C	-1.45725300	0.14742500	-0.01591500
C	-0.71550500	1.30311700	-0.13062600	C	-0.71539300	1.30375800	-0.13594800
H	-1.16076600	2.28129400	-0.26295700	H	-1.16107700	2.28136200	-0.27305900
C	0.68035300	1.04911000	-0.09824700	C	0.68174800	1.04934100	-0.10259100
C	-2.91883400	0.01117800	-0.00607200	C	-2.91987700	0.01043800	-0.00442000
C	-3.55155000	-1.16293500	-0.45280700	C	-3.55466700	-1.15179600	-0.48200700
H	-2.95126500	-1.98472700	-0.83206200	H	-2.95647500	-1.96498300	-0.88273600
C	-4.93990400	-1.27416500	-0.44041000	C	-4.94509900	-1.26228000	-0.47237500
H	-5.40675300	-2.18944200	-0.79226300	H	-5.41265600	-2.16747100	-0.84892900
C	-5.72834500	-0.21343700	0.00814500	C	-5.73371100	-0.21222600	0.00552400
C	-5.11343500	0.95873900	0.45326300	C	-5.11619100	0.94803100	0.48257800
H	-5.71645300	1.78670100	0.81453600	H	-5.71781400	1.76656000	0.86729400
C	-3.72566600	1.06864300	0.45457100	C	-3.72621800	1.05624800	0.48606700
H	-3.25728700	1.97026100	0.83634200	H	-3.25789500	1.94760100	0.89170800
H	-6.81063300	-0.30002500	0.01419300	H	-6.81618400	-0.29785300	0.00950000

Cartesian coordinates of compound 5 for the cationic geometry optimization

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-2.08161100	2.11205600	-0.00065700	S	-2.08251100	2.11197000	-0.00031200
S	0.40522800	-1.29863400	0.00008600	S	0.40544000	-1.29787100	0.00015400
C	-3.12841600	0.67257600	-0.00004800	C	-3.12922100	0.67259700	-0.00007900
C	-4.51456900	0.67775000	0.00009900	C	-4.51664300	0.67836800	-0.00006900
H	-5.07555000	1.60605200	-0.00009200	H	-5.07773800	1.60693600	-0.00020200
C	-5.18169700	-0.55469100	0.00040800	C	-5.18550200	-0.55461000	0.00011100
H	-6.26689300	-0.56437100	0.00048900	H	-6.27086800	-0.56352500	0.00012000
C	-4.47992300	-1.77524800	0.00055200	C	-4.48352200	-1.77624800	0.00027600
H	-5.03061700	-2.70921600	0.00077900	H	-5.03434000	-2.71041400	0.00041400
C	-3.09662700	-1.78774900	0.00039700	C	-3.09863600	-1.78882900	0.00026000
H	-2.54898700	-2.72485600	0.00052700	H	-2.55226000	-2.72688500	0.00038600
C	-2.39677700	-0.55675100	0.00009900	C	-2.39772800	-0.55750300	0.00008300
C	-1.00905100	-0.29925900	-0.00005900	C	-1.00889000	-0.29985400	0.00002500
C	1.45294500	0.14350500	-0.00006500	C	1.45249000	0.14426700	-0.00002400
C	0.69476100	1.32961600	-0.00034100	C	0.69452500	1.33159700	-0.00018400
H	1.13789300	2.31625400	-0.00072600	H	1.13770400	2.31839400	-0.00038000
C	-0.67201300	1.08609700	-0.00034600	C	-0.67331400	1.08730600	-0.00016200
C	2.88392100	0.01289000	0.00000400	C	2.88510000	0.01318600	0.00000100
C	3.50725700	-1.26321500	-0.00099800	C	3.50865100	-1.26366400	-0.00058100
H	2.90380100	-2.16560400	-0.00205400	H	2.90581600	-2.16651800	-0.00109600
C	4.88693400	-1.37602800	-0.00088800	C	4.88991900	-1.37744000	-0.00057200
H	5.34879600	-2.35734800	-0.00170700	H	5.35096600	-2.35941700	-0.00104000
C	5.68495500	-0.22353600	0.00020100	C	5.68946900	-0.22471900	0.00002000
C	5.09076900	1.04622900	0.00116700	C	5.09471000	1.04610800	0.00062000
H	5.71092400	1.93611100	0.00203000	H	5.71499700	1.93620900	0.00110900

C	3.71200400	1.16866400	0.00108200	C	3.71434300	1.16894800	0.00061500
H	3.26957200	2.15772300	0.00200300	H	3.27335100	2.15875800	0.00115000
H	6.76636200	-0.31461000	0.00028600	H	6.77100300	-0.31619000	0.00002700

Cartesian coordinates of compound 5 for the anionic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-2.11214100	2.09752000	-0.00025700	S	-2.11416700	2.09802600	-0.00021400
S	0.41452500	-1.30083800	-0.00013200	S	0.41392200	-1.29639400	-0.00038600
C	-3.17790500	0.66595400	0.00008700	C	-3.17683600	0.66670300	0.00013700
C	-4.56256400	0.67443100	0.00030700	C	-4.56388200	0.67280500	0.00044400
H	-5.10628100	1.61627000	0.00035900	H	-5.11058900	1.61282100	0.00054300
C	-5.25937600	-0.54916500	0.00040200	C	-5.25872600	-0.55442300	0.00056100
H	-6.34573500	-0.55507000	0.00057400	H	-6.34507800	-0.56236500	0.00080800
C	-4.54076300	-1.75353900	0.00028800	C	-4.53769100	-1.76002500	0.00039500
H	-5.08254200	-2.69773200	0.00038600	H	-5.07777100	-2.70477000	0.00052300
C	-3.14978400	-1.77325900	0.00003600	C	-3.14380900	-1.77581500	0.00004300
H	-2.61243000	-2.71779700	-0.00002300	H	-2.60419300	-2.71906400	-0.00005000
C	-2.42061000	-0.55483400	-0.00009300	C	-2.41935600	-0.55386800	-0.00012800
C	-1.03431600	-0.29409200	-0.00034200	C	-1.03143400	-0.29033900	-0.00050700
C	1.48857300	0.15159100	-0.00001200	C	1.48588000	0.15288600	-0.00017900
C	0.69763200	1.32510100	-0.00023600	C	0.69892000	1.33090200	-0.00032700
H	1.12728700	2.31944900	-0.00044900	H	1.12933800	2.32477800	-0.00066800
C	-0.66872300	1.06237100	-0.00036400	C	-0.67110000	1.06708500	-0.00048500
C	2.90787600	0.01847900	0.00003300	C	2.90643900	0.01817500	0.00001200
C	3.56477400	-1.25175600	-0.00028400	C	3.56122000	-1.25447600	-0.00015700
H	2.96363300	-2.15719000	-0.00082600	H	2.96068100	-2.16021800	-0.00054100
C	4.94712300	-1.36037200	-0.00015700	C	4.94600900	-1.36526800	0.00003600
H	5.39690800	-2.35233600	-0.00038100	H	5.39435300	-2.35752600	-0.00009300
C	5.77006900	-0.22374800	0.00026000	C	5.77121000	-0.22694500	0.00041000
C	5.14854700	1.03700600	0.00050300	C	5.15011300	1.03690300	0.00057100
H	5.75889700	1.93924900	0.00073800	H	5.76105400	1.93838000	0.00082200
C	3.76935900	1.16210900	0.00036600	C	3.76825600	1.16299900	0.00035900
H	3.33004200	2.15541400	0.00062200	H	3.33117800	2.15709400	0.00053700
H	6.85262300	-0.31482900	0.00044600	H	6.85366500	-0.31903400	0.00061800

Frequency coordinates of compound 5 for the optimized neutral geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	2.10219800	2.07841200	-0.20841500	S	2.10289300	2.07695500	-0.22038600
S	-0.41646200	-1.27354000	0.13885900	S	-0.41645900	-1.27272000	0.14689700
C	3.15487100	0.65953400	-0.06399400	C	3.15526300	0.65983800	-0.06833100
C	4.55034500	0.66771400	-0.06675400	C	4.55245400	0.66871100	-0.07298700
H	5.09904700	1.59955200	-0.16233300	H	5.10104600	1.60016000	-0.17529000
C	5.22555200	-0.54413200	0.05474700	C	5.22997600	-0.54301800	0.05570900

H	6.31112700	-0.55325600	0.05385300	H	6.31566500	-0.55116000	0.05363400
C	4.51784300	-1.75091200	0.17748600	C	4.52212700	-1.75104000	0.18740300
H	5.06298700	-2.68514100	0.27076800	H	5.06782000	-2.68449200	0.28643200
C	3.12896800	-1.76334800	0.18120000	C	3.13142800	-1.76374500	0.19239800
H	2.58607200	-2.69918700	0.27643900	H	2.59005200	-2.69989500	0.29445600
C	2.42442300	-0.55363300	0.06037700	C	2.42536100	-0.55407400	0.06440500
C	1.01415600	-0.28777200	0.03623900	C	1.01414700	-0.28854300	0.03929000
C	-1.45791500	0.14830500	-0.01772100	C	-1.45725300	0.14742500	-0.01591500
C	-0.71550500	1.30311700	-0.13062600	C	-0.71539300	1.30375800	-0.13594800
H	-1.16076600	2.28129400	-0.26295700	H	-1.16107700	2.28136200	-0.27305900
C	0.68035300	1.04911000	-0.09824700	C	0.68174800	1.04934100	-0.10259100
C	-2.91883400	0.01117800	-0.00607200	C	-2.91987700	0.01043800	-0.00442000
C	-3.55155000	-1.16293500	-0.45280700	C	-3.55466700	-1.15179600	-0.48200700
H	-2.95126500	-1.98472700	-0.83206200	H	-2.95647500	-1.96498300	-0.88273600
C	-4.93990400	-1.27416500	-0.44041000	C	-4.94509900	-1.26228000	-0.47237500
H	-5.40675300	-2.18944200	-0.79226300	H	-5.41265600	-2.16747100	-0.84892900
C	-5.72834500	-0.21343700	0.00814500	C	-5.73371100	-0.21222600	0.00552400
C	-5.11343500	0.95873900	0.45326300	C	-5.11619100	0.94803100	0.48257800
H	-5.71645300	1.78670100	0.81453600	H	-5.71781400	1.76656000	0.86729400
C	-3.72566600	1.06864300	0.45457100	C	-3.72621800	1.05624800	0.48606700
H	-3.25728700	1.97026100	0.83634200	H	-3.25789500	1.94760100	0.89170800
H	-6.81063300	-0.30002500	0.01419300	H	-6.81618400	-0.29785300	0.00950000

Frequency coordinates of compound 5 for the optimized cationic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-2.08161100	2.11205600	-0.00065700	S	-2.08251100	2.11197000	-0.00031200
S	0.40522800	-1.29863400	0.00008600	S	0.40544000	-1.29787100	0.00015400
C	-3.12841600	0.67257600	-0.00004800	C	-3.12922100	0.67259700	-0.00007900
C	-4.51456900	0.67775000	0.00009900	C	-4.51664300	0.67836800	-0.00006900
H	-5.07555000	1.60605200	-0.00009200	H	-5.07773800	1.60693600	-0.00020200
C	-5.18169700	-0.55469100	0.00040800	C	-5.18550200	-0.55461000	0.00011100
H	-6.26689300	-0.56437100	0.00048900	H	-6.27086800	-0.56352500	0.00012000
C	-4.47992300	-1.77524800	0.00055200	C	-4.48352200	-1.77624800	0.00027600
H	-5.03061700	-2.70921600	0.00077900	H	-5.03434000	-2.71041400	0.00041400
C	-3.09662700	-1.78774900	0.00039700	C	-3.09863600	-1.78882900	0.00026000
H	-2.54898700	-2.72485600	0.00052700	H	-2.55226000	-2.72688500	0.00038600
C	-2.39677700	-0.55675100	0.00009900	C	-2.39772800	-0.55750300	0.00008300
C	-1.00905100	-0.29925900	-0.00005900	C	-1.00889000	-0.29985400	0.00002500
C	1.45294500	0.14350500	-0.00006500	C	1.45249000	0.14426700	-0.00002400
C	0.69476100	1.32961600	-0.00034100	C	0.69452500	1.33159700	-0.00018400
H	1.13789300	2.31625400	-0.00072600	H	1.13770400	2.31839400	-0.00038000
C	-0.67201300	1.08609700	-0.00034600	C	-0.67331400	1.08730600	-0.00016200
C	2.88392100	0.01289000	0.00000400	C	2.88510000	0.01318600	0.00000100

C	3.50725700	-1.26321500	-0.00099800	C	3.50865100	-1.26366400	-0.00058100
H	2.90380100	-2.16560400	-0.00205400	H	2.90581600	-2.16651800	-0.00109600
C	4.88693400	-1.37602800	-0.00088800	C	4.88991900	-1.37744000	-0.00057200
H	5.34879600	-2.35734800	-0.00170700	H	5.35096600	-2.35941700	-0.00104000
C	5.68495500	-0.22353600	0.00020100	C	5.68946900	-0.22471900	0.00002000
C	5.09076900	1.04622900	0.00116700	C	5.09471000	1.04610800	0.00062000
H	5.71092400	1.93611100	0.00203000	H	5.71499700	1.93620900	0.00110900
C	3.71200400	1.16866400	0.00108200	C	3.71434300	1.16894800	0.00061500
H	3.26957200	2.15772300	0.00200300	H	3.27335100	2.15875800	0.00115000
H	6.76636200	-0.31461000	0.00028600	H	6.77100300	-0.31619000	0.00002700

Frequency coordinates of compound 5 for the optimized anionic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-2.11214100	2.09752000	-0.00025700	S	-2.11416700	2.09802600	-0.00021400
S	0.41452500	-1.30083800	-0.00013200	S	0.41392200	-1.29639400	-0.00038600
C	-3.17790500	0.66595400	0.00008700	C	-3.17683600	0.66670300	0.00013700
C	-4.56256400	0.67443100	0.00030700	C	-4.56388200	0.67280500	0.00044400
H	-5.10628100	1.61627000	0.00035900	H	-5.11058900	1.61282100	0.00054300
C	-5.25937600	-0.54916500	0.00040200	C	-5.25872600	-0.55442300	0.00056100
H	-6.34573500	-0.55507000	0.00057400	H	-6.34507800	-0.56236500	0.00080800
C	-4.54076300	-1.75353900	0.00028800	C	-4.53769100	-1.76002500	0.00039500
H	-5.08254200	-2.69773200	0.00038600	H	-5.07777100	-2.70477000	0.00052300
C	-3.14978400	-1.77325900	0.00003600	C	-3.14380900	-1.77581500	0.00004300
H	-2.61243000	-2.71779700	-0.00002300	H	-2.60419300	-2.71906400	-0.00005000
C	-2.42061000	-0.55483400	-0.00009300	C	-2.41935600	-0.55386800	-0.00012800
C	-1.03431600	-0.29409200	-0.00034200	C	-1.03143400	-0.29033900	-0.00050700
C	1.48857300	0.15159100	-0.00001200	C	1.48588000	0.15288600	-0.00017900
C	0.69763200	1.32510100	-0.00023600	C	0.69892000	1.33090200	-0.00032700
H	1.12728700	2.31944900	-0.00044900	H	1.12933800	2.32477800	-0.00066800
C	-0.66872300	1.06237100	-0.00036400	C	-0.67110000	1.06708500	-0.00048500
C	2.90787600	0.01847900	0.00003300	C	2.90643900	0.01817500	0.00001200
C	3.56477400	-1.25175600	-0.00028400	C	3.56122000	-1.25447600	-0.00015700
H	2.96363300	-2.15719000	-0.00082600	H	2.96068100	-2.16021800	-0.00054100
C	4.94712300	-1.36037200	-0.00015700	C	4.94600900	-1.36526800	0.00003600
H	5.39690800	-2.35233600	-0.00038100	H	5.39435300	-2.35752600	-0.00009300
C	5.77006900	-0.22374800	0.00026000	C	5.77121000	-0.22694500	0.00041000
C	5.14854700	1.03700600	0.00050300	C	5.15011300	1.03690300	0.00057100
H	5.75889700	1.93924900	0.00073800	H	5.76105400	1.93838000	0.00082200
C	3.76935900	1.16210900	0.00036600	C	3.76825600	1.16299900	0.00035900
H	3.33004200	2.15541400	0.00062200	H	3.33117800	2.15709400	0.00053700
H	6.85262300	-0.31482900	0.00044600	H	6.85366500	-0.31903400	0.00061800

Cartesian coordinates of compound 6 for the neutral geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.14302500	2.00781400	-0.43345000	S	4.14468600	2.00662500	-0.43911400
S	1.51144700	-1.19810200	0.27224400	S	1.51362900	-1.19753300	0.27795800
C	5.14648100	0.57904300	-0.12640000	C	5.14851900	0.57977500	-0.12985300
C	6.54139100	0.53938600	-0.12306100	C	6.54518000	0.54094100	-0.12953100
H	7.12190800	1.43527500	-0.32022500	H	7.12517500	1.43658100	-0.33059100
C	7.17443400	-0.67322200	0.13803600	C	7.18106400	-0.67162800	0.13374400
H	8.25905200	-0.71921400	0.14380500	H	8.26584800	-0.71655200	0.13711000
C	6.42562700	-1.83366000	0.39292000	C	6.43254600	-1.83340600	0.39403400
H	6.93830300	-2.76923500	0.59419200	H	6.94618400	-2.76828600	0.59673400
C	5.03717200	-1.79853700	0.39043700	C	5.04224800	-1.79858600	0.39455400
H	4.46230800	-2.69860400	0.58790200	H	4.46926600	-2.69914700	0.59594500
C	4.37475300	-0.58701800	0.12984000	C	4.37776300	-0.58708400	0.13181200
C	2.97467100	-0.27825000	0.06806100	C	2.97659700	-0.27872300	0.07175200
C	0.51848400	0.23195400	-0.04672800	C	0.52070000	0.23070300	-0.04297000
C	1.30060200	1.34155200	-0.28408700	C	1.30201700	1.34189000	-0.28433400
H	0.88953200	2.31350300	-0.52667700	H	0.89038200	2.31340600	-0.52879500
C	2.68654400	1.04580200	-0.21661800	C	2.68937500	1.04604200	-0.21679800
C	-0.94416800	0.14566500	-0.02854700	C	-0.94376100	0.14408500	-0.02440700
C	-1.62011600	-1.05411300	-0.31368100	C	-1.62102900	-1.04797100	-0.34178300
H	-1.05169000	-1.94555400	-0.56235000	H	-1.05434400	-1.93395000	-0.61330000
C	-3.00848100	-1.11745400	-0.29717500	C	-3.01166600	-1.11093000	-0.32742600
H	-3.49735600	-2.06561500	-0.49856100	H	-3.49985800	-2.05335400	-0.55691800
C	-3.78835100	0.01410900	-0.00522100	C	-3.79123600	0.01345600	-0.00429200
C	-3.11103000	1.21298500	0.27814900	C	-3.11281900	1.20439200	0.31245300
H	-3.68187500	2.11141700	0.49193200	H	-3.68204600	2.09720100	0.55366300
C	-1.72335800	1.27776500	0.27482500	C	-1.72286400	1.26840800	0.31052800
H	-1.23332600	2.21401200	0.52276000	H	-1.23348300	2.19831600	0.58314900
C	-5.27018200	-0.05472100	0.00660600	C	-5.27464900	-0.05460300	0.00585600
C	-5.96380500	-0.84978000	-0.92211400	C	-5.97125200	-0.78624400	-0.97304500
H	-5.40721800	-1.39815000	-1.67618900	H	-5.41722900	-1.28577100	-1.76238100
C	-7.35575400	-0.91635100	-0.91027500	C	-7.36530600	-0.85232000	-0.96323100
H	-7.87035700	-1.53129500	-1.64302100	H	-7.88183000	-1.41650500	-1.73464300
C	-8.08700700	-0.18811200	0.02956200	C	-8.09511600	-0.18660100	0.02542800
H	-9.17166900	-0.23960900	0.03853900	H	-9.17992400	-0.23749000	0.03313300
C	-7.41262400	0.60676800	0.95783200	C	-7.41697800	0.54527400	1.00413100
H	-7.97103100	1.17061200	1.69955400	H	-7.97322400	1.05920300	1.78301000
C	-6.02059200	0.67218000	0.94685300	C	-6.02282400	0.60997000	0.99442100
H	-5.50628400	1.27113400	1.69235200	H	-5.50699300	1.15982500	1.77611400

Cartesian coordinates of compound 6 for the cationic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.11724400	2.06634800	-0.16667000	S	4.12025000	2.06559500	-0.17412700
S	1.50945300	-1.23951700	0.09813300	S	1.51059600	-1.23792000	0.10479800
C	5.11231100	0.59876800	-0.04480100	C	5.11457600	0.59828800	-0.04868700
C	6.50067800	0.55674400	-0.03817300	C	6.50433800	0.55620400	-0.04406200
H	7.09100400	1.46385000	-0.11030500	H	7.09504000	1.46307300	-0.12030600
C	7.12485400	-0.69013100	0.06406300	C	7.12989100	-0.69115000	0.06167900
H	8.20899600	-0.73761900	0.07034000	H	8.21421800	-0.73830400	0.06644800
C	6.37994000	-1.88090800	0.15853900	C	6.38438200	-1.88261700	0.16158200
H	6.89720000	-2.83078400	0.23649500	H	6.90160500	-2.83253400	0.24220500
C	4.99646100	-1.84627300	0.15276100	C	4.99936100	-1.84751900	0.15768800
H	4.41777000	-2.76172800	0.22543800	H	4.42167600	-2.76348400	0.23453400
C	4.33965700	-0.59889900	0.05058200	C	4.34181000	-0.59972800	0.05201600
C	2.95718600	-0.29230100	0.02336000	C	2.95842900	-0.29261000	0.02547700
C	0.50963000	0.22951700	-0.02323600	C	0.51165400	0.23093800	-0.02010500
C	1.30936000	1.38259100	-0.11609800	C	1.31160400	1.38498400	-0.11783900
H	0.90224200	2.38149700	-0.19847400	H	0.90471100	2.38383000	-0.20385800
C	2.66898700	1.09134900	-0.08999200	C	2.67206300	1.09253900	-0.09229600
C	-0.91947500	0.15051400	-0.01744100	C	-0.91886700	0.15184900	-0.01358200
C	-1.59958700	-1.09476400	0.07595200	C	-1.59933900	-1.09418900	0.07835900
H	-1.03368700	-2.01735700	0.15888400	H	-1.03428600	-2.01747500	0.16027400
C	-2.97486700	-1.15946800	0.07776500	C	-2.97633600	-1.15940200	0.07996900
H	-3.45397400	-2.12590000	0.18178000	H	-3.45398900	-2.12718400	0.18056900
C	-3.77150000	0.01191400	-0.00462400	C	-3.77366000	0.01225500	-0.00210000
C	-3.09226000	1.25490300	-0.09451700	C	-3.09431100	1.25613700	-0.08991800
H	-3.66423400	2.17004400	-0.19389700	H	-3.66534200	2.17249400	-0.18610900
C	-1.71763900	1.32598200	-0.10499300	C	-1.71796200	1.32761400	-0.09932500
H	-1.24576400	2.29755100	-0.19227900	H	-1.24740500	2.30011200	-0.18479900
C	-5.23407300	-0.05859400	0.00366400	C	-5.23792400	-0.05892900	0.00386400
C	-5.90782900	-1.21039400	-0.46344600	C	-5.91121800	-1.20520300	-0.47958600
H	-5.34206900	-2.04237700	-0.86867600	H	-5.34561900	-2.03358200	-0.89279400
C	-7.29507400	-1.27174000	-0.46159000	C	-7.30029400	-1.26736700	-0.48041800
H	-7.79601500	-2.15643700	-0.84063300	H	-7.80005200	-2.14740500	-0.87230400
C	-8.04491600	-0.19348800	0.02002700	C	-8.05233900	-0.19500700	0.01445900
H	-9.12897300	-0.24548900	0.02631900	H	-9.13654600	-0.24740200	0.01848000
C	-7.39619400	0.95185300	0.49358400	C	-7.40351600	0.94504700	0.50413800
H	-7.97513800	1.78470800	0.87892400	H	-7.98290400	1.77292000	0.90003900
C	-6.00954200	1.02360200	0.47934400	C	-6.01499300	1.01714400	0.49287300
H	-5.52114800	1.90611500	0.87826800	H	-5.52873600	1.89648500	0.90175400

Cartesian coordinates of compound 6 for the anionic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.16287200	2.05603200	-0.11055700	S	4.16700400	2.05625900	-0.10636200
S	1.52075600	-1.24017900	0.05615900	S	1.52231400	-1.23573100	0.05907700
C	5.17601000	0.59349400	-0.02608000	C	5.17732900	0.59347000	-0.02737400
C	6.56250200	0.55386500	-0.01648700	C	6.56592900	0.55154300	-0.02113700
H	7.13947200	1.47407000	-0.06291100	H	7.14536500	1.47024200	-0.06686900
C	7.21160800	-0.68888800	0.05411500	C	7.21375400	-0.69450800	0.04520100
H	8.29693800	-0.73273000	0.06233000	H	8.29905700	-0.74005400	0.05070300
C	6.45405000	-1.86785900	0.11370800	C	6.45378700	-1.87473700	0.10393400
H	6.96309900	-2.82774600	0.16855700	H	6.96135400	-2.83533800	0.15539900
C	5.06348000	-1.83748100	0.10452600	C	5.06076500	-1.84080900	0.09799600
H	4.49231100	-2.76057900	0.15147000	H	4.48805400	-2.76306600	0.14404300
C	4.38239200	-0.59841600	0.03401200	C	4.38316800	-0.59856000	0.03176000
C	3.00062900	-0.28976100	0.01014900	C	3.00019000	-0.28691500	0.01166900
C	0.50177800	0.24330100	-0.02253800	C	0.50577900	0.24557600	-0.01657700
C	1.32822700	1.38474200	-0.08286300	C	1.32941900	1.39043800	-0.07576500
H	0.93327400	2.39166700	-0.13000800	H	0.93427100	2.39732600	-0.12182600
C	2.68900900	1.07222700	-0.06423000	C	2.69349500	1.07634500	-0.05951700
C	-0.92020400	0.15844000	-0.01808200	C	-0.91841800	0.15983400	-0.01251100
C	-1.62473900	-1.07982000	0.08755800	C	-1.62171000	-1.07992300	0.08735600
H	-1.05981900	-2.00328300	0.18771500	H	-1.05881100	-2.00502100	0.18264800
C	-3.00231900	-1.14408000	0.08895200	C	-3.00246200	-1.14498900	0.08860200
H	-3.46965000	-2.11807400	0.20901800	H	-3.46536500	-2.12181400	0.19938300
C	-3.82119900	0.01313200	-0.00552200	C	-3.82243900	0.01308100	-0.00244600
C	-3.12186000	1.24773100	-0.10845400	C	-3.12299500	1.24924300	-0.10028300
H	-3.68614100	2.16961400	-0.22462200	H	-3.68386500	2.17380300	-0.20835100
C	-1.74598900	1.32211600	-0.11953200	C	-1.74389600	1.32446300	-0.10903300
H	-1.27789700	2.29664300	-0.22545900	H	-1.27830100	2.30055200	-0.20995400
C	-5.28049700	-0.05884700	0.00365100	C	-5.28299800	-0.05968500	0.00358900
C	-5.97754200	-1.24501300	-0.34520900	C	-5.97934100	-1.25326200	-0.32808600
H	-5.41338500	-2.11642000	-0.66273100	H	-5.41666000	-2.13260800	-0.62519800
C	-7.36583300	-1.31242100	-0.33155300	C	-7.36992600	-1.32161500	-0.31885900
H	-7.85488700	-2.24255200	-0.61463400	H	-7.85662900	-2.25684100	-0.58843400
C	-8.13704600	-0.19932800	0.02283300	C	-8.14485200	-0.20164600	0.01446800
H	-9.22221800	-0.25269900	0.03005400	H	-9.23001300	-0.25542300	0.01836700
C	-7.47419500	0.98428300	0.36743700	C	-7.48216900	0.98958300	0.34235800
H	-8.04841000	1.86213500	0.65754000	H	-8.05709100	1.87218800	0.61570000
C	-6.08583300	1.05357700	0.36221400	C	-6.09149300	1.05931200	0.34088400
H	-5.60531200	1.97633500	0.67242600	H	-5.61594100	1.99017800	0.63358400

Frequency coordinates of compound 2 for the optimized neutral geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.14302500	2.00781400	-0.43345000	S	4.14468600	2.00662500	-0.43911400
S	1.51144700	-1.19810200	0.27224400	S	1.51362900	-1.19753300	0.27795800
C	5.14648100	0.57904300	-0.12640000	C	5.14851900	0.57977500	-0.12985300
C	6.54139100	0.53938600	-0.12306100	C	6.54518000	0.54094100	-0.12953100
H	7.12190800	1.43527500	-0.32022500	H	7.12517500	1.43658100	-0.33059100
C	7.17443400	-0.67322200	0.13803600	C	7.18106400	-0.67162800	0.13374400
H	8.25905200	-0.71921400	0.14380500	H	8.26584800	-0.71655200	0.13711000
C	6.42562700	-1.83366000	0.39292000	C	6.43254600	-1.83340600	0.39403400
H	6.93830300	-2.76923500	0.59419200	H	6.94618400	-2.76828600	0.59673400
C	5.03717200	-1.79853700	0.39043700	C	5.04224800	-1.79858600	0.39455400
H	4.46230800	-2.69860400	0.58790200	H	4.46926600	-2.69914700	0.59594500
C	4.37475300	-0.58701800	0.12984000	C	4.37776300	-0.58708400	0.13181200
C	2.97467100	-0.27825000	0.06806100	C	2.97659700	-0.27872300	0.07175200
C	0.51848400	0.23195400	-0.04672800	C	0.52070000	0.23070300	-0.04297000
C	1.30060200	1.34155200	-0.28408700	C	1.30201700	1.34189000	-0.28433400
H	0.88953200	2.31350300	-0.52667700	H	0.89038200	2.31340600	-0.52879500
C	2.68654400	1.04580200	-0.21661800	C	2.68937500	1.04604200	-0.21679800
C	-0.94416800	0.14566500	-0.02854700	C	-0.94376100	0.14408500	-0.02440700
C	-1.62011600	-1.05411300	-0.31368100	C	-1.62102900	-1.04797100	-0.34178300
H	-1.05169000	-1.94555400	-0.56235000	H	-1.05434400	-1.93395000	-0.61330000
C	-3.00848100	-1.11745400	-0.29717500	C	-3.01166600	-1.11093000	-0.32742600
H	-3.49735600	-2.06561500	-0.49856100	H	-3.49985800	-2.05335400	-0.55691800
C	-3.78835100	0.01410900	-0.00522100	C	-3.79123600	0.01345600	-0.00429200
C	-3.11103000	1.21298500	0.27814900	C	-3.11281900	1.20439200	0.31245300
H	-3.68187500	2.11141700	0.49193200	H	-3.68204600	2.09720100	0.55366300
C	-1.72335800	1.27776500	0.27482500	C	-1.72286400	1.26840800	0.31052800
H	-1.23332600	2.21401200	0.52276000	H	-1.23348300	2.19831600	0.58314900
C	-5.27018200	-0.05472100	0.00660600	C	-5.27464900	-0.05460300	0.00585600
C	-5.96380500	-0.84978000	-0.92211400	C	-5.97125200	-0.78624400	-0.97304500
H	-5.40721800	-1.39815000	-1.67618900	H	-5.41722900	-1.28577100	-1.76238100
C	-7.35575400	-0.91635100	-0.91027500	C	-7.36530600	-0.85232000	-0.96323100
H	-7.87035700	-1.53129500	-1.64302100	H	-7.88183000	-1.41650500	-1.73464300
C	-8.08700700	-0.18811200	0.02956200	C	-8.09511600	-0.18660100	0.02542800
H	-9.17166900	-0.23960900	0.03853900	H	-9.17992400	-0.23749000	0.03313300
C	-7.41262400	0.60676800	0.95783200	C	-7.41697800	0.54527400	1.00413100
H	-7.97103100	1.17061200	1.69955400	H	-7.97322400	1.05920300	1.78301000
C	-6.02059200	0.67218000	0.94685300	C	-6.02282400	0.60997000	0.99442100
H	-5.50628400	1.27113400	1.69235200	H	-5.50699300	1.15982500	1.77611400

Frequency coordinates of compound 6 for the optimized cationic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.11724400	2.06634800	-0.16667000	S	4.12025000	2.06559500	-0.17412700
S	1.50945300	-1.23951700	0.09813300	S	1.51059600	-1.23792000	0.10479800
C	5.11231100	0.59876800	-0.04480100	C	5.11457600	0.59828800	-0.04868700
C	6.50067800	0.55674400	-0.03817300	C	6.50433800	0.55620400	-0.04406200
H	7.09100400	1.46385000	-0.11030500	H	7.09504000	1.46307300	-0.12030600
C	7.12485400	-0.69013100	0.06406300	C	7.12989100	-0.69115000	0.06167900
H	8.20899600	-0.73761900	0.07034000	H	8.21421800	-0.73830400	0.06644800
C	6.37994000	-1.88090800	0.15853900	C	6.38438200	-1.88261700	0.16158200
H	6.89720000	-2.83078400	0.23649500	H	6.90160500	-2.83253400	0.24220500
C	4.99646100	-1.84627300	0.15276100	C	4.99936100	-1.84751900	0.15768800
H	4.41777000	-2.76172800	0.22543800	H	4.42167600	-2.76348400	0.23453400
C	4.33965700	-0.59889900	0.05058200	C	4.34181000	-0.59972800	0.05201600
C	2.95718600	-0.29230100	0.02336000	C	2.95842900	-0.29261000	0.02547700
C	0.50963000	0.22951700	-0.02323600	C	0.51165400	0.23093800	-0.02010500
C	1.30936000	1.38259100	-0.11609800	C	1.31160400	1.38498400	-0.11783900
H	0.90224200	2.38149700	-0.19847400	H	0.90471100	2.38383000	-0.20385800
C	2.66898700	1.09134900	-0.08999200	C	2.67206300	1.09253900	-0.09229600
C	-0.91947500	0.15051400	-0.01744100	C	-0.91886700	0.15184900	-0.01358200
C	-1.59958700	-1.09476400	0.07595200	C	-1.59933900	-1.09418900	0.07835900
H	-1.03368700	-2.01735700	0.15888400	H	-1.03428600	-2.01747500	0.16027400
C	-2.97486700	-1.15946800	0.07776500	C	-2.97633600	-1.15940200	0.07996900
H	-3.45397400	-2.12590000	0.18178000	H	-3.45398900	-2.12718400	0.18056900
C	-3.77150000	0.01191400	-0.00462400	C	-3.77366000	0.01225500	-0.00210000
C	-3.09226000	1.25490300	-0.09451700	C	-3.09431100	1.25613700	-0.08991800
H	-3.66423400	2.17004400	-0.19389700	H	-3.66534200	2.17249400	-0.18610900
C	-1.71763900	1.32598200	-0.10499300	C	-1.71796200	1.32761400	-0.09932500
H	-1.24576400	2.29755100	-0.19227900	H	-1.24740500	2.30011200	-0.18479900
C	-5.23407300	-0.05859400	0.00366400	C	-5.23792400	-0.05892900	0.00386400
C	-5.90782900	-1.21039400	-0.46344600	C	-5.91121800	-1.20520300	-0.47958600
H	-5.34206900	-2.04237700	-0.86867600	H	-5.34561900	-2.03358200	-0.89279400
C	-7.29507400	-1.27174000	-0.46159000	C	-7.30029400	-1.26736700	-0.48041800
H	-7.79601500	-2.15643700	-0.84063300	H	-7.80005200	-2.14740500	-0.87230400
C	-8.04491600	-0.19348800	0.02002700	C	-8.05233900	-0.19500700	0.01445900
H	-9.12897300	-0.24548900	0.02631900	H	-9.13654600	-0.24740200	0.01848000
C	-7.39619400	0.95185300	0.49358400	C	-7.40351600	0.94504700	0.50413800
H	-7.97513800	1.78470800	0.87892400	H	-7.98290400	1.77292000	0.90003900
C	-6.00954200	1.02360200	0.47934400	C	-6.01499300	1.01714400	0.49287300
H	-5.52114800	1.90611500	0.87826800	H	-5.52873600	1.89648500	0.90175400

Frequency coordinates of compound 6 for the optimized anionic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	4.16287200	2.05603200	-0.11055700	S	4.16700400	2.05625900	-0.10636200
S	1.52075600	-1.24017900	0.05615900	S	1.52231400	-1.23573100	0.05907700
C	5.17601000	0.59349400	-0.02608000	C	5.17732900	0.59347000	-0.02737400
C	6.56250200	0.55386500	-0.01648700	C	6.56592900	0.55154300	-0.02113700
H	7.13947200	1.47407000	-0.06291100	H	7.14536500	1.47024200	-0.06686900
C	7.21160800	-0.68888800	0.05411500	C	7.21375400	-0.69450800	0.04520100
H	8.29693800	-0.73273000	0.06233000	H	8.29905700	-0.74005400	0.05070300
C	6.45405000	-1.86785900	0.11370800	C	6.45378700	-1.87473700	0.10393400
H	6.96309900	-2.82774600	0.16855700	H	6.96135400	-2.83533800	0.15539900
C	5.06348000	-1.83748100	0.10452600	C	5.06076500	-1.84080900	0.09799600
H	4.49231100	-2.76057900	0.15147000	H	4.48805400	-2.76306600	0.14404300
C	4.38239200	-0.59841600	0.03401200	C	4.38316800	-0.59856000	0.03176000
C	3.00062900	-0.28976100	0.01014900	C	3.00019000	-0.28691500	0.01166900
C	0.50177800	0.24330100	-0.02253800	C	0.50577900	0.24557600	-0.01657700
C	1.32822700	1.38474200	-0.08286300	C	1.32941900	1.39043800	-0.07576500
H	0.93327400	2.39166700	-0.13000800	H	0.93427100	2.39732600	-0.12182600
C	2.68900900	1.07222700	-0.06423000	C	2.69349500	1.07634500	-0.05951700
C	-0.92020400	0.15844000	-0.01808200	C	-0.91841800	0.15983400	-0.01251100
C	-1.62473900	-1.07982000	0.08755800	C	-1.62171000	-1.07992300	0.08735600
H	-1.05981900	-2.00328300	0.18771500	H	-1.05881100	-2.00502100	0.18264800
C	-3.00231900	-1.14408000	0.08895200	C	-3.00246200	-1.14498900	0.08860200
H	-3.46965000	-2.11807400	0.20901800	H	-3.46536500	-2.12181400	0.19938300
C	-3.82119900	0.01313200	-0.00552200	C	-3.82243900	0.01308100	-0.00244600
C	-3.12186000	1.24773100	-0.10845400	C	-3.12299500	1.24924300	-0.10028300
H	-3.68614100	2.16961400	-0.22462200	H	-3.68386500	2.17380300	-0.20835100
C	-1.74598900	1.32211600	-0.11953200	C	-1.74389600	1.32446300	-0.10903300
H	-1.27789700	2.29664300	-0.22545900	H	-1.27830100	2.30055200	-0.20995400
C	-5.28049700	-0.05884700	0.00365100	C	-5.28299800	-0.05968500	0.00358900
C	-5.97754200	-1.24501300	-0.34520900	C	-5.97934100	-1.25326200	-0.32808600
H	-5.41338500	-2.11642000	-0.66273100	H	-5.41666000	-2.13260800	-0.62519800
C	-7.36583300	-1.31242100	-0.33155300	C	-7.36992600	-1.32161500	-0.31885900
H	-7.85488700	-2.24255200	-0.61463400	H	-7.85662900	-2.25684100	-0.58843400
C	-8.13704600	-0.19932800	0.02283300	C	-8.14485200	-0.20164600	0.01446800
H	-9.22221800	-0.25269900	0.03005400	H	-9.23001300	-0.25542300	0.01836700
C	-7.47419500	0.98428300	0.36743700	C	-7.48216900	0.98958300	0.34235800
H	-8.04841000	1.86213500	0.65754000	H	-8.05709100	1.87218800	0.61570000
C	-6.08583300	1.05357700	0.36221400	C	-6.09149300	1.05931200	0.34088400
H	-5.60531200	1.97633500	0.67242600	H	-5.61594100	1.99017800	0.63358400

Cartesian coordinates of compound 7 for the neutral geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.44108600	1.97540400	-0.37719500	S	3.44175700	1.97381300	-0.38693400
S	0.59090800	-1.04853100	0.28274300	S	0.59262600	-1.04729700	0.29153800
C	4.34044200	0.46598600	-0.14289600	C	4.34165400	0.46664800	-0.14736500
C	5.72829300	0.32323200	-0.17166200	C	5.73126200	0.32473100	-0.17843800
H	6.37010300	1.18021200	-0.35106900	H	6.37247100	1.18133900	-0.36301800
C	6.27397700	-0.94122700	0.03483600	C	6.27983200	-0.93956500	0.03262300
H	7.35205800	-1.06743000	0.01552500	H	7.35813000	-1.06455100	0.01169900
C	5.44571200	-2.05141200	0.26692300	C	5.45186500	-2.05094900	0.27175100
H	5.89097600	-3.02874200	0.42573400	H	5.89820000	-3.02738500	0.43380900
C	4.06396800	-1.91375300	0.29566200	C	4.06829700	-1.91362500	0.30275800
H	3.42745500	-2.77520200	0.47549300	H	3.43370400	-2.77555800	0.48772900
C	3.48882900	-0.64815400	0.09052200	C	3.49106200	-0.64818200	0.09322800
C	2.11480100	-0.23443600	0.07105200	C	2.11598500	-0.23498400	0.07398000
C	-0.29768000	0.46206400	0.03712600	C	-0.29636000	0.46105900	0.04133300
C	0.56075000	1.51823100	-0.17967700	C	0.56154400	1.51849400	-0.18227800
H	0.22033400	2.52730700	-0.37542000	H	0.22090400	2.52709600	-0.38113100
C	1.92150100	1.11690400	-0.16012800	C	1.92352200	1.11677500	-0.16315100
C	-1.76241100	0.48613600	0.08349100	C	-1.76268000	0.48503400	0.08813300
C	-2.52531000	-0.63336000	-0.21324800	C	-2.52683400	-0.63303600	-0.21562200
H	-2.03849800	-1.55825600	-0.51118200	H	-2.04134200	-1.55726400	-0.51799800
C	-3.94149600	-0.60504300	-0.16758100	C	-3.94467700	-0.60417000	-0.17087600
C	-4.60414100	0.61522200	0.18441200	C	-4.60785900	0.61445900	0.18811100
C	-3.80701400	1.75346200	0.48371400	C	-3.80967200	1.75151700	0.49539400
C	-2.43702500	1.69372100	0.44133500	C	-2.43777500	1.69128800	0.45352500
H	-1.85086800	2.56725000	0.70700700	H	-1.85323100	2.56446200	0.72425400
H	-4.30145100	2.67997900	0.76371300	H	-4.30281700	2.67702000	0.78146900
C	-4.72967100	-1.74900700	-0.47008700	C	-4.73333700	-1.74758300	-0.48079300
C	-6.02204100	0.64293900	0.22563500	C	-6.02719500	0.64267200	0.22792000
H	-6.51978900	1.57080400	0.49524000	H	-6.52583500	1.56879600	0.50232400
H	-4.22714700	-2.67430100	-0.73930100	H	-4.23147100	-2.67196200	-0.75487400
C	-6.75728200	-0.48331900	-0.07082000	C	-6.76395900	-0.48298800	-0.07625900
H	-7.84216900	-0.45027800	-0.03688600	H	-7.84895700	-0.44931500	-0.04325500
C	-6.10398000	-1.68984800	-0.42243300	C	-6.10974000	-1.68886500	-0.43437000
H	-6.69425400	-2.57133600	-0.65467000	H	-6.69948600	-2.56931900	-0.67230200

Cartesian coordinates of compound 7 for the cationic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.44735400	2.01776200	0.00029500	S	-3.44881800	2.01764100	-0.00028900
S	0.57079600	-1.06617100	-0.00053100	S	-0.57127500	-1.06536400	0.00011400
C	4.31495000	0.46562100	0.00028200	C	-4.31632100	0.46567500	-0.00006800
C	5.69418000	0.30652100	0.00051500	C	-5.69690800	0.30696900	-0.00002700
H	6.35943100	1.16325800	0.00079600	H	-6.36239000	1.16388400	-0.00011100
C	6.21078400	-0.99351400	0.00026100	C	-6.21513400	-0.99389400	0.00007300
H	7.28706800	-1.13229800	0.00037800	H	-7.29168100	-1.13193800	0.00007200
C	5.36822400	-2.12097300	-0.00022100	C	-5.37219800	-2.12250800	0.00013400
H	5.80319400	-3.11425500	-0.00043900	H	-5.80731600	-3.11596000	0.00020500
C	3.99254800	-1.96915700	-0.00042800	C	-3.99490300	-1.97056700	0.00010700
H	3.33835800	-2.83533100	-0.00077700	H	-3.34187900	-2.83784200	0.00017100
C	3.44373100	-0.66629000	-0.00018300	C	-3.44513300	-0.66712600	0.00000100
C	2.09250700	-0.24321900	-0.00021900	C	-2.09290100	-0.24380800	-0.00000500
C	-0.30157800	0.49018300	-0.00007900	C	0.30047700	0.49113100	0.00006600
C	0.59300800	1.57335300	0.00023900	C	-0.59420200	1.57555100	-0.00001800
H	0.27200000	2.60622900	0.00038500	H	-0.27361500	2.60870000	-0.00011300
C	1.92322000	1.16662300	0.00014300	C	-1.92530000	1.16771700	-0.00009400
C	-1.73393600	0.53849200	-0.00011500	C	1.73428000	0.53913000	0.00014300
C	-2.49943900	-0.64696200	0.00011600	C	2.49999700	-0.64688200	0.00001200
H	-2.00458300	-1.61415500	0.00031100	H	2.00560700	-1.61436700	-0.00009200
C	-3.90246500	-0.62495100	0.00015300	C	3.90453900	-0.62496700	-0.00001800
C	-4.57944300	0.64236600	-0.00014700	C	4.58237200	0.64243200	0.00008500
C	-3.79340100	1.83649300	-0.00049600	C	3.79604000	1.83766300	0.00028600
C	-2.42798200	1.79464700	-0.00049100	C	2.42906900	1.79583300	0.00032300
H	-1.86882800	2.72218700	-0.00091900	H	1.87112000	2.72418800	0.00053100
H	-4.30428800	2.79462400	-0.00088200	H	4.30633100	2.79634200	0.00041000
C	-4.67053700	-1.82644600	0.00048000	C	4.67287700	-1.82764200	-0.00018600
C	-5.98619100	0.66273900	-0.00009000	C	5.99050200	0.66258400	0.00000000
H	-6.50503700	1.61648400	-0.00033200	H	6.51019300	1.61609200	0.00007300
H	-4.15433000	-2.78192600	0.00071400	H	4.15720800	-2.78363200	-0.00024700
C	-6.70673200	-0.52381100	0.00026900	C	6.71183100	-0.52498100	-0.00016200
H	-7.79161500	-0.49287300	0.00031100	H	7.79688600	-0.49411900	-0.00022100
C	-6.04690500	-1.77320500	0.00056900	C	6.05080000	-1.77510300	-0.00024100
H	-6.62902900	-2.68847000	0.00089500	H	6.63231700	-2.69100800	-0.00035100

Cartesian coordinates of compound 2 for the anionic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.47867000	2.00820800	0.00013700	S	-3.48218300	2.00827500	-0.00028900
S	0.57796100	-1.06924300	-0.00045000	S	-0.57863800	-1.06497800	-0.00015200
C	4.37076600	0.46550200	0.00011400	C	-4.37115500	0.46538600	0.00004000
C	5.74905000	0.31388500	0.00017200	C	-5.75114500	0.31112800	0.00028300
H	6.39823800	1.18603500	0.00024600	H	-6.40289500	1.18137800	0.00029800
C	6.29680000	-0.97966700	0.00009400	C	-6.29726300	-0.98582100	0.00055700
H	7.37512100	-1.11099300	0.00011500	H	-7.37538800	-1.11894600	0.00078800
C	5.44609300	-2.09478500	-0.00005200	C	-5.44363000	-2.10163400	0.00056500
H	5.87569200	-3.09442600	-0.00013500	H	-5.87135500	-3.10183700	0.00078600
C	4.06241700	-1.95231500	-0.00009500	C	-4.05775200	-1.95531300	0.00026500
H	3.41885500	-2.82778700	-0.00021300	H	-3.41253900	-2.82964600	0.00025600
C	3.48226600	-0.65999800	0.00000000	C	-3.48149100	-0.65994500	-0.00000700
C	2.13091300	-0.24069900	0.00003700	C	-2.12971000	-0.23758500	-0.00053700
C	-0.31759300	0.49234000	-0.00011100	C	0.31494000	0.49453900	-0.00013100
C	0.59864500	1.56571300	-0.00001800	C	-0.59974000	1.57174100	-0.00033500
H	0.28884700	2.60315800	0.00002700	H	-0.28993100	2.60916600	-0.00044600
C	1.92905600	1.14518100	0.00009400	C	-1.93263200	1.14953100	-0.00058100
C	-1.74414400	0.50906200	0.00002000	C	1.74323600	0.51100200	-0.00014600
C	-2.53916400	-0.66618400	0.00021700	C	2.53733800	-0.66625200	-0.00047200
H	-2.05435100	-1.63935500	0.00061800	H	2.05293000	-1.63956200	-0.00123000
C	-3.94558500	-0.63064500	0.00016200	C	3.94594600	-0.63097500	-0.00020000
C	-4.63132000	0.63865200	-0.00004600	C	4.63269500	0.63841000	0.00034200
C	-3.82226500	1.82108700	-0.00014400	C	3.82414300	1.82294100	0.00052000
C	-2.45576700	1.75752900	-0.00010600	C	2.45488800	1.76001700	0.00028600
H	-1.88885900	2.68435100	-0.00021200	H	1.89019900	2.68792900	0.00051300
H	-4.31916400	2.78986600	-0.00022300	H	4.32023000	2.79209500	0.00086600
C	-4.75116500	-1.81162800	0.00031000	C	4.75122700	-1.81432000	-0.00046500
C	-6.03780100	0.67219100	-0.00013000	C	6.04105900	0.67160500	0.00062500
H	-6.53352400	1.64209400	-0.00029700	H	6.53822700	1.64067200	0.00104000
H	-4.25216300	-2.77845500	0.00048100	H	4.25218300	-2.78113600	-0.00086400
C	-6.79319600	-0.49702900	-0.00001100	C	6.79757300	-0.49954000	0.00037400
H	-7.87912300	-0.45229300	-0.00008300	H	7.88344400	-0.45525300	0.00059000
C	-6.13145300	-1.74226700	0.00022000	C	6.13349200	-1.74682200	-0.00017900
H	-6.71499000	-2.66116900	0.00032300	H	6.71591200	-2.66617800	-0.00037200

Frequency coordinates of compound 7 for the optimized neutral geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.44108600	1.97540400	-0.37719500	S	3.44175700	1.97381300	-0.38693400
S	0.59090800	-1.04853100	0.28274300	S	0.59262600	-1.04729700	0.29153800
C	4.34044200	0.46598600	-0.14289600	C	4.34165400	0.46664800	-0.14736500
C	5.72829300	0.32323200	-0.17166200	C	5.73126200	0.32473100	-0.17843800
H	6.37010300	1.18021200	-0.35106900	H	6.37247100	1.18133900	-0.36301800
C	6.27397700	-0.94122700	0.03483600	C	6.27983200	-0.93956500	0.03262300
H	7.35205800	-1.06743000	0.01552500	H	7.35813000	-1.06455100	0.01169900
C	5.44571200	-2.05141200	0.26692300	C	5.45186500	-2.05094900	0.27175100
H	5.89097600	-3.02874200	0.42573400	H	5.89820000	-3.02738500	0.43380900
C	4.06396800	-1.91375300	0.29566200	C	4.06829700	-1.91362500	0.30275800
H	3.42745500	-2.77520200	0.47549300	H	3.43370400	-2.77555800	0.48772900
C	3.48882900	-0.64815400	0.09052200	C	3.49106200	-0.64818200	0.09322800
C	2.11480100	-0.23443600	0.07105200	C	2.11598500	-0.23498400	0.07398000
C	-0.29768000	0.46206400	0.03712600	C	-0.29636000	0.46105900	0.04133300
C	0.56075000	1.51823100	-0.17967700	C	0.56154400	1.51849400	-0.18227800
H	0.22033400	2.52730700	-0.37542000	H	0.22090400	2.52709600	-0.38113100
C	1.92150100	1.11690400	-0.16012800	C	1.92352200	1.11677500	-0.16315100
C	-1.76241100	0.48613600	0.08349100	C	-1.76268000	0.48503400	0.08813300
C	-2.52531000	-0.63336000	-0.21324800	C	-2.52683400	-0.63303600	-0.21562200
H	-2.03849800	-1.55825600	-0.51118200	H	-2.04134200	-1.55726400	-0.51799800
C	-3.94149600	-0.60504300	-0.16758100	C	-3.94467700	-0.60417000	-0.17087600
C	-4.60414100	0.61522200	0.18441200	C	-4.60785900	0.61445900	0.18811100
C	-3.80701400	1.75346200	0.48371400	C	-3.80967200	1.75151700	0.49539400
C	-2.43702500	1.69372100	0.44133500	C	-2.43777500	1.69128800	0.45352500
H	-1.85086800	2.56725000	0.70700700	H	-1.85323100	2.56446200	0.72425400
H	-4.30145100	2.67997900	0.76371300	H	-4.30281700	2.67702000	0.78146900
C	-4.72967100	-1.74900700	-0.47008700	C	-4.73333700	-1.74758300	-0.48079300
C	-6.02204100	0.64293900	0.22563500	C	-6.02719500	0.64267200	0.22792000
H	-6.51978900	1.57080400	0.49524000	H	-6.52583500	1.56879600	0.50232400
H	-4.22714700	-2.67430100	-0.73930100	H	-4.23147100	-2.67196200	-0.75487400
C	-6.75728200	-0.48331900	-0.07082000	C	-6.76395900	-0.48298800	-0.07625900
H	-7.84216900	-0.45027800	-0.03688600	H	-7.84895700	-0.44931500	-0.04325500
C	-6.10398000	-1.68984800	-0.42243300	C	-6.10974000	-1.68886500	-0.43437000
H	-6.69425400	-2.57133600	-0.65467000	H	-6.69948600	-2.56931900	-0.67230200

Frequency coordinates of compound 7 for the optimized cationic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.44735400	2.01776200	0.00029500	S	-3.44881800	2.01764100	-0.00028900
S	0.57079600	-1.06617100	-0.00053100	S	-0.57127500	-1.06536400	0.00011400
C	4.31495000	0.46562100	0.00028200	C	-4.31632100	0.46567500	-0.00006800
C	5.69418000	0.30652100	0.00051500	C	-5.69690800	0.30696900	-0.00002700
H	6.35943100	1.16325800	0.00079600	H	-6.36239000	1.16388400	-0.00011100
C	6.21078400	-0.99351400	0.00026100	C	-6.21513400	-0.99389400	0.00007300
H	7.28706800	-1.13229800	0.00037800	H	-7.29168100	-1.13193800	0.00007200
C	5.36822400	-2.12097300	-0.00022100	C	-5.37219800	-2.12250800	0.00013400
H	5.80319400	-3.11425500	-0.00043900	H	-5.80731600	-3.11596000	0.00020500
C	3.99254800	-1.96915700	-0.00042800	C	-3.99490300	-1.97056700	0.00010700
H	3.33835800	-2.83533100	-0.00077700	H	-3.34187900	-2.83784200	0.00017100
C	3.44373100	-0.66629000	-0.00018300	C	-3.44513300	-0.66712600	0.00000100
C	2.09250700	-0.24321900	-0.00021900	C	-2.09290100	-0.24380800	-0.00000500
C	-0.30157800	0.49018300	-0.00007900	C	0.30047700	0.49113100	0.00006600
C	0.59300800	1.57335300	0.00023900	C	-0.59420200	1.57555100	-0.00001800
H	0.27200000	2.60622900	0.00038500	H	-0.27361500	2.60870000	-0.00011300
C	1.92322000	1.16662300	0.00014300	C	-1.92530000	1.16771700	-0.00009400
C	-1.73393600	0.53849200	-0.00011500	C	1.73428000	0.53913000	0.00014300
C	-2.49943900	-0.64696200	0.00011600	C	2.49999700	-0.64688200	0.00001200
H	-2.00458300	-1.61415500	0.00031100	H	2.00560700	-1.61436700	-0.00009200
C	-3.90246500	-0.62495100	0.00015300	C	3.90453900	-0.62496700	-0.00001800
C	-4.57944300	0.64236600	-0.00014700	C	4.58237200	0.64243200	0.00008500
C	-3.79340100	1.83649300	-0.00049600	C	3.79604000	1.83766300	0.00028600
C	-2.42798200	1.79464700	-0.00049100	C	2.42906900	1.79583300	0.00032300
H	-1.86882800	2.72218700	-0.00091900	H	1.87112000	2.72418800	0.00053100
H	-4.30428800	2.79462400	-0.00088200	H	4.30633100	2.79634200	0.00041000
C	-4.67053700	-1.82644600	0.00048000	C	4.67287700	-1.82764200	-0.00018600
C	-5.98619100	0.66273900	-0.00009000	C	5.99050200	0.66258400	0.00000000
H	-6.50503700	1.61648400	-0.00033200	H	6.51019300	1.61609200	0.00007300
H	-4.15433000	-2.78192600	0.00071400	H	4.15720800	-2.78363200	-0.00024700
C	-6.70673200	-0.52381100	0.00026900	C	6.71183100	-0.52498100	-0.00016200
H	-7.79161500	-0.49287300	0.00031100	H	7.79688600	-0.49411900	-0.00022100
C	-6.04690500	-1.77320500	0.00056900	C	6.05080000	-1.77510300	-0.00024100
H	-6.62902900	-2.68847000	0.00089500	H	6.63231700	-2.69100800	-0.00035100

Frequency coordinates of compound 7 for the optimized anionic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.47867000	2.00820800	0.00013700	S	-3.48218300	2.00827500	-0.00028900
S	0.57796100	-1.06924300	-0.00045000	S	-0.57863800	-1.06497800	-0.00015200
C	4.37076600	0.46550200	0.00011400	C	-4.37115500	0.46538600	0.00004000
C	5.74905000	0.31388500	0.00017200	C	-5.75114500	0.31112800	0.00028300
H	6.39823800	1.18603500	0.00024600	H	-6.40289500	1.18137800	0.00029800
C	6.29680000	-0.97966700	0.00009400	C	-6.29726300	-0.98582100	0.00055700
H	7.37512100	-1.11099300	0.00011500	H	-7.37538800	-1.11894600	0.00078800
C	5.44609300	-2.09478500	-0.00005200	C	-5.44363000	-2.10163400	0.00056500
H	5.87569200	-3.09442600	-0.00013500	H	-5.87135500	-3.10183700	0.00078600
C	4.06241700	-1.95231500	-0.00009500	C	-4.05775200	-1.95531300	0.00026500
H	3.41885500	-2.82778700	-0.00021300	H	-3.41253900	-2.82964600	0.00025600
C	3.48226600	-0.65999800	0.00000000	C	-3.48149100	-0.65994500	-0.00000700
C	2.13091300	-0.24069900	0.00003700	C	-2.12971000	-0.23758500	-0.00053700
C	-0.31759300	0.49234000	-0.00011100	C	0.31494000	0.49453900	-0.00013100
C	0.59864500	1.56571300	-0.00001800	C	-0.59974000	1.57174100	-0.00033500
H	0.28884700	2.60315800	0.00002700	H	-0.28993100	2.60916600	-0.00044600
C	1.92905600	1.14518100	0.00009400	C	-1.93263200	1.14953100	-0.00058100
C	-1.74414400	0.50906200	0.00002000	C	1.74323600	0.51100200	-0.00014600
C	-2.53916400	-0.66618400	0.00021700	C	2.53733800	-0.66625200	-0.00047200
H	-2.05435100	-1.63935500	0.00061800	H	2.05293000	-1.63956200	-0.00123000
C	-3.94558500	-0.63064500	0.00016200	C	3.94594600	-0.63097500	-0.00020000
C	-4.63132000	0.63865200	-0.00004600	C	4.63269500	0.63841000	0.00034200
C	-3.82226500	1.82108700	-0.00014400	C	3.82414300	1.82294100	0.00052000
C	-2.45576700	1.75752900	-0.00010600	C	2.45488800	1.76001700	0.00028600
H	-1.88885900	2.68435100	-0.00021200	H	1.89019900	2.68792900	0.00051300
H	-4.31916400	2.78986600	-0.00022300	H	4.32023000	2.79209500	0.00086600
C	-4.75116500	-1.81162800	0.00031000	C	4.75122700	-1.81432000	-0.00046500
C	-6.03780100	0.67219100	-0.00013000	C	6.04105900	0.67160500	0.00062500
H	-6.53352400	1.64209400	-0.00029700	H	6.53822700	1.64067200	0.00104000
H	-4.25216300	-2.77845500	0.00048100	H	4.25218300	-2.78113600	-0.00086400
C	-6.79319600	-0.49702900	-0.00001100	C	6.79757300	-0.49954000	0.00037400
H	-7.87912300	-0.45229300	-0.00008300	H	7.88344400	-0.45525300	0.00059000
C	-6.13145300	-1.74226700	0.00022000	C	6.13349200	-1.74682200	-0.00017900
H	-6.71499000	-2.66116900	0.00032300	H	6.71591200	-2.66617800	-0.00037200

Cartesian coordinates of compound 8 for the neutral geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.24584400	2.09052300	-0.32542100	S	3.24740200	2.08401800	-0.35552700
S	0.67802900	-1.19760800	0.23095100	S	0.67787600	-1.19422500	0.25232800
C	4.27558800	0.66771100	-0.08481800	C	4.27651800	0.66584200	-0.09298800
C	5.67099900	0.65439300	-0.08263300	C	5.67366800	0.65270600	-0.09232900
H	6.23452500	1.56929500	-0.23695700	H	6.23736000	1.56511600	-0.26167200
C	6.32656100	-0.55722900	0.12063300	C	6.33118000	-0.55651800	0.12932000
H	7.41183100	-0.58309000	0.12457700	H	7.41658200	-0.58175600	0.13219800
C	5.60000900	-1.74256200	0.31964600	C	5.60412700	-1.74036500	0.34795300
H	6.13041300	-2.67676200	0.47608700	H	6.13480600	-2.67214700	0.51813200
C	4.21127900	-1.73365000	0.31876700	C	4.21358800	-1.73111700	0.34856800
H	3.65367500	-2.65277800	0.47306900	H	3.65715900	-2.64848800	0.51778200
C	3.52637700	-0.52352200	0.11589000	C	3.52751500	-0.52328600	0.12756200
C	2.12086700	-0.23846100	0.06944900	C	2.12104200	-0.23863800	0.07813100
C	-0.33902300	0.22642900	-0.02930400	C	-0.33826300	0.22543300	-0.03016800
C	0.41819500	1.36382900	-0.21992700	C	0.41886300	1.36121300	-0.23885600
H	-0.01819900	2.33320500	-0.42534000	H	-0.01742700	2.32713700	-0.46122400
C	1.80784500	1.09276000	-0.15470800	C	1.80986600	1.09048000	-0.16749300
C	-1.78589000	0.13110800	-0.00484500	C	-1.78700800	0.13022700	-0.00344300
C	-2.67515200	1.10961700	0.35051600	C	-2.67470700	1.09799600	0.38882800
S	-2.61221900	-1.35870200	-0.49380200	S	-2.61494600	-1.34046000	-0.54154900
C	-4.04866700	0.70962600	0.24796700	C	-4.04976800	0.70169400	0.27420300
H	-2.36207700	2.08343900	0.70928300	H	-2.35954200	2.05798700	0.78196000
C	-4.18218700	-0.63239300	-0.19033600	C	-4.18372500	-0.62524900	-0.21061900
C	-5.43378000	-1.23365800	-0.34590600	C	-5.43720400	-1.22159600	-0.38439400
C	-5.21394600	1.44725600	0.53296700	C	-5.21544300	1.42980600	0.58741100
H	-5.52058300	-2.26222700	-0.68175600	H	-5.52537800	-2.23806400	-0.75555300
H	-5.13209100	2.47590500	0.87223800	H	-5.13348500	2.44628000	0.96208200
C	-6.45726100	0.85188600	0.37702100	C	-6.46101600	0.83972500	0.41331800
H	-7.35694200	1.41922100	0.59519300	H	-7.36030700	1.39918800	0.65289900
C	-6.56798300	-0.48058400	-0.06010800	C	-6.57261600	-0.47858900	-0.07020700
H	-7.55000500	-0.92894600	-0.17566400	H	-7.55478300	-0.92317000	-0.19941600

Cartesian coordinates of compound 8 for the cationic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.19904300	2.14512500	-0.00008300	S	-3.20089900	2.14483300	-0.00022300
S	0.69487500	-1.25674600	0.00016200	S	-0.69499100	-1.25615600	-0.00043300
C	4.23657700	0.70395600	-0.00007600	C	-4.23746500	0.70402500	-0.00011400
C	5.62614700	0.70344100	-0.00013400	C	-5.62870500	0.70388700	-0.00010000
H	6.18870400	1.63080300	-0.00020900	H	-6.19109800	1.63170000	-0.00034700
C	6.28721300	-0.52765700	-0.00006800	C	-6.29146100	-0.52743700	0.00033000
H	7.37231900	-0.54274100	-0.00010300	H	-7.37673900	-0.54188700	0.00036700
C	5.57915500	-1.74559100	0.00006000	C	-5.58305000	-1.74677300	0.00074400
H	6.12600400	-2.68195800	0.00010900	H	-6.13005700	-2.68330200	0.00113600
C	4.19618200	-1.75356400	0.00012400	C	-4.19861800	-1.75483100	0.00067700
H	3.64594600	-2.68923700	0.00021500	H	-3.64968500	-2.69149200	0.00090500
C	3.50135100	-0.52188600	0.00005800	C	-3.50261900	-0.52277500	0.00022800
C	2.11168000	-0.25685300	0.00007400	C	-2.11175300	-0.25748000	0.00007600
C	-0.34440400	0.18232900	0.00000700	C	0.34399800	0.18258200	-0.00023700
C	0.41412900	1.37182300	-0.00004400	C	-0.41481300	1.37344700	-0.00054400
H	-0.03376500	2.35707800	-0.00013500	H	0.03239100	2.35918100	-0.00036700
C	1.77963800	1.12263400	-0.00002500	C	-1.78122900	1.12322600	-0.00027400
C	-1.75574600	0.07666400	-0.00000500	C	1.75683300	0.07702200	-0.00061300
C	-2.66188200	1.14877600	0.00016600	C	2.66321400	1.15057600	0.00021800
S	-2.59233100	-1.47715800	-0.00010600	S	2.59352400	-1.47622000	-0.00021700
C	-4.01212600	0.74880400	0.00009000	C	4.01425600	0.74945300	0.00042300
H	-2.34873500	2.18605800	0.00031800	H	2.35059000	2.18812100	-0.00026500
C	-4.15402700	-0.67231300	-0.00009100	C	4.15502600	-0.67245600	-0.00008500
C	-5.40546200	-1.27806400	-0.00020300	C	5.40749100	-1.27966600	-0.00044000
C	-5.17592100	1.56112300	0.00017100	C	5.17954900	1.56138400	0.00082500
H	-5.51266000	-2.35725100	-0.00033200	H	5.51416400	-2.35918300	-0.00092700
H	-5.07955400	2.64208300	0.00030900	H	5.08478400	2.64273600	0.00123200
C	-6.41713000	0.95665700	0.00007000	C	6.42185200	0.95571700	0.00071000
H	-7.31641500	1.56272000	0.00013600	H	7.32158700	1.56150400	0.00113400
C	-6.53046600	-0.45082400	-0.00012200	C	6.53442000	-0.45315900	0.00002600
H	-7.51668500	-0.90383400	-0.00018600	H	7.52035000	-0.90717200	0.00001200

Cartesian coordinates of compound 8 for the anionic geometry optimization

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	-3.25669600	2.12683000	-0.00000500	S	-3.25717900	2.12735400	0.00002000
S	-0.68156200	-1.23138700	-0.00003200	S	-0.68313300	-1.23020300	-0.00020700
C	-4.29918800	0.68128300	0.00002300	C	-4.29843500	0.68269300	0.00008500
C	-5.68548500	0.66874700	0.00007900	C	-5.68668100	0.66939200	0.00025300
H	-6.24376100	1.60169400	0.00012500	H	-6.24659900	1.60137000	0.00039000
C	-6.36042400	-0.56309000	0.00010700	C	-6.36184700	-0.56518200	0.00029700
H	-7.44645900	-0.58549600	0.00017500	H	-7.44789800	-0.58812100	0.00046700
C	-5.62589000	-1.75782300	0.00006200	C	-5.62589500	-1.76176800	0.00014500
H	-6.15363700	-2.70928500	0.00008800	H	-6.15301100	-2.71334100	0.00018900
C	-4.23482900	-1.75507300	-0.00002200	C	-4.23225400	-1.75707600	-0.00006600
H	-3.68269700	-2.69090500	-0.00005600	H	-3.67941400	-2.69255500	-0.00018700
C	-3.52786700	-0.52768400	-0.00004500	C	-3.52737900	-0.52710600	-0.00010700
C	-2.14209900	-0.24596000	-0.00018900	C	-2.14043400	-0.24408800	-0.00045800
C	0.36333900	0.23315100	0.00000700	C	0.36168000	0.23185900	-0.00006000
C	-0.43794300	1.40148900	-0.00001600	C	-0.43619800	1.40438800	-0.00004000
H	-0.01230900	2.39701000	-0.00004200	H	-0.00976400	2.39963900	-0.00008800
C	-1.80047200	1.11409100	-0.00013900	C	-1.80192400	1.11708000	-0.00032300
C	1.76874700	0.14777400	0.00000200	C	1.76887000	0.14555000	0.00001800
C	2.71396800	1.18528100	0.00000600	C	2.71233900	1.18707000	-0.00004600
S	2.60893200	-1.43800400	-0.00000800	S	2.60841900	-1.43805900	0.00006100
C	4.06331900	0.75946200	0.00002600	C	4.06351000	0.75987700	0.00004000
H	2.42343400	2.22987600	0.00012100	H	2.42114200	2.23150800	0.00014400
C	4.19799200	-0.66447900	0.00003400	C	4.19649700	-0.66508400	0.00008500
C	5.43511200	-1.29362200	0.00002600	C	5.43497200	-1.29603000	0.00011600
C	5.25904700	1.52289600	0.00002500	C	5.26046600	1.52405500	0.00002000
H	5.50144500	-2.37890300	0.00001300	H	5.50126100	-2.38134600	0.00013900
H	5.19937800	2.60883600	0.00001800	H	5.20166200	2.61009200	-0.00003900
C	6.49667300	0.88881800	0.00002800	C	6.50000900	0.88941100	0.00006000
H	7.40293900	1.49149800	0.00003100	H	7.40644900	1.49139600	0.00004500
C	6.60023900	-0.51085100	0.00002300	C	6.60256800	-0.51350200	0.00011800
H	7.57544600	-0.98980000	0.00003000	H	7.57729100	-0.99336700	0.00015500

Frequency coordinates of compound 8 for the optimized neutral geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.24584400	2.09052300	-0.32542100	S	3.24740200	2.08401800	-0.35552700
S	0.67802900	-1.19760800	0.23095100	S	0.67787600	-1.19422500	0.25232800
C	4.27558800	0.66771100	-0.08481800	C	4.27651800	0.66584200	-0.09298800
C	5.67099900	0.65439300	-0.08263300	C	5.67366800	0.65270600	-0.09232900
H	6.23452500	1.56929500	-0.23695700	H	6.23736000	1.56511600	-0.26167200
C	6.32656100	-0.55722900	0.12063300	C	6.33118000	-0.55651800	0.12932000
H	7.41183100	-0.58309000	0.12457700	H	7.41658200	-0.58175600	0.13219800
C	5.60000900	-1.74256200	0.31964600	C	5.60412700	-1.74036500	0.34795300
H	6.13041300	-2.67676200	0.47608700	H	6.13480600	-2.67214700	0.51813200
C	4.21127900	-1.73365000	0.31876700	C	4.21358800	-1.73111700	0.34856800
H	3.65367500	-2.65277800	0.47306900	H	3.65715900	-2.64848800	0.51778200
C	3.52637700	-0.52352200	0.11589000	C	3.52751500	-0.52328600	0.12756200
C	2.12086700	-0.23846100	0.06944900	C	2.12104200	-0.23863800	0.07813100
C	-0.33902300	0.22642900	-0.02930400	C	-0.33826300	0.22543300	-0.03016800
C	0.41819500	1.36382900	-0.21992700	C	0.41886300	1.36121300	-0.23885600
H	-0.01819900	2.33320500	-0.42534000	H	-0.01742700	2.32713700	-0.46122400
C	1.80784500	1.09276000	-0.15470800	C	1.80986600	1.09048000	-0.16749300
C	-1.78589000	0.13110800	-0.00484500	C	-1.78700800	0.13022700	-0.00344300
C	-2.67515200	1.10961700	0.35051600	C	-2.67470700	1.09799600	0.38882800
S	-2.61221900	-1.35870200	-0.49380200	S	-2.61494600	-1.34046000	-0.54154900
C	-4.04866700	0.70962600	0.24796700	C	-4.04976800	0.70169400	0.27420300
H	-2.36207700	2.08343900	0.70928300	H	-2.35954200	2.05798700	0.78196000
C	-4.18218700	-0.63239300	-0.19033600	C	-4.18372500	-0.62524900	-0.21061900
C	-5.43378000	-1.23365800	-0.34590600	C	-5.43720400	-1.22159600	-0.38439400
C	-5.21394600	1.44725600	0.53296700	C	-5.21544300	1.42980600	0.58741100
H	-5.52058300	-2.26222700	-0.68175600	H	-5.52537800	-2.23806400	-0.75555300
H	-5.13209100	2.47590500	0.87223800	H	-5.13348500	2.44628000	0.96208200
C	-6.45726100	0.85188600	0.37702100	C	-6.46101600	0.83972500	0.41331800
H	-7.35694200	1.41922100	0.59519300	H	-7.36030700	1.39918800	0.65289900
C	-6.56798300	-0.48058400	-0.06010800	C	-6.57261600	-0.47858900	-0.07020700
H	-7.55000500	-0.92894600	-0.17566400	H	-7.55478300	-0.92317000	-0.19941600

Frequency coordinates of compound 8 for the optimized cationic geometry

B3LYP/6-31G(d, p)				B3LYP/6-31++G(d, p)			
S	3.19904300	2.14512500	-0.00008300	S	-3.20089900	2.14483300	-0.00022300
S	0.69487500	-1.25674600	0.00016200	S	-0.69499100	-1.25615600	-0.00043300
C	4.23657700	0.70395600	-0.00007600	C	-4.23746500	0.70402500	-0.00011400
C	5.62614700	0.70344100	-0.00013400	C	-5.62870500	0.70388700	-0.00010000
H	6.18870400	1.63080300	-0.00020900	H	-6.19109800	1.63170000	-0.00034700
C	6.28721300	-0.52765700	-0.00006800	C	-6.29146100	-0.52743700	0.00033000
H	7.37231900	-0.54274100	-0.00010300	H	-7.37673900	-0.54188700	0.00036700

C	5.57915500	-1.74559100	0.00006000	C	-5.58305000	-1.74677300	0.00074400
H	6.12600400	-2.68195800	0.00010900	H	-6.13005700	-2.68330200	0.00113600
C	4.19618200	-1.75356400	0.00012400	C	-4.19861800	-1.75483100	0.00067700
H	3.64594600	-2.68923700	0.00021500	H	-3.64968500	-2.69149200	0.00090500
C	3.50135100	-0.52188600	0.00005800	C	-3.50261900	-0.52277500	0.00022800
C	2.11168000	-0.25685300	0.00007400	C	-2.11175300	-0.25748000	0.00007600
C	-0.34440400	0.18232900	0.00000700	C	0.34399800	0.18258200	-0.00023700
C	0.41412900	1.37182300	-0.00004400	C	-0.41481300	1.37344700	-0.00054400
H	-0.03376500	2.35707800	-0.00013500	H	0.03239100	2.35918100	-0.00036700
C	1.77963800	1.12263400	-0.00002500	C	-1.78122900	1.12322600	-0.00027400
C	-1.75574600	0.07666400	-0.00000500	C	1.75683300	0.07702200	-0.00061300
C	-2.66188200	1.14877600	0.00016600	C	2.66321400	1.15057600	0.00021800
S	-2.59233100	-1.47715800	-0.00010600	S	2.59352400	-1.47622000	-0.00021700
C	-4.01212600	0.74880400	0.00009000	C	4.01425600	0.74945300	0.00042300
H	-2.34873500	2.18605800	0.00031800	H	2.35059000	2.18812100	-0.00026500
C	-4.15402700	-0.67231300	-0.00009100	C	4.15502600	-0.67245600	-0.00008500
C	-5.40546200	-1.27806400	-0.00020300	C	5.40749100	-1.27966600	-0.00044000
C	-5.17592100	1.56112300	0.00017100	C	5.17954900	1.56138400	0.00082500
H	-5.51266000	-2.35725100	-0.00033200	H	5.51416400	-2.35918300	-0.00092700
H	-5.07955400	2.64208300	0.00030900	H	5.08478400	2.64273600	0.00123200
C	-6.41713000	0.95665700	0.00007000	C	6.42185200	0.95571700	0.00071000
H	-7.31641500	1.56272000	0.00013600	H	7.32158700	1.56150400	0.00113400
C	-6.53046600	-0.45082400	-0.00012200	C	6.53442000	-0.45315900	0.00002600
H	-7.51668500	-0.90383400	-0.00018600	H	7.52035000	-0.90717200	0.00001200

Frequency coordinates of compound 8 for the optimized anionic geometry

B3LYP/6-31G(d, p)				**B3LYP/6-31++G(d, p)**			
S	-3.25669600	2.12683000	-0.00000500	S	-3.25717900	2.12735400	0.00002000
S	-0.68156200	-1.23138700	-0.00003200	S	-0.68313300	-1.23020300	-0.00020700
C	-4.29918800	0.68128300	0.00002300	C	-4.29843500	0.68269300	0.00008500
C	-5.68548500	0.66874700	0.00007900	C	-5.68668100	0.66939200	0.00025300
H	-6.24376100	1.60169400	0.00012500	H	-6.24659900	1.60137000	0.00039000
C	-6.36042400	-0.56309000	0.00010700	C	-6.36184700	-0.56518200	0.00029700
H	-7.44645900	-0.58549600	0.00017500	H	-7.44789800	-0.58812100	0.00046700
C	-5.62589000	-1.75782300	0.00006200	C	-5.62589500	-1.76176800	0.00014500
H	-6.15363700	-2.70928500	0.00008800	H	-6.15301100	-2.71334100	0.00018900
C	-4.23482900	-1.75507300	-0.00002200	C	-4.23225400	-1.75707600	-0.00006600
H	-3.68269700	-2.69090500	-0.00005600	H	-3.67941400	-2.69255500	-0.00018700
C	-3.52786700	-0.52768400	-0.00004500	C	-3.52737900	-0.52710600	-0.00010700
C	-2.14209900	-0.24596000	-0.00018900	C	-2.14043400	-0.24408800	-0.00045800
C	0.36333900	0.23315100	0.00000700	C	0.36168000	0.23185900	-0.00006000
C	-0.43794300	1.40148900	-0.00001600	C	-0.43619800	1.40438800	-0.00004000
H	-0.01230900	2.39701000	-0.00004200	H	-0.00976400	2.39963900	-0.00008800

C	-1.80047200	1.11409100	-0.00013900	C	-1.80192400	1.11708000	-0.00032300
C	1.76874700	0.14777400	0.00000200	C	1.76887000	0.14555000	0.00001800
C	2.71396800	1.18528100	0.00000600	C	2.71233900	1.18707000	-0.00004600
S	2.60893200	-1.43800400	-0.00000800	S	2.60841900	-1.43805900	0.00006100
C	4.06331900	0.75946200	0.00002600	C	4.06351000	0.75987700	0.00004000
H	2.42343400	2.22987600	0.00012100	H	2.42114200	2.23150800	0.00014400
C	4.19799200	-0.66447900	0.00003400	C	4.19649700	-0.66508400	0.00008500
C	5.43511200	-1.29362200	0.00002600	C	5.43497200	-1.29603000	0.00011600
C	5.25904700	1.52289600	0.00002500	C	5.26046600	1.52405500	0.00002000
H	5.50144500	-2.37890300	0.00001300	H	5.50126100	-2.38134600	0.00013900
H	5.19937800	2.60883600	0.00001800	H	5.20166200	2.61009200	-0.00003900
C	6.49667300	0.88881800	0.00002800	C	6.50000900	0.88941100	0.00006000
H	7.40293900	1.49149800	0.00003100	H	7.40644900	1.49139600	0.00004500
C	6.60023900	-0.51085100	0.00002300	C	6.60256800	-0.51350200	0.00011800
H	7.57544600	-0.98980000	0.00003000	H	7.57729100	-0.99336700	0.00015500

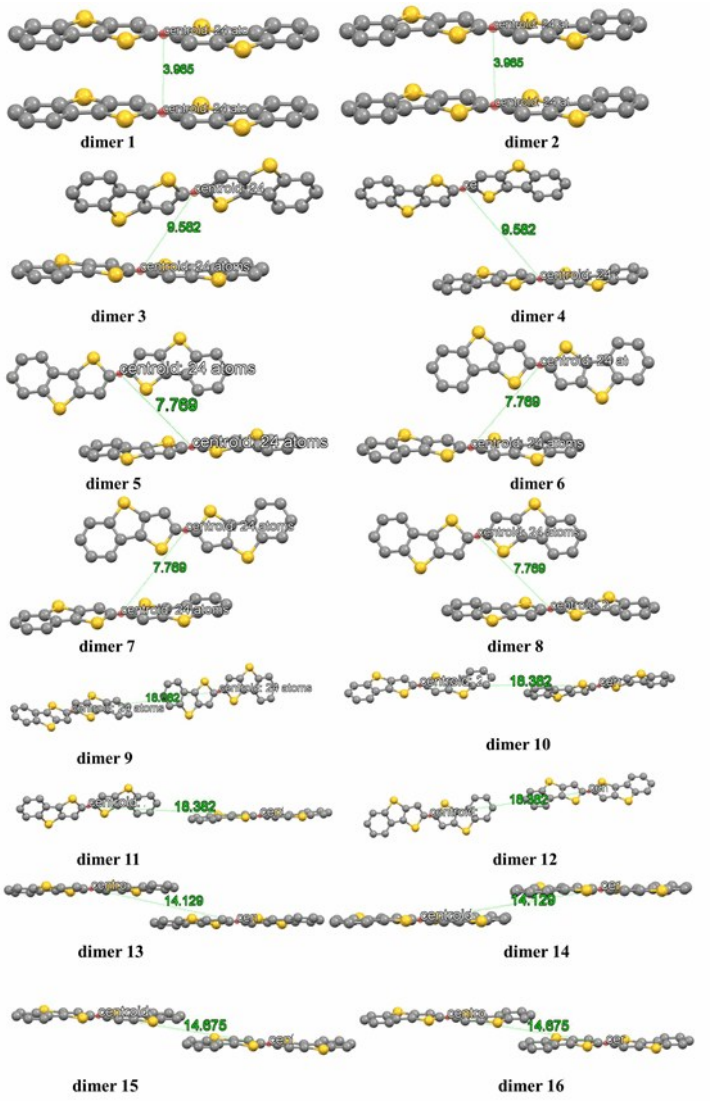

Figure S7 The centroid-centroid distance for all the main pathways of compound 1

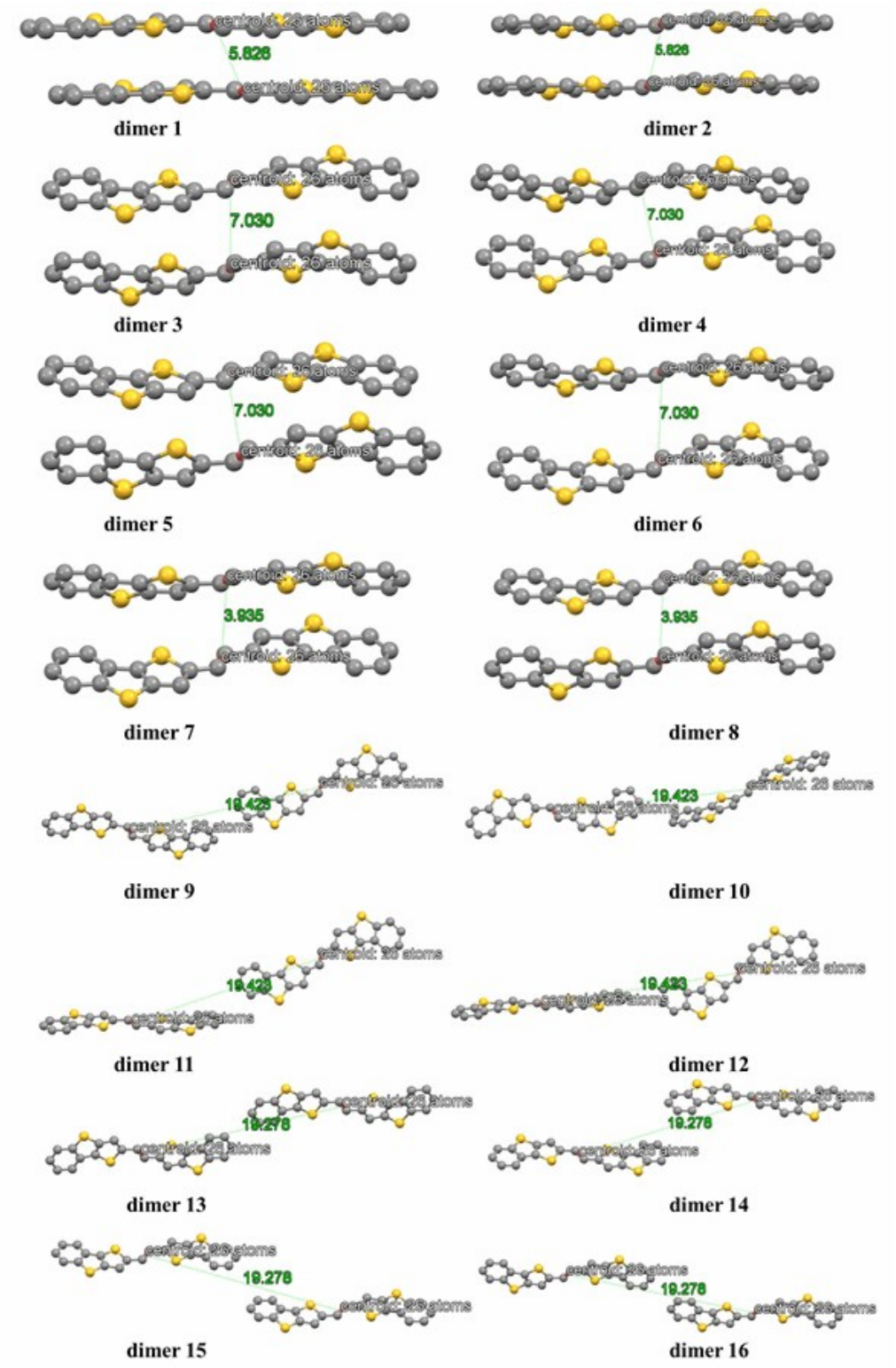

Figure S8 The centroid-centroid distance for all the main pathways of compound 2

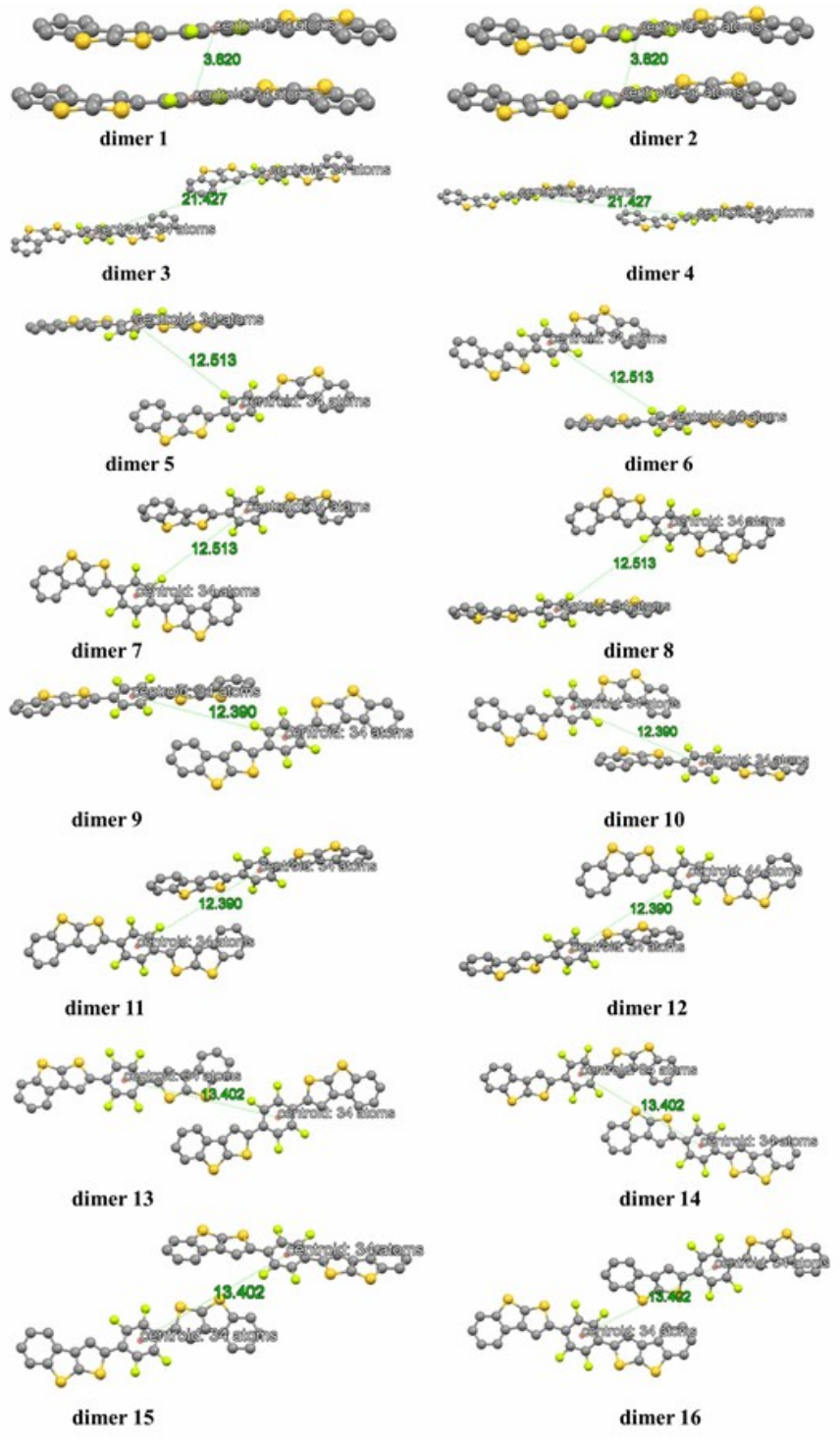

Figure S9 The centroid-centroid distance for all the main pathways of compound 4

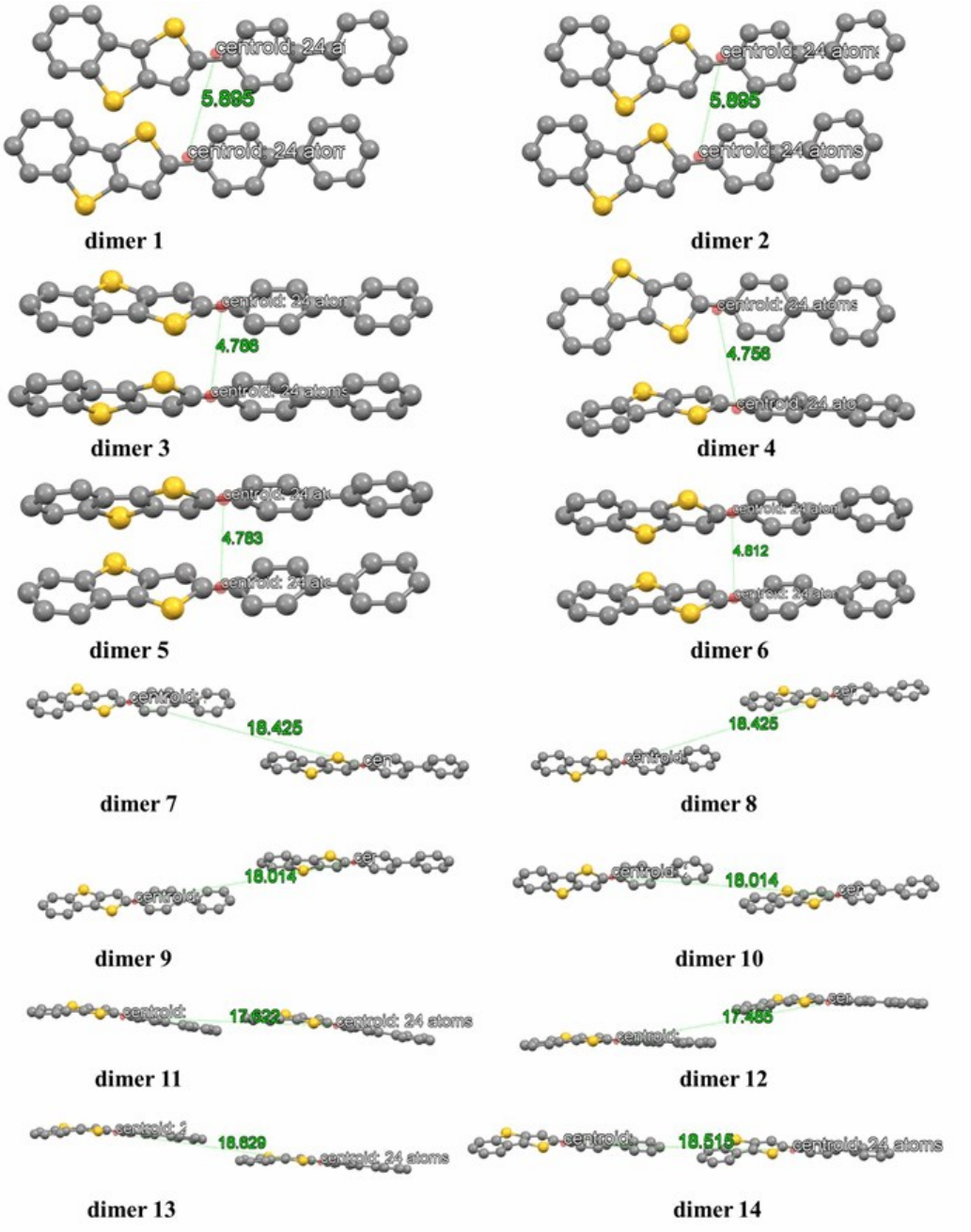

Figure S10 The centroid-centroid distance for all the main pathways of compound 6