ELECTRONIC SUPPLEMENTARY INFORMATION

Relating circular dichroism to atomic structure by means of MD simulations and computed CD spectra: the example α-peptoids

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Ac-$(stbe)_6$-COOtBu	ω	ϕ	ψ	χ1
1	-11.8	-73.8	-175.0	-100.4
2	-9.1	-74.0	-170.3	-102.2
3	-7.8	-73.3	-172.0	-101.8
4	-9.4	-72.6	-171.4	-102.5
5	-7.8	-73.5	-170.2	-102.9
6	-6.6	-74.7		-103.5
Ac-$(stbe)_5$-COOtBu	ω	ϕ	ψ	χ1
1	-11.1	-74.7	-171.2	-100.9
2	-9.8	-73.2	-172.7	-100.8
3	-8.9	-73.0	-171.9	-102.9
4	-8.7	-73.0	-170.5	-102.8
5	-6.6	-75.2		-103.0
Ac-$(stbe)_4$-COOtBu	ω	ϕ	ψ	χ1
1	-9.6	-75.0	-175.5	-101.8
2	-9.3	-73.3	-174.4	-103.1
3	-9.1	-72.9	-171.9	-102.6
4	-7.2	-74.7		-102.7
Ac-$(stbe)_3$-COOtBu	ω	ϕ	ψ	χ1
1	-10.9	-74.3	-174.1	-101.0
2	-9.0	-73.1	-172.2	-102.5
3	-6.0	-74.8		-103.0
Ac-$(stbe)_2$-COOtBu	ω	ϕ	ψ	χ1
1	-10.5	-73.9	-173.5	-101.2
2	-6.9	-74.9		-102.6

Table S1. Selected backbone angles for right-handed helix conformation. ω, ψ, ϕ and χ1 angles are defined as follow: ω = C_α(i-1)-C(i-1)-N(i)-C_α(i), ϕ = C(i-1)-N(i)-C_α(i)-C(i), ψ = N(i)-C_α(i)-C(i)-N(i+1) and χ1 = C(i-1)-N(i)-NC_α(i)-NC_β(i)

Ac-(stbe)$_6$-COOtBu	ω	ϕ	ψ	χ1
1	-0.9	79.4	173.2	-111.6
2	-1.8	77.0	173.1	-110.6
3	-1.8	76.4	172.4	-110.4
4	-1.6	77.2	170.3	-109.9
5	-2.1	76.3	172.3	-111.0
6	-2.5	76.8		-110.1
Ac-(stbe)$_5$-COOtBu	ω	ϕ	ψ	χ1
1	-1.2	78.9	173.5	-112.4
2	-2.7	77.5	172.6	-110.4
3	-2.1	76.5	172.7	-110.8
4	-3.0	77.1	171.0	-111.5
5	-3.1	76.4		-110.3
Ac-(stbe)$_4$-COOtBu	ω	ϕ	ψ	χ1
1	-0.6	79.6	171.1	-112.4
2	-2.4	76.1	174.0	-112.0
3	-2.7	77.3	171.3	-111.7
4	-4.9	76.7		-110.5
Ac-(stbe)$_3$-COOtBu	ω	ϕ	ψ	χ1
1	-1.1	79.4	172.3	-112.2
2	-1.4	77.0	171.7	-110.5
3	-2.3	73.3		-110.6
Ac-(stbe)$_2$-COOtBu	ω	ϕ	ψ	χ1
1	-0.7	78.7	172.9	-111.2
2	-3.3	76.6		-110.9

Table S2. Selected backbone angles for left-handed helix conformation. ω, ψ, ϕ and χ1 angles are defined as follow: ω = C_α(i-1)-C(i-1)-N(i)-C_α(i), ϕ = C(i-1)-N(i)-C_α(i)-C(i), ψ = N(i)-C_α(i)-C(i)-N(i+1) and χ1 = C(i-1)-N(i)-NC_α(i)-NC_β(i).

Ac-$(tBu)_3$-$(stbe)_4$-$(tBu)_3$-CO_2tBu[a]	ω	ϕ	ψ	χ1
1(tbu)	5.6 ± 13.9	-87.8 ± 11.8	175.9 ± 13.7	
2(tbu)	5.9 ± 15.9	-84.7 ± 11.9	176.6 ± 14.8	
3(tbu)	8.6 ± 17.5	-87.4 ± 10.8	-174.8 ± 15.0	
4(stbe)	-4.8 ± 11.2	-71.8 ± 8.1	177.5 ± 11.1	-98.8 ± 7.7
5(stbe)	-10.0 ± 9.5	-70.8 ± 7.8	176.4 ± 9.2	-97.5 ± 7.5
6(stbe)	-11.4 ± 9.4	-69.3 ± 8.0	-179.3 ± 10.0	-98.3 ± 7.7
7(stbe)	-5.7 ± 9.2	-67.5 ± 8.6	172.5 ± 11.6	-98.7 ± 7.8
8(tbu)	6.1 ± 13.6	-83.4 ± 11.7	178.9 ± 14.7	
9(tbu)	9.4 ± 14.2	-84.7 ± 11.4	175.4 ± 13.8	
10(tbu)	4.4 ± 15.7	-87.1 ±12.3	-174.4 ± 13.1	
Ac-$(tBu)_2$-$(stbe)_4$-$(tBu)_2$-CO_2tBu[b]	ω	ϕ	ψ	χ1
1(tbu)	-1.1	-89.2	-175.3	
2(tbu)	-14.0	-76.6	-170.0	
3(stbe)	-4.7	-71.7	-176.8	-99.9
4(stbe)	-6.3	-69.4	177.4	-98.4
5(stbe)	-6.9	-66.5	171.0	-100.9
6(stbe)	-0.9	-68.4	169.2	-105.2
7(tbu)	7.1	-84.6	-178.9	
8(tbu)	-2.0	-85.4	-172.4	

Table S3. Selected backbone angles of hetero-oligomer with all ϕ angles being negatives. ω, ψ, ϕ and χ1 angles are defined as follow: ω = C_α(i-1)-C(i-1)-N(i)-C_α(i), ϕ = C(i-1)-N(i)-C_α(i)-C(i), ψ = N(i)-C_α(i)-C(i)-N(i+1) and χ1 = C(i-1)-N(i)-NC_α(i)-NC_β(i). a) $(-)_{10}$ this work; b) Ref 4

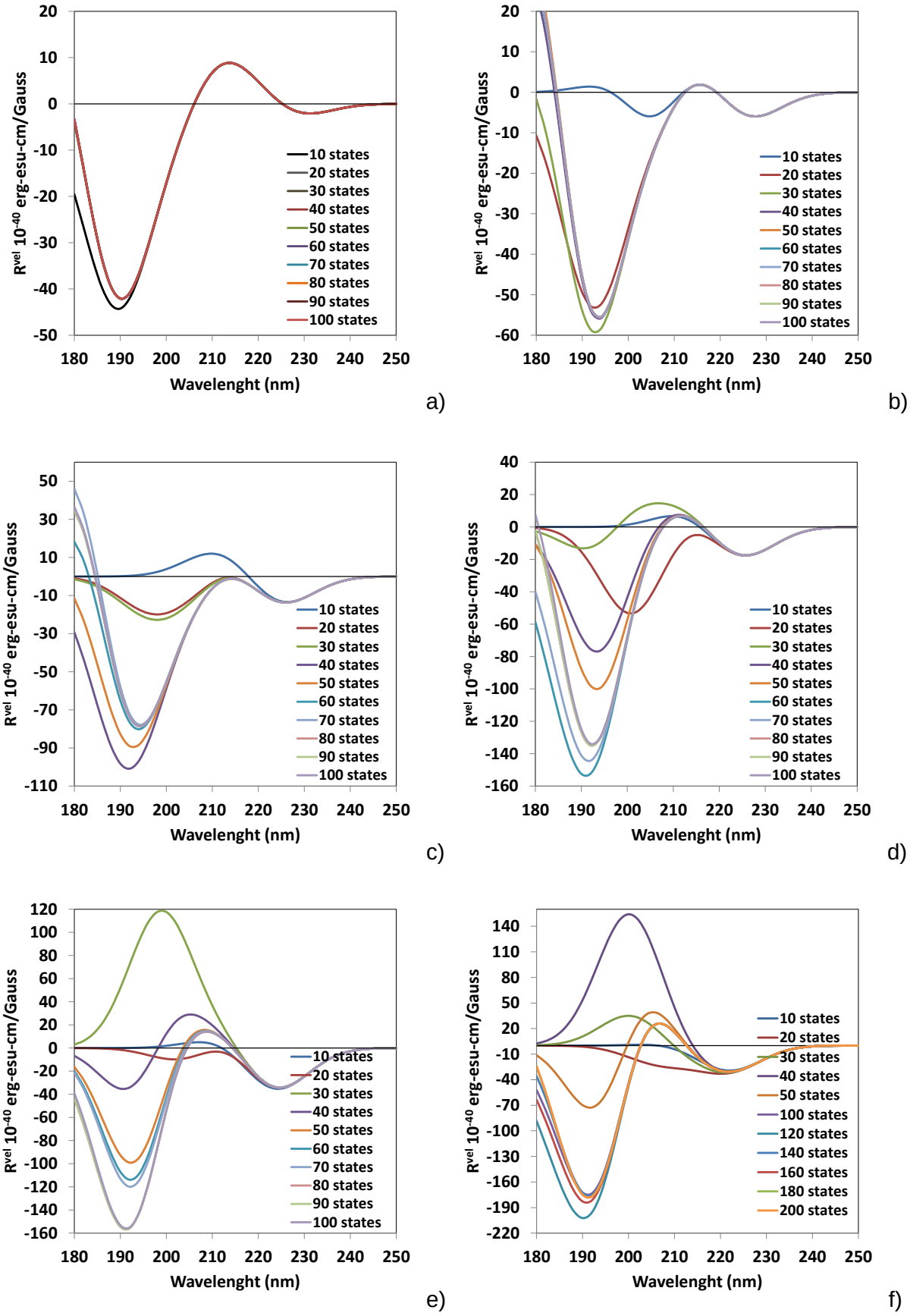


Figure S1. Theoretical CD spectra of Ac-(stbe)$_n$-COOtBu as a function of the number of states calculated in the TD-DFT procedure. a) n=1; b) n=2; c) n=3; d) n=4 ; e) n=5; f) n=6.

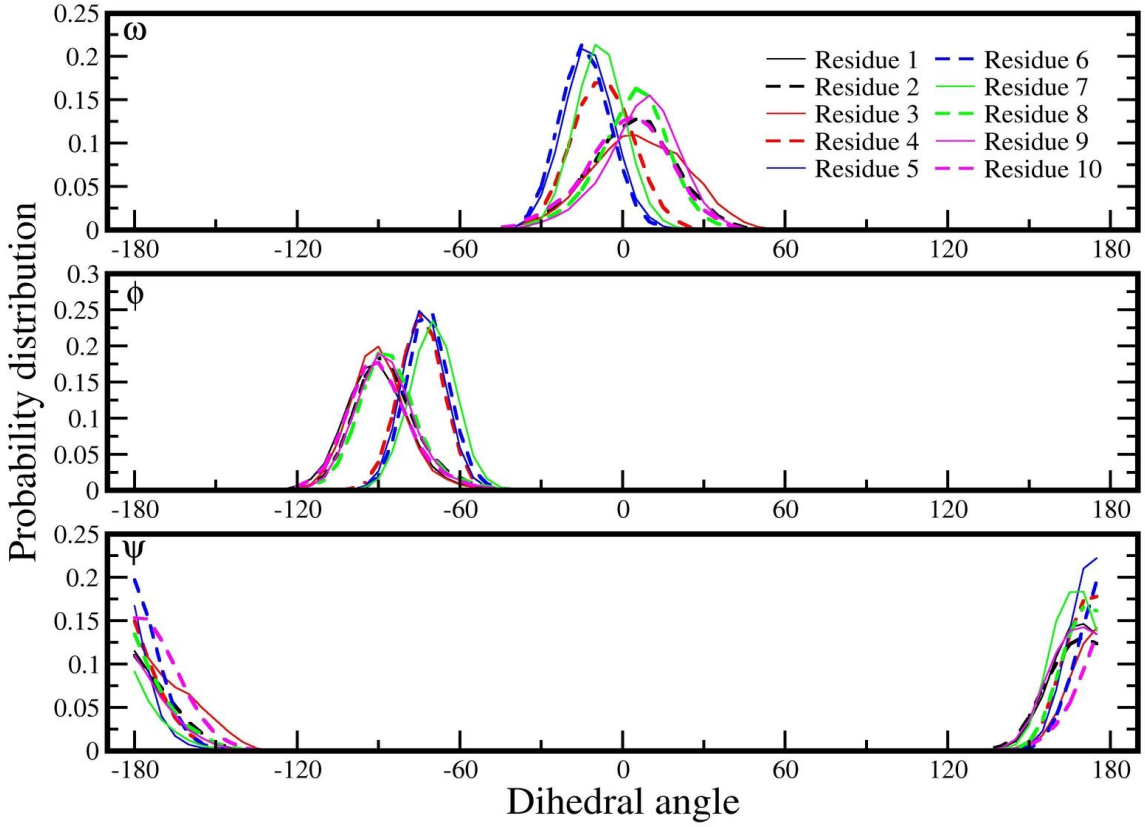


Figure S2. Probability distribution of ϕ dihedral angles from 50 ns simulation of $(–)_{10}$ *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

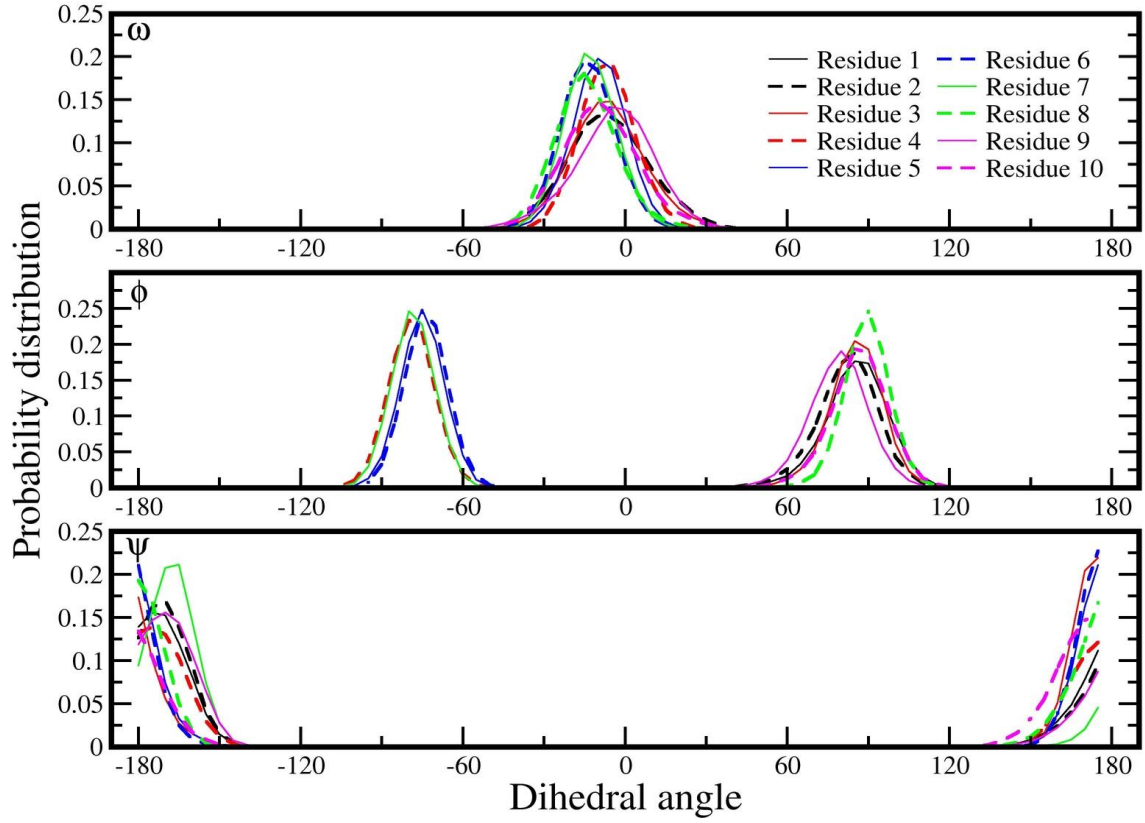


Figure S3. Probability distribution of ϕ dihedral angles from 50 ns simulation of $(+)_3$-$(–)_4$-$(+)_3$ *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

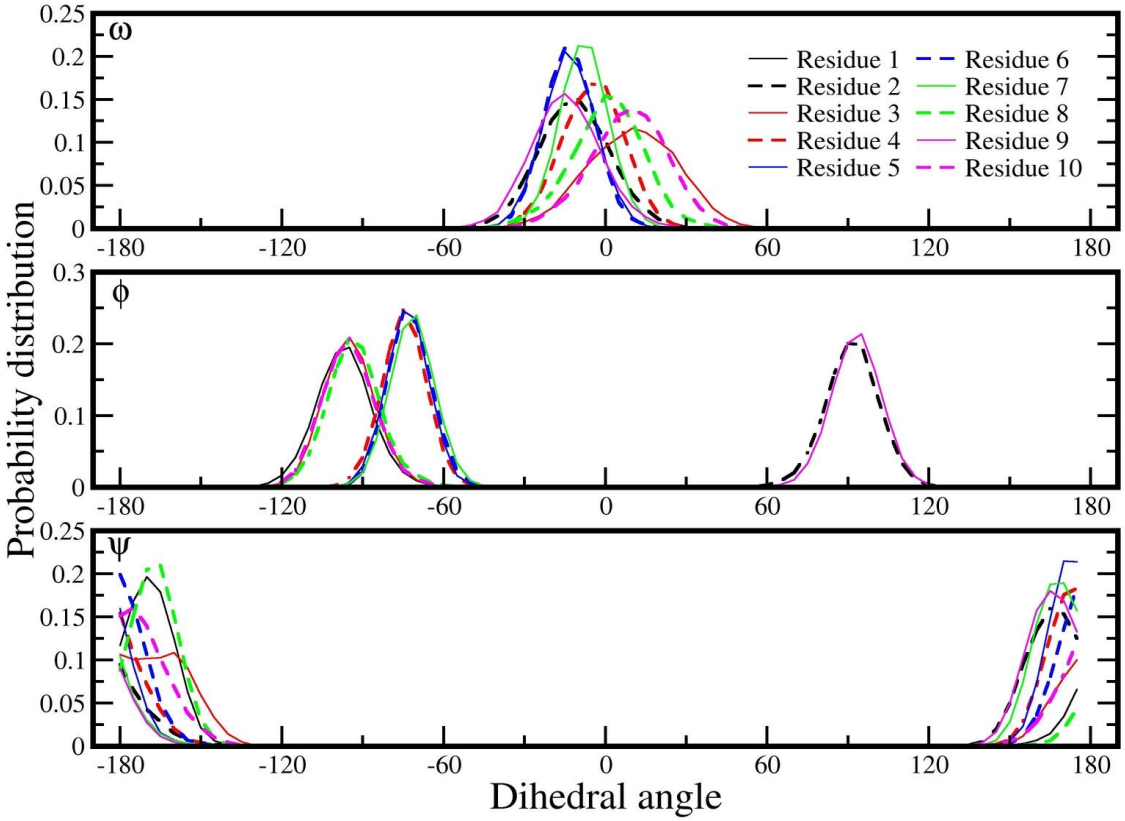


Figure S4. Probability distribution of ϕ dihedral angles from 50 ns simulation of (+–+)-(–)$_4$-(+–+) *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

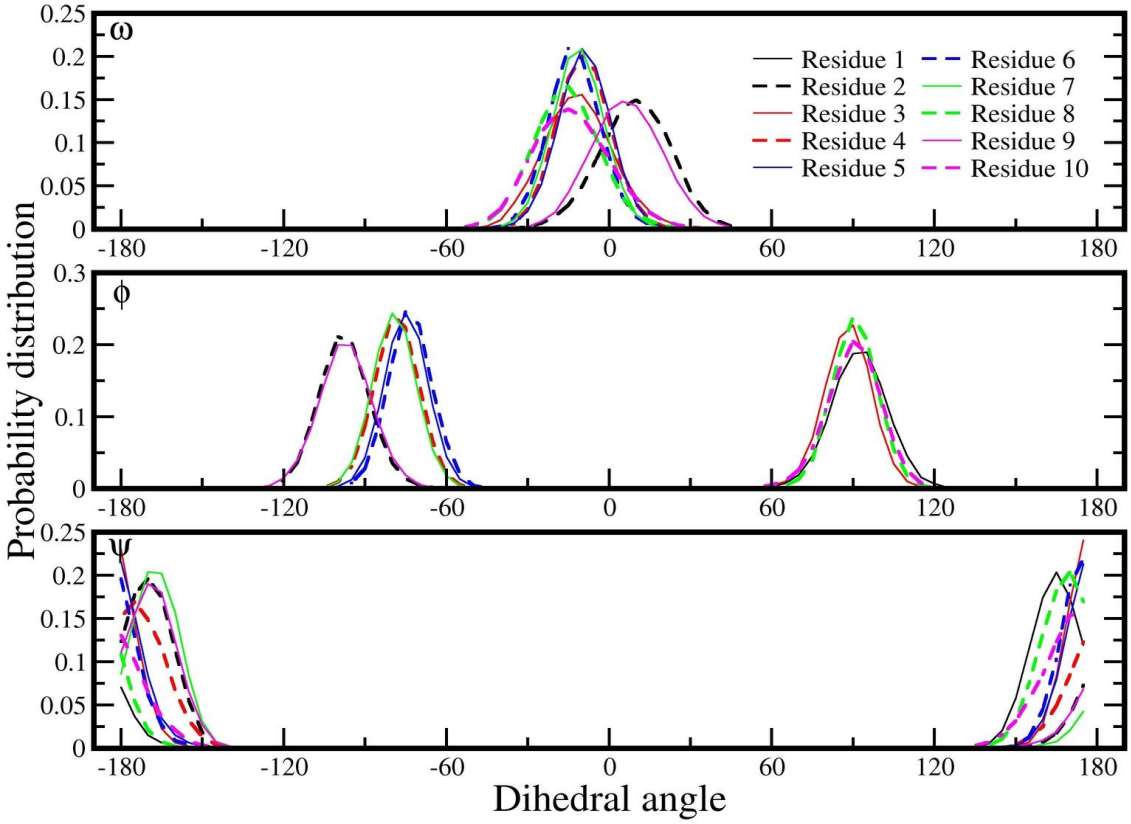


Figure S5. Probability distribution of ϕ dihedral angles from 50 ns simulation of (–+–)-(–)$_4$-(–+–) *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

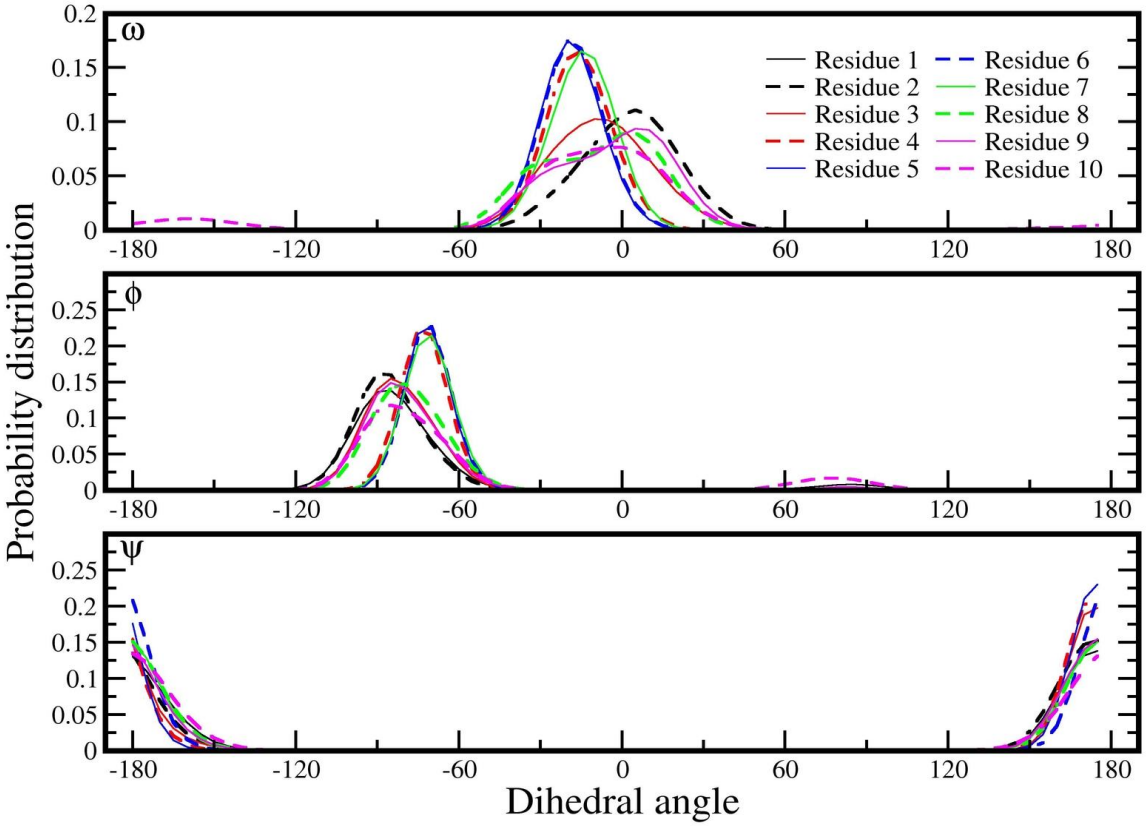


Figure S6. Probability distribution of ϕ dihedral angles from REMD simulation of $(–)_{10}$ *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

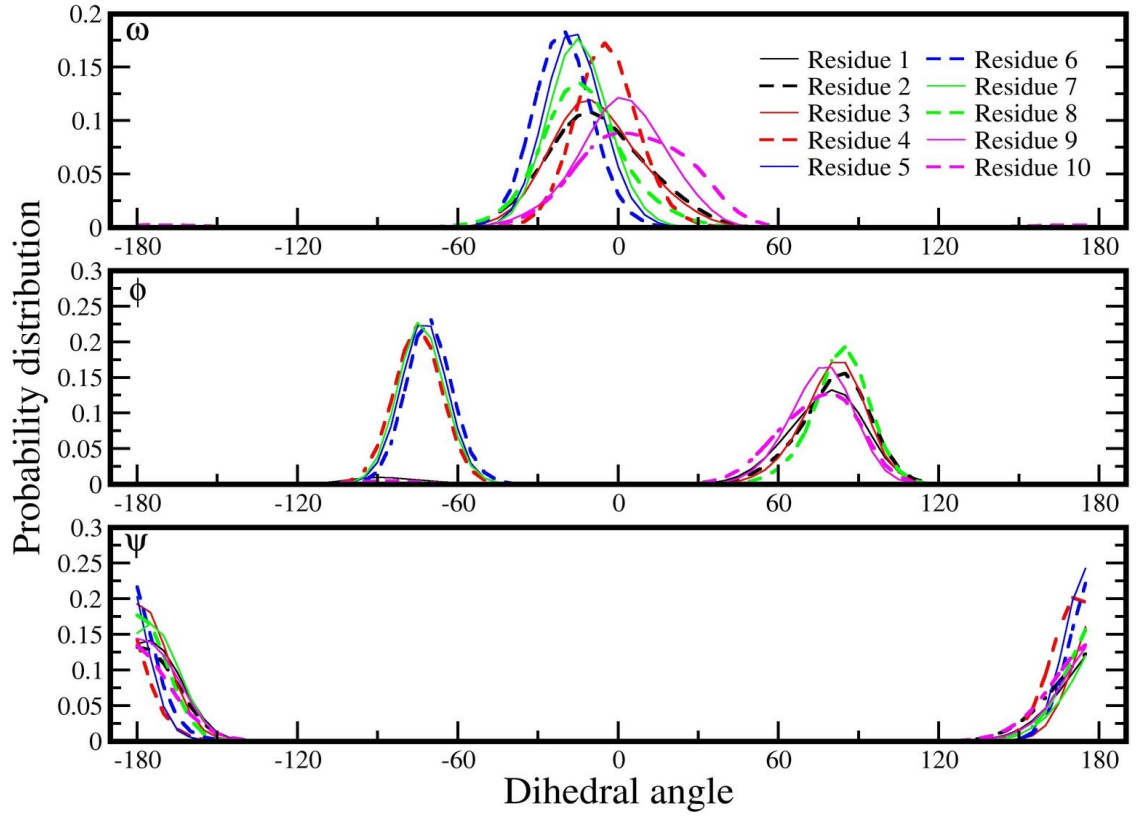


Figure S7. Probability distribution of ϕ dihedral angles from REMD simulation of $(+)_3$-$(–)_4(+)_3$ *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

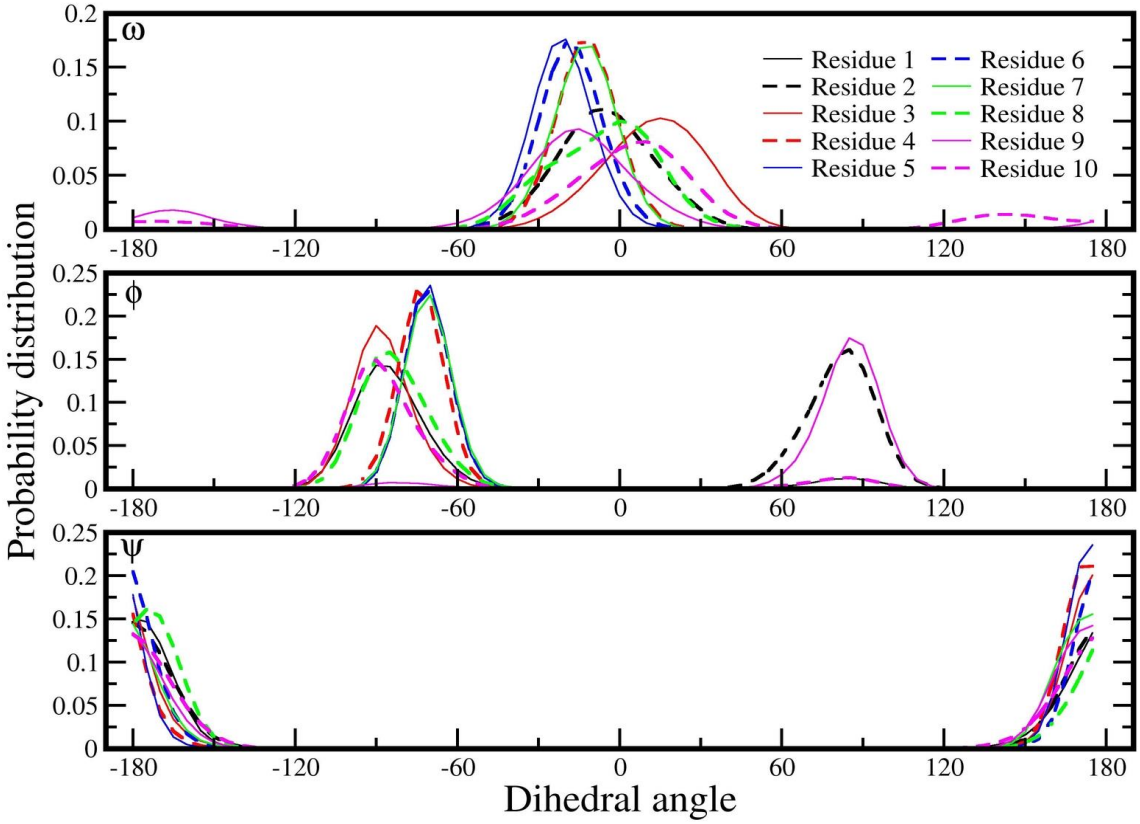


Figure S8. Probability distribution of ϕ dihedral angles from REMD simulation of (+–+)-(–)$_4$-(+–+) *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

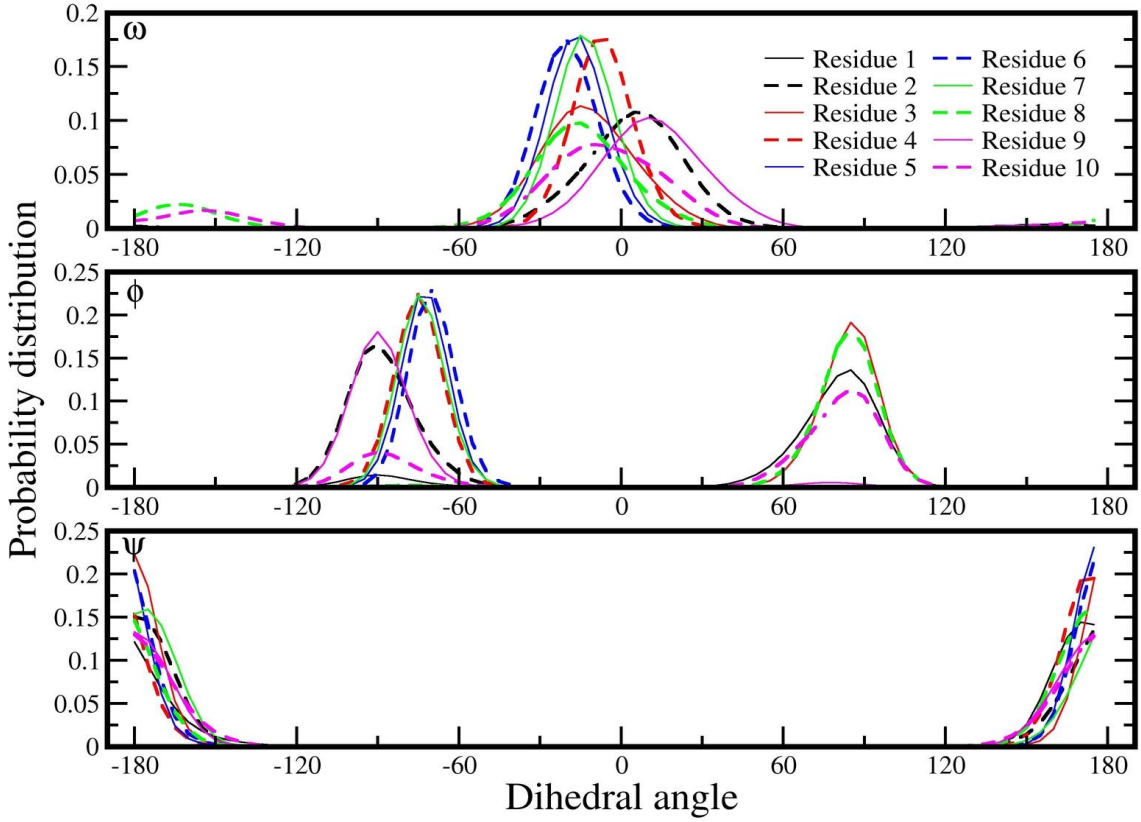


Figure S9. Probability distribution of ϕ dihedral angles from REMD simulation of (–+–)-(–)$_4$-(–+–) *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer

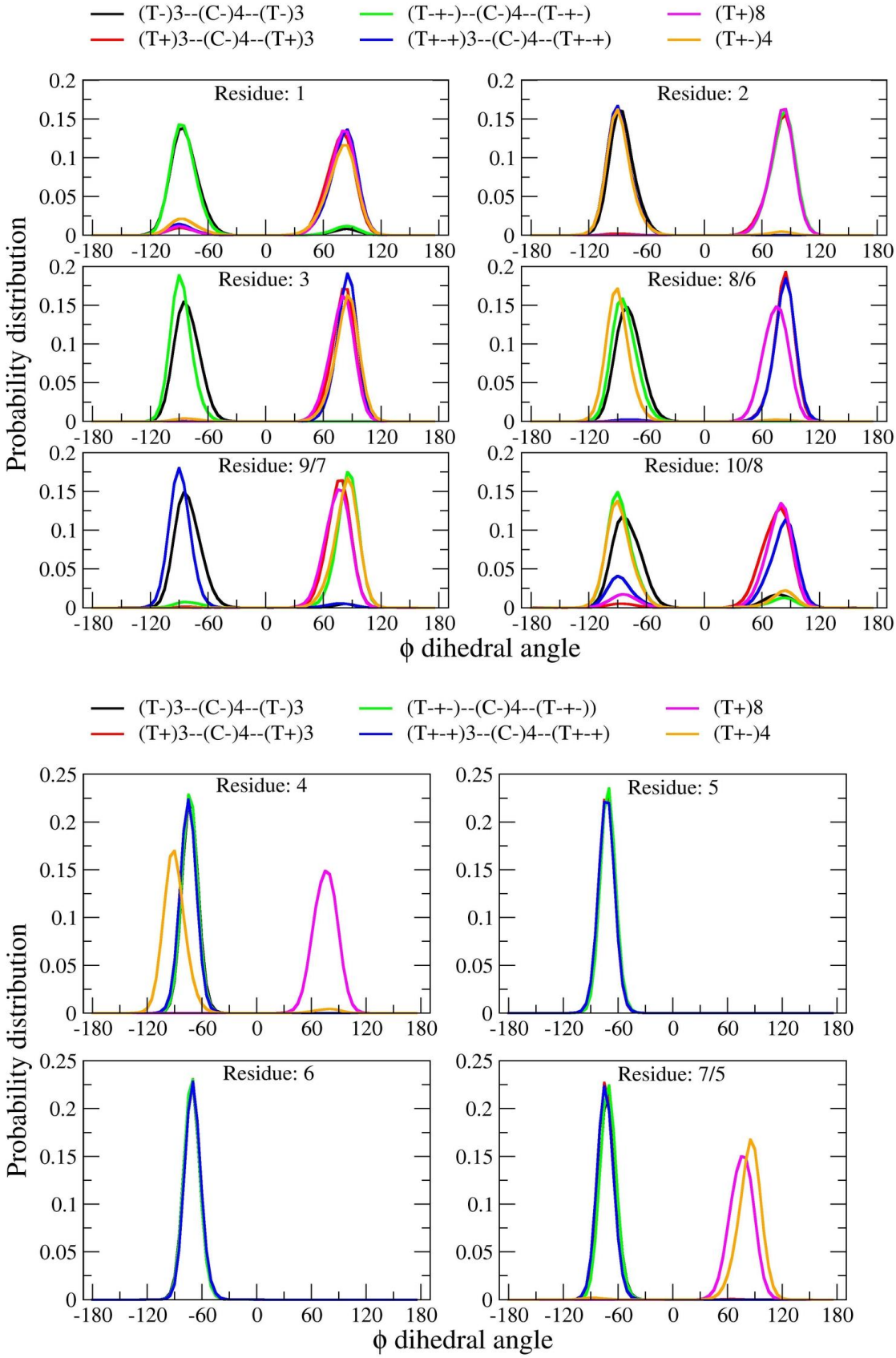


Figure S10. Probability distribution of φ angles from REMD simulations *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer and *Ac-(tBu)$_8$COOtBu* octamer obtained from previous work.

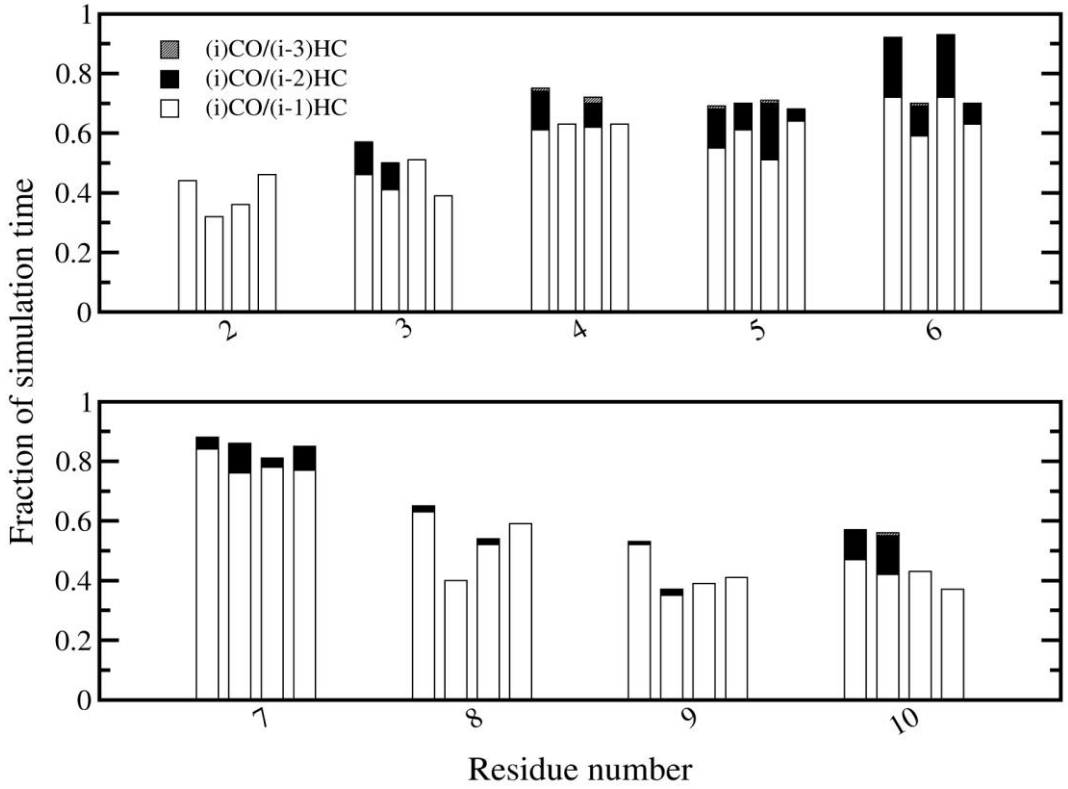


Figure S11. Hydrogen bonding probabilities between carbonyl oxygen and Cα methylene backbone. The bars from left to right represent respectively $(–)_{10}$, $(+)_3$-$(–)_4(+)_3$, (+ – +)-$(–)_4$-(+– +), and (–+–)-$(–)_4$-(–+–) *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

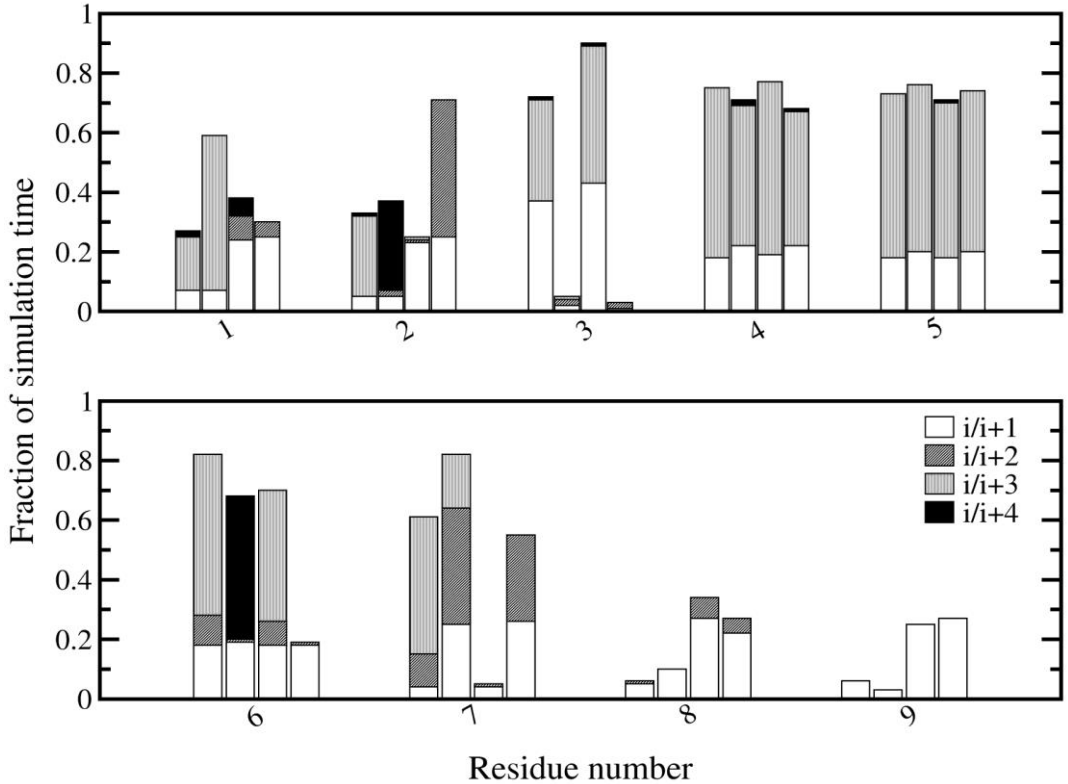
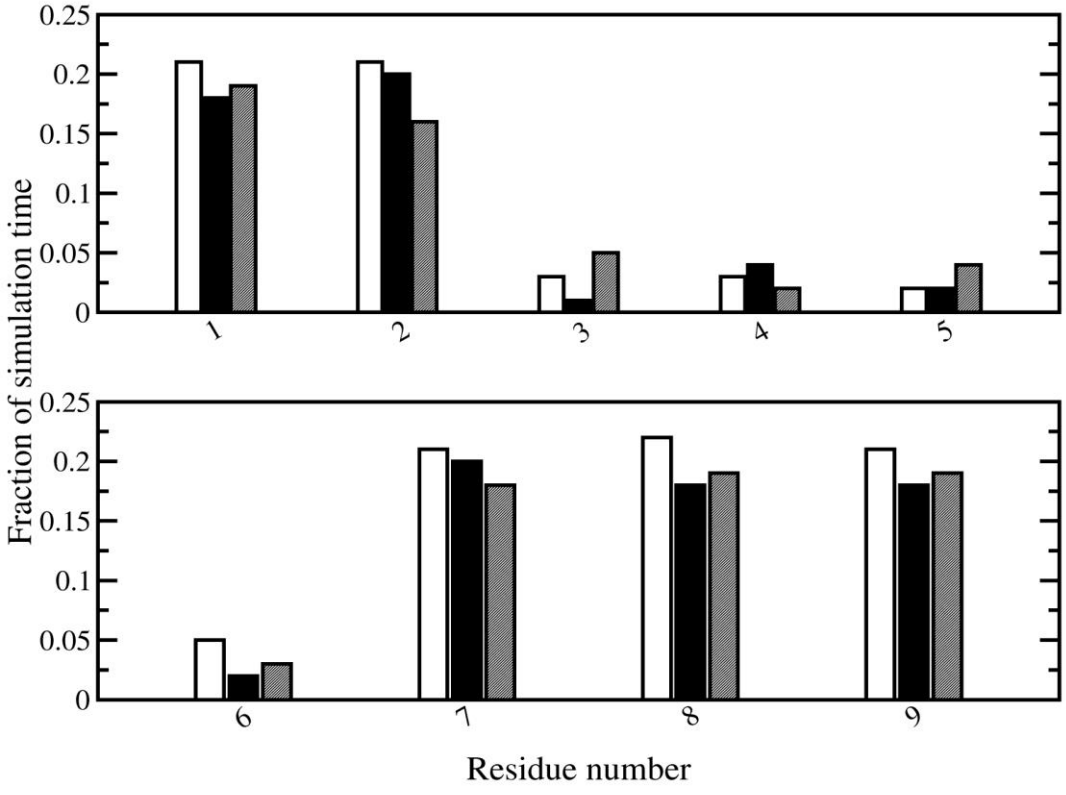
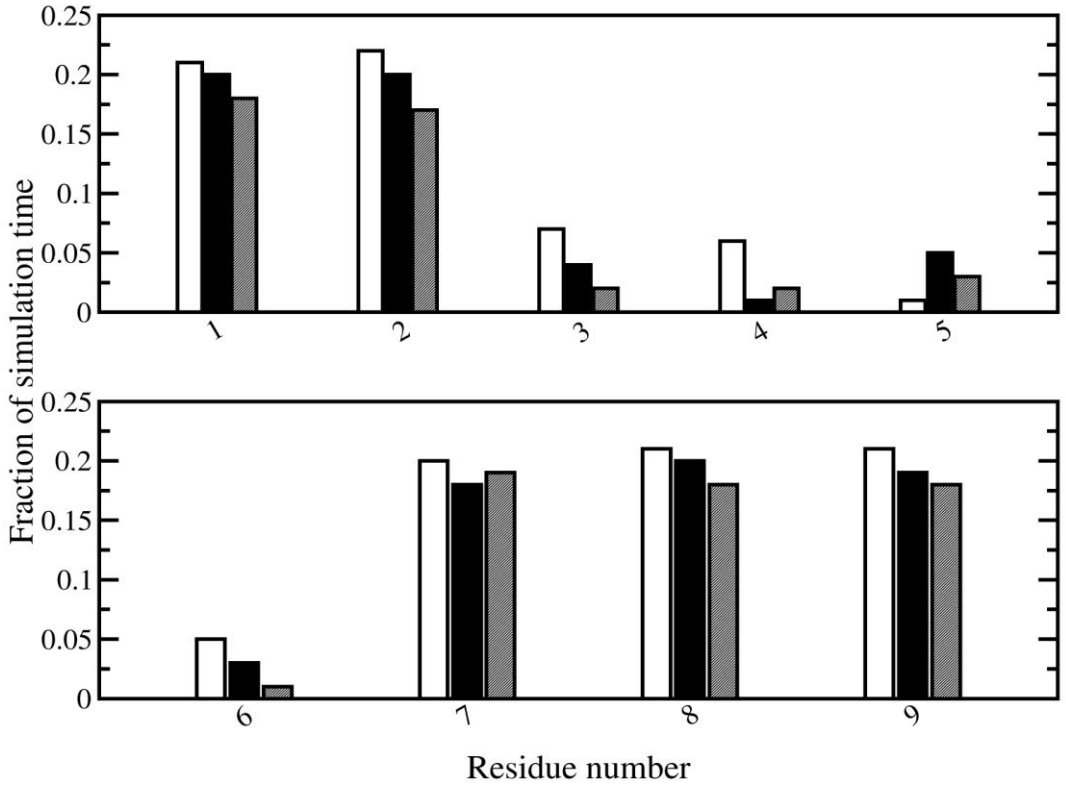


Figure S12. Fraction of simulation time during which CH_3 (for tBu & stbe) and CH (for stbe) groups interact. The bars from left to right represent respectively $(–)_{10}$, $(+)_3$-$(–)_4(+)_3$, (+–+)-$(–)_4$-(+–+), and (–+–)-$(–)_4$-(–+–) *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer.

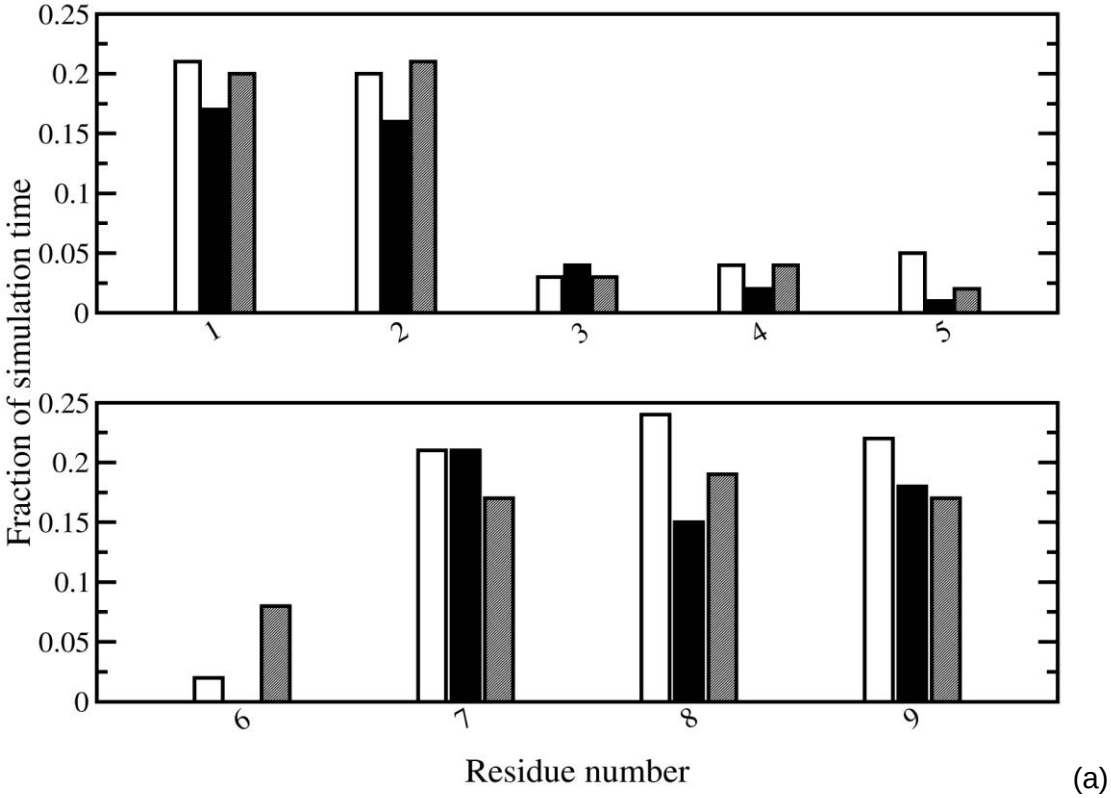


(a)

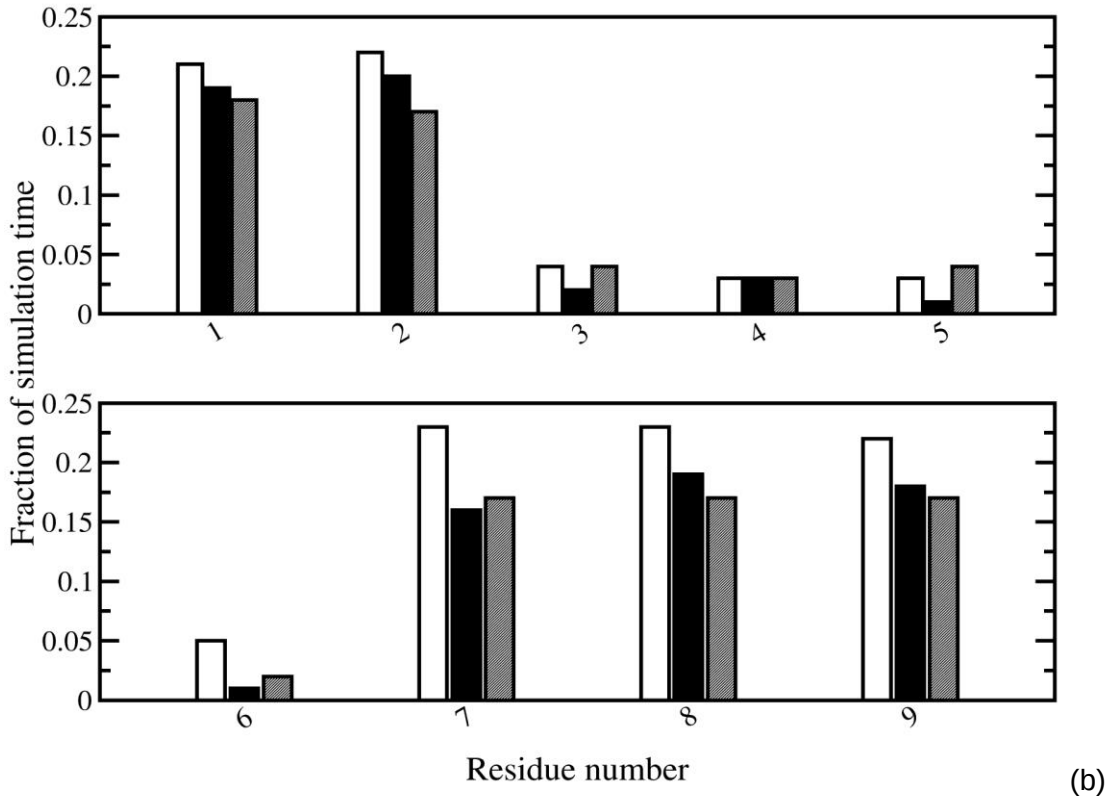


(b)

Figure S13. Hydrogen bonding probabilities between carbonyl oxygen and methyl side chain (i+1 residue) obtained from MD simulation of $(–)_{10}$ (a) and $(+)_3$-$(–)_4(+)_3$ (b) conformation of Ac-$(tBu)_3$-$(stbe)_4$-$(tBu)_3$-COOtBu decamer. For stbe sidechain three methyl groups (CD1, CD2 & CD3) are considered. Result of fourth methyl (CG) is shown separately. Separate bar for each methyl.



(a)



(b)

Figure S14. Hydrogen bonding probabilities between carbonyl oxygen and methyl side chain (i+1 residue) obtained from MD simulation of (+–+)-(–)$_4$-(+–+) (a) and (–+–)-(–)$_4$-(– + –) (b) conformation of *Ac-(tBu)$_3$-(stbe)$_4$-(tBu)$_3$-COOtBu* decamer. For stbe sidechain three methyl groups (CD1, CD2 & CD3) are considered. Result of fourth methyl (CG) is shown separately. Separate bar for each methyl.

Cartesian coordinates for *cis* - Ac-stbe-COOtBu - B3LYP/6-31+G(d,p), gas phase
Energy = -830.279542 hartree

C	7.368342	-0.963356	-11.082424
C	5.943526	-1.387806	-10.714026
C	5.856858	-1.794733	-9.241777
C	5.410519	-2.499706	-11.622572
O	5.036446	-0.212327	-10.777298
C	4.820884	0.472547	-11.913793
O	5.310166	0.232480	-12.997105
C	3.863437	1.637866	-11.614769
N	3.405573	2.378822	-12.773661
C	2.105162	2.032084	-13.408243
C	1.952798	0.509788	-13.552928
C	4.231966	3.276285	-13.426786
O	3.896127	3.828035	-14.473284
C	5.574891	3.599880	-12.787482
C	0.875716	2.769285	-12.761923
C	1.126787	4.291391	-12.765257
C	-0.371024	2.488099	-13.631690
C	0.575051	2.323797	-11.315079
H	7.441899	-0.674581	-12.131845
H	8.050760	-1.800849	-10.903256
H	7.692189	-0.125056	-10.456952
H	6.194061	-0.980504	-8.593393
H	6.490680	-2.668110	-9.059646
H	4.828248	-2.050319	-8.970437
H	4.372997	-2.738476	-11.367543
H	6.010939	-3.403745	-11.476008
H	5.462048	-2.215434	-12.674509
H	3.009165	1.227522	-11.076996
H	4.369843	2.294795	-10.899990
H	2.196656	2.445027	-14.415165
H	2.835766	0.095527	-14.045706
H	1.084248	0.273844	-14.171873
H	1.819561	-0.007945	-12.596712
H	-0.346654	2.802215	-10.964294
H	1.369509	2.620646	-10.622328
H	0.427762	1.240982	-11.232965
H	1.320970	4.662564	-13.775722
H	1.987514	4.557895	-12.144110
H	0.251952	4.816833	-12.365084
H	-0.696274	1.444784	-13.568542
H	-0.182108	2.723332	-14.685659
H	-1.208180	3.111368	-13.298087
H	6.213192	2.714815	-12.718969
H	6.062523	4.340448	-13.420735
H	5.456003	4.019942	-11.782200

Cartesian coordinates for *trans* - Ac-stbe-COOtBu - B3LYP/6-31+G(d,p), gas phase.
Energy = -830.279917 hartree

C	7.345125	-0.800739	-11.465819
C	6.100421	-1.282448	-10.714088
C	6.382083	-1.411604	-9.215418
C	5.541632	-2.592059	-11.279477
O	5.057193	-0.229249	-10.754827
C	4.533430	0.215104	-11.908006
O	4.792529	-0.201179	-13.018414
C	3.487775	1.296393	-11.604544
N	3.222851	2.163683	-12.744522
C	1.945438	2.067708	-13.487296
C	1.638895	0.606120	-13.863404
C	4.305505	2.920547	-13.138483
O	5.337310	2.919896	-12.463492
C	4.232954	3.731313	-14.422672
C	0.751165	2.837638	-12.805320
C	1.127193	4.322461	-12.624155
C	-0.476880	2.763637	-13.740763
C	0.354004	2.268576	-11.426981
H	7.154312	-0.708723	-12.535714
H	8.158241	-1.518865	-11.313812
H	7.669086	0.171804	-11.083192
H	6.733076	-0.460024	-8.805535
H	7.153022	-2.169560	-9.044631
H	5.477893	-1.708984	-8.675286
H	4.622042	-2.873546	-10.755579
H	6.274484	-3.392090	-11.129179
H	5.331810	-2.507948	-12.346667
H	2.569367	0.785868	-11.313240
H	3.836883	1.876528	-10.747504
H	2.119353	2.593550	-14.428398
H	2.538624	0.135123	-14.265708
H	0.854154	0.562766	-14.622460
H	1.301966	0.008546	-13.010594
H	-0.540795	2.785033	-11.061597
H	1.139436	2.419468	-10.680558
H	0.114182	1.200628	-11.469549
H	1.307262	4.810917	-13.588642
H	2.022531	4.440785	-12.006421
H	0.309513	4.862060	-12.133536
H	-0.893397	1.753662	-13.798765
H	-0.226497	3.087311	-14.758605
H	-1.269257	3.423726	-13.371034
H	3.422511	4.464303	-14.418836
H	5.184083	4.254469	-14.520694
H	4.098930	3.079193	-15.292658

Cartesian coordinates for *Right* - Ac-(stbe)$_2$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -1274.207028 hartree

O	5.052445	0.123544	-10.745843
O	5.340003	0.472465	-12.980086
O	3.700068	3.835078	-14.696374
O	7.165293	5.539828	-15.559205
N	6.060856	4.876902	-13.668471
N	3.279350	2.466852	-12.911499
C	7.440776	-0.484182	-10.946084
H	7.529041	-0.268116	-12.011745
H	8.172495	-1.256206	-10.687725
H	7.684895	0.418055	-10.376534
C	5.939778	-1.300025	-9.091138
H	6.204222	-0.424144	-8.491199
H	6.627530	-2.112400	-8.838878
H	4.924603	-1.611929	-8.828349
C	5.602885	-2.183693	-11.429605
H	4.576199	-2.471981	-11.183378
H	6.256203	-3.033707	-11.208770
H	5.666399	-1.966958	-12.497019
C	6.041197	-0.986051	-10.584198
C	4.813331	0.726030	-11.912411
C	3.764865	1.828756	-11.696038
H	2.927215	1.380966	-11.164918
H	4.188880	2.559180	-11.000884
C	1.995554	2.000128	-13.516365
H	2.046942	2.366145	-14.543079
C	1.951852	0.465780	-13.582271
H	2.867170	0.086576	-14.043400
H	1.111269	0.142481	-14.199558
H	1.839129	-0.010154	-12.603184
C	0.723425	2.679270	-12.889948
C	0.488795	2.322522	-11.406569
H	-0.471060	2.737938	-11.079355
H	1.258044	2.747989	-10.754281
H	0.446530	1.240827	-11.238136
C	0.842220	4.212289	-13.011595
H	0.945799	4.522147	-14.056345
H	1.704124	4.595567	-12.457302
H	-0.055385	4.689830	-12.602874
C	-0.511847	2.228989	-13.703644
H	-0.749622	1.172869	-13.545455
H	-0.363361	2.388992	-14.778175
H	-1.388091	2.810998	-13.397957
C	4.041888	3.369870	-13.605443
C	5.377018	3.808452	-12.953271
H	5.179990	4.149500	-11.938383
H	6.028234	2.936021	-12.863794
C	5.919039	6.284890	-13.202121

H	6.191195	6.877888	-14.077353
C	4.455408	6.611366	-12.866890
H	3.805603	6.284921	-13.681985
H	4.329159	7.689784	-12.749427
H	4.105736	6.140098	-11.942712
C	6.956690	6.676426	-12.085601
C	6.800584	8.184549	-11.784892
H	5.858423	8.410649	-11.276509
H	6.844077	8.780919	-12.704133
H	7.614155	8.519254	-11.131867
C	6.777895	5.889521	-10.770432
H	7.462054	6.284495	-10.010766
H	7.015784	4.828328	-10.894904
H	5.762965	5.974558	-10.367023
C	8.390416	6.438965	-12.603253
H	9.117538	6.734278	-11.838289
H	8.590012	7.024311	-13.506444
H	8.564398	5.384332	-12.838076
C	6.705072	4.628052	-14.853238
C	6.893114	3.179567	-15.271553
H	7.479592	2.626784	-14.529960
H	5.939203	2.663780	-15.398958
H	7.430886	3.172606	-16.219401

Cartesian coordinates for *Right* - Ac-(stbe)$_3$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -1718.122183 hartree

O	4.996910	0.146640	-10.536001
O	5.434777	0.480092	-12.748560
O	3.779489	3.731578	-14.657385
O	7.208206	5.516868	-15.474766
O	7.973443	3.287148	-18.651614
N	6.093437	4.838294	-13.595890
N	3.317311	2.420079	-12.840503
N	7.743637	2.959736	-16.399093
C	7.407903	-0.392147	-10.546069
H	7.568502	-0.176358	-11.603271
H	8.140683	-1.141629	-10.230839
H	7.582671	0.517986	-9.963700
C	5.793740	-1.235637	-8.801970
H	5.990240	-0.347841	-8.193451
H	6.480237	-2.028026	-8.489768
H	4.769608	-1.570797	-8.612855
C	5.662788	-2.151822	-11.147919
H	4.628774	-2.467351	-10.977322
H	6.320887	-2.979711	-10.865647
H	5.802042	-1.945611	-12.210146
C	6.000363	-0.933177	-10.286444
C	4.832866	0.735572	-11.721656
C	3.765821	1.832829	-11.585612
H	2.914425	1.397966	-11.066718
H	4.159752	2.593731	-10.905246
C	2.057341	1.919224	-13.468586
H	2.136179	2.254110	-14.504028
C	2.036353	0.383140	-13.487468
H	2.969795	0.002798	-13.910213
H	1.218939	0.028643	-14.118521
H	1.901501	-0.063712	-12.497802
C	0.757095	2.600392	-12.904477
C	0.466707	2.274114	-11.424005
H	-0.509430	2.687050	-11.145656
H	1.204347	2.722306	-10.750806
H	0.427716	1.196172	-11.233195
C	0.867488	4.131464	-13.055204
H	1.007953	4.420189	-14.101663
H	1.703953	4.534741	-12.476625
H	-0.049158	4.608820	-12.691163
C	-0.441346	2.120724	-13.756001
H	-0.677402	1.066622	-13.582519
H	-0.250988	2.256796	-14.827205
H	-1.333540	2.702237	-13.499517
C	4.092530	3.303722	-13.542433
C	5.412542	3.767644	-12.877385
H	5.199526	4.122844	-11.871077

H	6.069655	2.902818	-12.760617
C	5.916405	6.249689	-13.140927
H	6.200039	6.841056	-14.013182
C	4.438395	6.550356	-12.848046
H	3.817444	6.208431	-13.679110
H	4.290210	7.626932	-12.741322
H	4.071538	6.078467	-11.931058
C	6.917907	6.668623	-12.002650
C	6.729451	8.177954	-11.726310
H	5.771175	8.395111	-11.244919
H	6.787051	8.763113	-12.651891
H	7.520676	8.533802	-11.057394
C	6.717411	5.896959	-10.681426
H	7.371380	6.317593	-9.909149
H	6.981116	4.839333	-10.781568
H	5.689990	5.967063	-10.307853
C	8.367787	6.448363	-12.480446
H	9.070069	6.767204	-11.702001
H	8.580733	7.023924	-13.386960
H	8.565540	5.393988	-12.695034
C	6.748424	4.607756	-14.776275
C	6.921178	3.130041	-15.208501
H	7.377871	2.571312	-14.392773
H	5.933419	2.693115	-15.364608
C	9.183156	2.602333	-16.263347
H	9.617466	2.903907	-17.218445
C	9.861948	3.440520	-15.169622
H	9.637259	4.498622	-15.320633
H	10.945784	3.316678	-15.220500
H	9.549529	3.167766	-14.156638
C	9.430400	1.051831	-16.158409
C	8.864924	0.420783	-14.868947
H	9.163493	-0.632456	-14.814793
H	7.771221	0.445369	-14.844178
H	9.243348	0.911180	-13.965559
C	8.793532	0.339937	-17.370026
H	9.205727	0.711951	-18.313348
H	7.708710	0.482087	-17.395924
H	8.987251	-0.737269	-17.314158
C	10.955290	0.800182	-16.203961
H	11.460221	1.143443	-15.295794
H	11.417266	1.303768	-17.061561
H	11.152305	-0.273140	-16.302179
C	7.253357	3.275984	-17.639368
C	5.767109	3.563901	-17.767975
H	5.176371	2.678734	-17.507581
H	5.441878	4.381958	-17.122785
H	5.566283	3.825018	-18.806956

Cartesian coordinates for *Right* - Ac-(stbe)$_4$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2162.037462 hartree

O	5.186520	0.150183	-10.168207
O	5.545967	0.425499	-12.402650
O	3.696486	3.465107	-14.417488
O	7.010492	5.295822	-15.525808
O	7.690420	2.862356	-18.576955
O	4.890657	4.532718	-20.877115
N	6.012158	4.721394	-13.548508
N	3.358713	2.281340	-12.489010
N	7.578857	2.693023	-16.297683
N	4.978760	3.328159	-18.933474
C	7.608995	-0.327906	-10.231812
H	7.735067	-0.136231	-11.298410
H	8.369264	-1.050212	-9.918203
H	7.776077	0.601492	-9.678308
C	6.064734	-1.166481	-8.422632
H	6.250244	-0.257475	-7.842693
H	6.782295	-1.929997	-8.108432
H	5.056211	-1.526167	-8.197974
C	5.895993	-2.146751	-10.740085
H	4.874269	-2.482072	-10.536596
H	6.580617	-2.950685	-10.451746
H	6.005794	-1.966069	-11.810325
C	6.223878	-0.897698	-9.919330
C	4.972682	0.700158	-11.364123
C	3.892222	1.784326	-11.228247
H	3.082635	1.370896	-10.631035
H	4.312631	2.594097	-10.624257
C	2.082035	1.706283	-13.012472
H	2.098572	1.960469	-14.073582
C	2.096061	0.173054	-12.911195
H	3.013814	-0.223281	-13.353164
H	1.255261	-0.244905	-13.468258
H	2.022854	-0.196762	-11.884096
C	0.797490	2.402402	-12.431029
C	0.607901	2.198629	-10.912903
H	-0.361074	2.610000	-10.608419
H	1.372781	2.721174	-10.329548
H	0.613132	1.140633	-10.629240
C	0.854555	3.916842	-12.717428
H	0.931574	4.117229	-13.790764
H	1.707898	4.389794	-12.222299
H	-0.055488	4.400466	-12.345224
C	-0.435719	1.823157	-13.162010
H	-0.632755	0.783887	-12.882227
H	-0.313415	1.866836	-14.250684
H	-1.326086	2.406341	-12.902973
C	4.072543	3.131269	-13.289882

C	5.404443	3.683926	-12.723258
H	5.225799	4.104533	-11.735632
H	6.097328	2.852172	-12.577508
C	5.811094	6.156107	-13.185525
H	6.034134	6.691062	-14.110224
C	4.339712	6.434987	-12.843049
H	3.692220	6.024359	-13.621093
H	4.165281	7.511879	-12.797500
H	4.028859	6.013739	-11.882008
C	6.851750	6.685117	-12.131753
C	6.637349	8.207503	-11.967845
H	5.696086	8.441765	-11.461477
H	6.638811	8.717904	-12.938401
H	7.448149	8.633221	-11.366660
C	6.729951	6.019548	-10.744698
H	7.406429	6.516772	-10.040414
H	7.016143	4.963208	-10.769851
H	5.718649	6.097393	-10.331016
C	8.283779	6.458511	-12.658107
H	9.011711	6.861333	-11.944964
H	8.438610	6.956604	-13.620554
H	8.501118	5.394356	-12.789649
C	6.614882	4.427759	-14.740915
C	6.817711	2.928701	-15.075895
H	7.345994	2.452515	-14.251645
H	5.843236	2.440597	-15.132000
C	9.037039	2.386538	-16.209882
H	9.407454	2.602930	-17.213225
C	9.746051	3.351269	-15.247679
H	9.473617	4.381037	-15.488627
H	10.828782	3.255416	-15.353442
H	9.504430	3.173160	-14.195349
C	9.342040	0.862043	-15.968956
C	8.879877	0.342238	-14.591730
H	9.226943	-0.688447	-14.455388
H	7.789585	0.326455	-14.499828
H	9.290177	0.932253	-13.765015
C	8.660213	0.017729	-17.064942
H	8.998611	0.312149	-18.063650
H	7.571384	0.120410	-17.032476
H	8.899409	-1.042238	-16.923161
C	10.869714	0.653833	-16.085280
H	11.414389	1.108252	-15.252070
H	11.260559	1.075079	-17.019193
H	11.099335	-0.417436	-16.081132
C	7.031423	2.913356	-17.532899
C	5.511631	3.207416	-17.582398
H	4.980665	2.404454	-17.072913
H	5.304364	4.114314	-17.012172
C	4.298890	2.168683	-19.573917

H	4.321360	2.413483	-20.637405
C	5.112138	0.879367	-19.387445
H	6.142029	1.041874	-19.712810
H	4.688374	0.076138	-19.994399
H	5.136800	0.527927	-18.351408
C	2.772788	2.050924	-19.204927
C	2.136006	0.989091	-20.131285
H	1.047608	0.990290	-20.005277
H	2.489536	-0.022041	-19.907545
H	2.349899	1.199113	-21.186137
C	2.514576	1.640981	-17.739843
H	3.018705	0.704956	-17.475884
H	1.440334	1.483081	-17.588525
H	2.827035	2.414059	-17.031535
C	2.067939	3.397557	-19.468401
H	0.997725	3.307288	-19.250447
H	2.177973	3.708283	-20.512115
H	2.471658	4.192788	-18.834002
C	5.217150	4.451324	-19.680787
C	5.853631	5.645662	-18.990564
H	6.021867	6.415886	-19.743168
H	6.801537	5.398286	-18.509632
H	5.185682	6.047196	-18.220364

Cartesian coordinates for *Right* - Ac-(stbe)$_5$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2605.952915 hartree

O	-3.878035	4.007102	19.298821
O	-3.953120	4.059848	17.021153
O	-7.213036	2.567154	15.038344
O	-8.288589	5.926342	13.290691
O	-5.689624	5.709986	10.338358
O	-7.689215	3.083669	8.210778
O	-10.434273	5.562288	6.847193
N	-6.234015	2.320228	17.091439
N	-7.994540	5.197569	15.439431
N	-5.601753	5.856006	12.619776
N	-6.696511	3.136514	10.271567
N	-9.785597	4.761997	8.890316
C	-1.455148	4.092692	18.824310
H	-1.551926	4.068659	17.737969
H	-1.377260	3.067587	19.199588
H	-0.529356	4.618246	19.078811
C	-2.852272	6.223117	18.922215
H	-2.969021	6.211020	17.837633
H	-1.985251	6.843472	19.170377
H	-3.737795	6.682167	19.373009
C	-2.480947	4.844010	21.001970
H	-2.375241	3.830319	21.399738
H	-3.349458	5.316306	21.470504
H	-1.588334	5.415821	21.271906
C	-2.632752	4.816037	19.480839
C	-4.401265	3.729384	18.104086
C	-5.704730	2.939633	18.299052
H	-5.519354	2.172216	19.047226
H	-6.434284	3.615920	18.754496
C	-5.917130	0.885177	16.815700
H	-6.106278	0.779676	15.746342
C	-4.423228	0.607147	17.043177
H	-4.162919	-0.377385	16.649561
H	-4.130856	0.623898	18.097652
H	-3.819829	1.345565	16.509070
C	-6.899269	-0.121171	17.518760
C	-8.350482	0.197124	17.104310
H	-8.476067	0.141518	16.018308
H	-8.653808	1.196759	17.429530
H	-9.035852	-0.524057	17.563389
C	-6.562406	-1.546047	17.021615
H	-6.531107	-1.591159	15.926560
H	-7.332302	-2.247092	17.361746
H	-5.602144	-1.903877	17.405306
C	-6.814849	-0.106807	19.059447
H	-5.795582	-0.275449	19.423235
H	-7.439942	-0.909697	19.466097

H	-7.186716	0.831430	19.483383
C	-6.863347	3.050052	16.119891
C	-7.134276	4.545699	16.420040
H	-7.607211	4.641124	17.395149
H	-6.176037	5.064466	16.497120
C	-9.452261	5.347622	15.730948
H	-9.898538	5.504348	14.747563
C	-10.036561	4.042576	16.292313
H	-9.730967	3.835016	17.322394
H	-9.731608	3.199833	15.667965
H	-11.127524	4.088253	16.280549
C	-9.792854	6.639419	16.559971
C	-9.196678	6.642733	17.983576
H	-9.477470	5.751782	18.555672
H	-9.572214	7.512095	18.534978
H	-8.104650	6.720240	17.971130
C	-11.330999	6.747812	16.672317
H	-11.754358	5.973058	17.318695
H	-11.811021	6.672390	15.689417
H	-11.602666	7.718152	17.102057
C	-9.278823	7.885977	15.811417
H	-8.190294	7.870811	15.702762
H	-9.545268	8.791911	16.367336
H	-9.717483	7.958970	14.811112
C	-7.546037	5.508454	14.185685
C	-6.031886	5.331578	13.911551
H	-5.463938	5.840573	14.687958
H	-5.781230	4.272593	13.999007
C	-4.990503	7.217181	12.544986
H	-5.108653	7.497178	11.496870
C	-5.794706	8.227457	13.376719
H	-5.683410	8.089600	14.456601
H	-6.856078	8.150210	13.131167
H	-5.470061	9.243638	13.143565
C	-3.440039	7.223040	12.809876
C	-2.743201	6.250810	11.836080
H	-3.073348	5.219477	11.992159
H	-1.658875	6.280213	11.991565
H	-2.944743	6.517213	10.793573
C	-2.909131	8.647143	12.524613
H	-3.247495	9.373740	13.269560
H	-3.223685	9.000928	11.535402
H	-1.813722	8.644979	12.543660
C	-3.053132	6.832509	14.250934
H	-3.277416	5.783375	14.465859
H	-3.552400	7.455982	15.000352
H	-1.973859	6.964013	14.388120
C	-5.912149	5.218749	11.450625
C	-6.553809	3.812627	11.557024
H	-5.946299	3.185359	12.207060

H	-7.522302	3.904094	12.051974
C	-5.665323	2.144430	9.841714
H	-5.765879	2.116656	8.754987
C	-4.247745	2.647189	10.153488
H	-4.000350	2.620105	11.219149
H	-4.130197	3.674313	9.801665
H	-3.512649	2.029460	9.633382
C	-5.969256	0.681542	10.334584
C	-4.908391	-0.266059	9.729643
H	-3.916732	-0.110269	10.164834
H	-4.829105	-0.135987	8.643596
H	-5.190287	-1.307466	9.920611
C	-7.353249	0.235554	9.820699
H	-8.152809	0.870095	10.213301
H	-7.555888	-0.792665	10.141032
H	-7.401350	0.268189	8.727667
C	-5.947744	0.534273	11.869474
H	-4.998371	0.861350	12.307337
H	-6.080042	-0.520115	12.138073
H	-6.759142	1.092651	12.345751
C	-7.643337	3.526894	9.363500
C	-8.701543	4.552280	9.842423
H	-9.130680	4.215449	10.784367
H	-8.199035	5.496313	10.061145
C	-11.071479	4.027893	9.054925
H	-11.517347	4.059301	8.058923
C	-10.829142	2.550256	9.398293
H	-10.463721	2.395144	10.418097
H	-10.100103	2.122240	8.706818
H	-11.758690	1.985858	9.297029
C	-12.093411	4.765169	9.997551
C	-13.435270	3.998918	9.952132
H	-13.372753	3.024139	10.445554
H	-13.769483	3.837959	8.920165
H	-14.210466	4.577504	10.466825
C	-11.627362	4.855413	11.464996
H	-10.746719	5.494479	11.578238
H	-11.398577	3.872272	11.890317
H	-12.424942	5.294220	12.075768
C	-12.343970	6.195470	9.476142
H	-11.427108	6.792940	9.482862
H	-13.076830	6.702106	10.114404
H	-12.732824	6.183892	8.452956
C	-9.584121	5.496074	7.750866
C	-8.295640	6.292640	7.632617
H	-7.409834	5.657775	7.694484
H	-8.226459	7.043899	8.426872
H	-8.305378	6.801510	6.668786

Cartesian coordinates for *Right* - Ac-(stbe)$_6$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -3049.868505 hartree

C	-3.275198	6.378645	-1.216687
C	-3.149207	6.998226	-2.616430
C	-1.772416	7.701269	-2.907224
C	-0.565917	6.740822	-2.875657
N	-3.554764	6.022352	-3.671598
C	-3.081157	4.643802	-3.597591
C	-4.096279	3.666185	-2.954574
O	-5.250479	4.043445	-2.722243
C	-4.504471	6.404386	-4.579527
O	-5.027398	7.524367	-4.571191
C	-4.900307	5.372435	-5.666191
N	-5.830166	5.900199	-6.657112
C	-5.322572	6.397692	-7.966145
C	-4.052576	7.243505	-7.787828
C	-7.146549	6.105632	-6.335626
C	-7.662154	5.521135	-5.031454
O	-7.927906	6.703016	-7.094766
C	-5.216116	5.268841	-9.056656
C	-6.587453	4.584908	-9.233345
C	-4.170706	4.184852	-8.720980
C	-4.832267	5.925830	-10.401999
N	-3.654068	2.405436	-2.664340
C	-2.339679	1.938912	-3.095569
C	-2.245685	1.643595	-4.612804
O	-3.189932	1.933173	-5.356403
C	-4.623582	1.430299	-2.078848
C	-4.645661	0.124526	-2.888095
C	-4.461169	1.241960	-0.526304
C	-5.593547	0.313437	-0.030831
C	-3.105952	0.630219	-0.116231
C	-4.616158	2.603124	0.182167
N	-1.100973	1.045944	-5.061368
C	0.064099	0.883723	-4.197422
C	0.821669	2.204949	-3.917053
O	0.338379	3.281117	-4.285315
C	-0.981164	0.744742	-6.519900
C	0.307166	1.346222	-7.101138
C	-1.225434	-0.769628	-6.865062
C	-1.236512	-0.918435	-8.404136
C	-2.605968	-1.205862	-6.333271
C	-0.155794	-1.719220	-6.287856
N	2.021839	2.113130	-3.268386
C	2.496225	0.853783	-2.705942
C	1.754711	0.421518	-1.416326
O	0.737254	1.023581	-1.059415
C	2.763936	3.374092	-2.965431
C	3.972008	3.640894	-3.936838

C	3.473578	3.650322	-5.396347
C	3.101675	3.465275	-1.469637
N	2.277507	-0.633793	-0.719661
C	3.392736	-1.418007	-1.232537
C	3.036374	-2.386099	-2.371094
O	4.066515	-3.207154	-2.578954
C	4.084625	-4.247563	-3.653387
C	2.964275	-5.259494	-3.404280
C	1.567918	-1.102335	0.509753
C	2.261912	-0.649442	1.846629
C	2.395053	0.887256	1.864174
C	1.251054	-2.602568	0.413049
O	1.985022	-2.370097	-2.984958
C	-1.817568	8.384025	-4.289471
C	-1.557028	8.798819	-1.839628
C	5.110932	2.606413	-3.816554
C	4.545387	5.040715	-3.617488
C	5.458344	-4.890932	-3.461568
C	3.980025	-3.569127	-5.020648
C	3.659512	-1.264494	2.069223
C	1.349549	-1.064365	3.024182
H	0.738891	0.174632	-4.672681
H	-0.220564	0.436410	-3.242886
H	-4.001784	5.032961	-6.180284
H	-5.324388	4.492522	-5.179811
H	-2.152492	4.633953	-3.030657
H	-2.826734	4.271358	-4.591785
H	-2.102384	1.034789	-2.538218
H	-1.568428	2.664125	-2.830909
H	3.557895	0.961435	-2.493896
H	2.416139	0.048638	-3.440155
H	3.822633	-2.004836	-0.424059
H	4.204897	-0.775713	-1.586236
H	0.758197	-2.820057	-0.538039
H	0.566630	-2.891132	1.213246
H	2.135483	-3.241617	0.494490
H	-4.208424	7.986957	-7.003075
H	-3.825630	7.775627	-8.714240
H	-3.169186	6.652295	-7.527171
H	-3.900958	7.786049	-2.689656
H	-0.691265	9.413577	-2.109806
H	-1.363915	8.379364	-0.847674
H	-2.427086	9.462292	-1.766833
H	-0.592934	6.016695	-3.695091
H	-0.495454	6.191229	-1.930666
H	0.360885	7.315814	-2.984890
H	-0.867529	8.894448	-4.484083
H	-2.619438	9.127498	-4.341037
H	-1.976230	7.658358	-5.092567
H	-4.254896	5.909089	-1.104639

H	-3.188558	7.156474	-0.455086
H	-2.509167	5.626822	-1.003632
H	-5.593292	1.912064	-2.216298
H	-4.735501	0.347533	-3.953384
H	-5.509589	-0.477433	-2.598668
H	-3.754080	-0.492630	-2.740700
H	-5.589619	3.055419	-0.032458
H	-3.839696	3.308883	-0.126885
H	-4.532863	2.470658	1.266817
H	-5.607482	0.298274	1.064505
H	-5.461438	-0.718075	-0.371020
H	-6.575580	0.662498	-0.371998
H	-2.270449	1.303741	-0.329349
H	-2.913548	-0.328499	-0.610120
H	-3.101188	0.442930	0.963648
H	-1.817921	1.284742	-6.966150
H	0.391510	2.395502	-6.809544
H	0.279010	1.304379	-8.191940
H	1.215688	0.828801	-6.778093
H	-0.187400	-1.758635	-5.194892
H	0.857668	-1.441803	-6.597376
H	-0.337206	-2.737431	-6.650420
H	-1.566294	-1.927216	-8.675701
H	-0.244765	-0.769286	-8.841594
H	-1.926409	-0.205365	-8.870932
H	-2.796780	-2.250299	-6.604128
H	-3.407883	-0.592111	-6.755936
H	-2.660278	-1.129723	-5.243334
H	2.037347	4.159474	-3.180078
H	5.279763	5.322026	-4.380125
H	5.052352	5.069111	-2.648372
H	3.758833	5.804575	-3.614243
H	3.053825	2.682219	-5.685499
H	4.307603	3.866598	-6.073373
H	2.703892	4.413116	-5.550631
H	4.806820	1.617695	-4.174652
H	5.479386	2.509182	-2.789667
H	5.958031	2.922981	-4.435524
H	2.207554	3.271807	-0.872813
H	3.451928	4.470905	-1.227936
H	3.881546	2.765146	-1.154327
H	5.545052	-5.330215	-2.463336
H	5.599086	-5.683913	-4.201763
H	6.254793	-4.151960	-3.590212
H	3.005203	-3.100816	-5.163829
H	4.761917	-2.811742	-5.134636
H	4.120288	-4.321607	-5.803009
H	3.033254	-5.666144	-2.390529
H	1.978776	-4.812732	-3.543162
H	3.072251	-6.088772	-4.110495

H	-7.622403	4.426440	-5.059918
H	-7.087577	5.849874	-4.164104
H	-8.700780	5.830304	-4.914474
H	4.396132	-0.879246	1.357184
H	4.017542	-1.001633	3.070968
H	3.649953	-2.357941	2.006418
H	0.319172	-0.721543	2.872764
H	1.330608	-2.148373	3.171325
H	1.717472	-0.614238	3.952553
H	2.846026	1.211322	2.808743
H	3.033322	1.246720	1.051545
H	1.418930	1.373664	1.769145
H	0.617053	-0.568342	0.478509
H	-6.110908	7.068487	-8.313698
H	-3.173773	4.605414	-8.550404
H	-4.455336	3.600233	-7.840777
H	-4.087293	3.484192	-9.559766
H	-4.902055	5.188375	-11.209421
H	-5.506631	6.754780	-10.648656
H	-3.807839	6.310451	-10.397122
H	-6.914428	4.095261	-8.310933
H	-7.357612	5.306208	-9.524250
H	-6.524544	3.818238	-10.013965

Cartesian coordinates for *Left*- Ac-(stbe)$_2$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -1274.203507 hartree

O	2.365218	1.134118	-12.745603
O	4.174222	1.010840	-14.125713
O	7.720347	2.885576	-12.650629
O	7.507803	5.885438	-15.513215
N	6.280616	4.987711	-13.802606
N	5.870344	1.756630	-11.915511
C	1.596182	-0.672692	-14.244717
H	2.510180	-0.721329	-14.838284
H	0.758618	-0.997131	-14.870282
H	1.679631	-1.366559	-13.402433
C	0.039107	0.798660	-12.913921
H	0.087827	0.092600	-12.079694
H	-0.815808	0.533195	-13.542587
H	-0.124235	1.804001	-12.514448
C	1.286466	1.779240	-14.873268
H	1.154128	2.787245	-14.467908
H	0.434814	1.561429	-15.525365
H	2.196866	1.752947	-15.473917
C	1.322133	0.746940	-13.744161
C	3.662981	1.231162	-13.043242
C	4.420291	1.687646	-11.788316
H	3.990148	2.644719	-11.474737
H	4.168172	0.988813	-10.991443
C	6.723328	0.815811	-11.125070
H	7.721656	1.241070	-11.232925
C	6.359786	0.898079	-9.632559
H	6.310145	1.945562	-9.320066
H	7.130489	0.410439	-9.031421
H	5.405790	0.423886	-9.383280
C	6.827371	-0.635506	-11.711279
C	5.522720	-1.453234	-11.604120
H	5.711421	-2.483803	-11.925423
H	4.731056	-1.062747	-12.248758
H	5.144620	-1.497790	-10.577261
C	7.257682	-0.559782	-13.190851
H	8.221794	-0.049943	-13.294692
H	6.519510	-0.024592	-13.793876
H	7.365301	-1.570382	-13.601128
C	7.930107	-1.384312	-10.926110
H	7.635187	-1.593360	-9.893170
H	8.865271	-0.812320	-10.905164
H	8.138202	-2.345658	-11.408357
C	6.492034	2.785390	-12.577928
C	5.579554	3.832777	-13.254612
H	5.000151	3.327515	-14.031406
H	4.855410	4.197899	-12.526994
C	6.088591	6.334293	-13.188139

H	6.517040	7.004811	-13.934340
C	4.588833	6.669105	-13.093582
H	4.093487	6.425116	-14.038481
H	4.452700	7.738620	-12.916909
H	4.067581	6.139435	-12.290241
C	6.912106	6.595016	-11.878822
C	6.769412	8.091758	-11.515176
H	5.759687	8.342055	-11.174943
H	7.011141	8.736226	-12.368824
H	7.460409	8.342452	-10.702756
C	6.446345	5.758939	-10.668143
H	6.988914	6.080907	-9.771940
H	6.652098	4.693535	-10.797525
H	5.378128	5.885607	-10.461877
C	8.402282	6.304473	-12.149871
H	8.993985	6.506913	-11.249432
H	8.785624	6.940942	-12.955086
H	8.554557	5.259920	-12.433345
C	6.936532	4.906436	-15.004705
C	6.925389	3.577000	-15.739610
H	7.328736	2.768419	-15.127312
H	5.908162	3.301656	-16.039166
H	7.534089	3.686492	-16.636907

Cartesian coordinates for *Left*- Ac-(stbe)$_3$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -1718.117046 hartree

O	7.319366	4.751940	-9.870247
O	7.905441	4.836848	-12.070839
O	4.702942	5.019218	-14.857943
O	5.512400	1.272382	-16.385484
O	8.342065	2.798314	-19.024966
N	5.023789	2.284558	-14.393136
N	5.217844	5.650950	-12.719597
N	7.908221	2.653441	-16.781797
C	9.667183	5.478289	-9.620944
H	9.872218	5.553777	-10.689796
H	10.605040	5.254651	-9.102682
H	9.300799	6.443561	-9.258041
C	8.373323	4.282852	-7.816156
H	8.027058	5.245570	-7.428605
H	9.289153	4.005528	-7.286256
H	7.610962	3.526049	-7.608712
C	9.074863	3.011671	-9.878119
H	8.297245	2.263694	-9.694301
H	9.987271	2.684214	-9.369742
H	9.276177	3.062050	-10.949209
C	8.655433	4.371765	-9.316209
C	7.090595	4.935328	-11.171728
C	5.606593	5.276259	-11.365439
H	5.023612	4.428559	-10.989721
H	5.375987	6.100078	-10.691423
C	4.758670	7.049632	-12.991058
H	4.323384	6.975939	-13.988057
C	3.618692	7.427412	-12.029168
H	2.878667	6.622242	-11.994767
H	3.111968	8.326768	-12.386040
H	3.952060	7.627288	-11.006560
C	5.907161	8.110243	-13.118868
C	6.636060	8.412267	-11.792565
H	7.336395	9.241542	-11.942323
H	7.225511	7.563491	-11.436168
H	5.944221	8.712609	-10.998635
C	6.934156	7.627312	-14.163596
H	6.460127	7.473472	-15.139142
H	7.402491	6.687804	-13.858277
H	7.724105	8.376820	-14.287579
C	5.277742	9.426695	-13.632577
H	4.632318	9.896754	-12.884186
H	4.684125	9.259862	-14.539185
H	6.069008	10.142659	-13.880111
C	5.067172	4.721585	-13.716063
C	5.381657	3.251309	-13.359586
H	6.441089	3.179759	-13.100239

H	4.836450	2.980073	-12.456897
C	3.921799	1.306557	-14.135523
H	4.037873	0.588244	-14.947711
C	4.183746	0.544163	-12.824186
H	5.220671	0.195445	-12.797548
H	3.538402	-0.335425	-12.767267
H	4.001628	1.137650	-11.923112
C	2.469271	1.878309	-14.296184
C	1.482512	0.688581	-14.237887
H	1.428102	0.241998	-13.240224
H	1.761001	-0.098045	-14.949226
H	0.475342	1.031939	-14.498346
C	2.067873	2.890073	-13.202177
H	1.011574	3.156524	-13.321438
H	2.637847	3.820271	-13.267130
H	2.185803	2.478755	-12.194104
C	2.333200	2.549103	-15.678553
H	1.309161	2.914927	-15.817063
H	2.548358	1.838114	-16.483788
H	3.015622	3.397251	-15.775916
C	5.788500	2.106806	-15.516890
C	7.038878	3.002506	-15.663106
H	6.703522	4.039488	-15.737393
H	7.630231	2.940615	-14.750273
C	9.263389	2.085102	-16.523003
H	9.742649	2.143183	-17.501041
C	10.055551	3.007902	-15.579387
H	9.971462	4.044886	-15.919053
H	11.114892	2.740981	-15.591478
H	9.721430	2.964969	-14.538525
C	9.291039	0.562568	-16.144272
C	8.692811	0.248181	-14.756576
H	8.848275	-0.811529	-14.523565
H	7.615333	0.426343	-14.718481
H	9.169916	0.827634	-13.958892
C	8.530224	-0.242042	-17.218100
H	8.985197	-0.105778	-18.205610
H	7.483642	0.067552	-17.273580
H	8.562589	-1.311407	-16.978327
C	10.766394	0.097803	-16.148524
H	11.341092	0.530471	-15.323590
H	11.266152	0.362592	-17.088050
H	10.811348	-0.991855	-16.042595
C	7.597922	3.041733	-18.059618
C	6.313620	3.822265	-18.279786
H	5.440002	3.287930	-17.902036
H	6.356288	4.796475	-17.780631
H	6.201092	3.985063	-19.351507

Cartesian coordinates for *Left*- Ac-(stbe)$_4$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2162.030788 hartree

O	2.143823	-3.433338	4.873946
O	0.761730	-3.512173	3.064041
O	0.110581	0.220711	1.071908
O	-3.890314	0.327313	2.136506
O	-4.987645	-1.762432	-1.249346
O	-5.028303	1.661476	-3.593904
N	-1.820199	0.151906	3.094825
N	1.702044	-0.896645	2.279774
N	-3.653718	-1.985863	0.596039
N	-3.608388	0.436857	-2.280159
C	2.216217	-5.861439	4.423548
H	1.588355	-5.826769	3.532135
H	2.102139	-6.844697	4.890788
H	3.263465	-5.745877	4.127559
C	2.711748	-4.840939	6.676270
H	3.767258	-4.752640	6.402419
H	2.565569	-5.796853	7.187584
H	2.460386	-4.034528	7.371567
C	0.341517	-4.836678	5.815523
H	0.088286	-4.013844	6.491401
H	0.144107	-5.777573	6.338719
H	-0.303033	-4.788600	4.936694
C	1.822305	-4.782278	5.434145
C	1.577834	-2.946179	3.768319
C	2.107982	-1.525552	3.531285
H	1.827879	-0.921923	4.401278
H	3.195403	-1.578530	3.561099
C	2.735243	-0.612768	1.234306
H	2.210887	0.048347	0.543833
C	3.894466	0.198247	1.837370
H	3.499011	1.041343	2.411901
H	4.518574	0.605327	1.038941
H	4.547178	-0.384610	2.493889
C	3.160581	-1.854508	0.374398
C	3.984374	-2.905997	1.147439
H	4.338067	-3.674499	0.451049
H	3.394768	-3.420858	1.910259
H	4.868717	-2.472564	1.626473
C	1.902152	-2.528087	-0.210571
H	1.331071	-1.826114	-0.827859
H	1.245469	-2.903787	0.578310
H	2.191119	-3.374159	-0.844388
C	4.022005	-1.339313	-0.802937
H	4.994906	-0.963460	-0.471470
H	3.514259	-0.536259	-1.350184
H	4.209367	-2.156250	-1.508289
C	0.446995	-0.376328	2.100031

C	-0.569290	-0.586539	3.244239
H	-0.753167	-1.659777	3.339575
H	-0.119232	-0.279939	4.186912
C	-2.140350	1.256842	4.051438
H	-3.190328	1.464064	3.843121
C	-2.065620	0.742492	5.499750
H	-2.610986	-0.202107	5.586916
H	-2.536101	1.459264	6.176709
H	-1.045116	0.579865	5.859032
C	-1.393904	2.610011	3.781876
C	-2.020629	3.685719	4.700128
H	-1.780880	3.521624	5.755357
H	-3.111957	3.712569	4.598078
H	-1.635980	4.674221	4.426258
C	0.122565	2.563086	4.064581
H	0.542635	3.570474	3.966831
H	0.659216	1.927806	3.355549
H	0.345761	2.217945	5.079729
C	-1.622591	3.033286	2.316461
H	-1.127416	3.991588	2.121506
H	-2.690544	3.158771	2.106078
H	-1.218524	2.290993	1.623218
C	-2.807046	-0.259588	2.239957
C	-2.518201	-1.513297	1.384437
H	-1.654241	-1.303799	0.749547
H	-2.214257	-2.327287	2.041370
C	-4.266153	-3.312181	0.911714
H	-4.920399	-3.489722	0.057486
C	-3.189494	-4.411684	0.885209
H	-2.583015	-4.314468	-0.020328
H	-3.659855	-5.397490	0.863700
H	-2.515855	-4.391996	1.747097
C	-5.212954	-3.332006	2.162684
C	-4.486473	-3.130104	3.509533
H	-5.192977	-3.289801	4.331990
H	-4.094895	-2.115960	3.621994
H	-3.663562	-3.839564	3.647981
C	-6.289899	-2.239820	2.001588
H	-6.876764	-2.398659	1.090004
H	-5.837930	-1.245856	1.953130
H	-6.979192	-2.264172	2.853678
C	-5.919048	-4.707861	2.198396
H	-5.229229	-5.521050	2.444787
H	-6.391625	-4.940700	1.236736
H	-6.704078	-4.700557	2.962506
C	-4.052036	-1.353447	-0.552097
C	-3.280829	-0.076540	-0.953855
H	-3.466092	0.678208	-0.186335
H	-2.210304	-0.275600	-0.925683
C	-2.599637	0.367103	-3.377134

H	-3.034577	1.003354	-4.149183
C	-1.285524	1.035166	-2.934174
H	-1.499036	2.010716	-2.486398
H	-0.638012	1.201476	-3.798118
H	-0.715316	0.447973	-2.208195
C	-2.435373	-1.040361	-4.051563
C	-1.546465	-0.865621	-5.305737
H	-1.540941	-1.794135	-5.887491
H	-0.507802	-0.634064	-5.049824
H	-1.923376	-0.067148	-5.956094
C	-1.777084	-2.099882	-3.142934
H	-0.811308	-1.765338	-2.749591
H	-1.592893	-3.012893	-3.720785
H	-2.414779	-2.380717	-2.301080
C	-3.816960	-1.552218	-4.508512
H	-3.709734	-2.520487	-5.011649
H	-4.278812	-0.855294	-5.216839
H	-4.491501	-1.677826	-3.657925
C	-4.743872	1.176648	-2.485031
C	-5.655294	1.434971	-1.297368
H	-6.546469	1.943978	-1.664230
H	-5.161343	2.082577	-0.564309
H	-5.947709	0.512969	-0.792419

Cartesian coordinates for *Left*- Ac-(stbe)$_5$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2605.944720 hartree

O	-1.561752	-1.183736	14.783636
O	-2.062668	0.548021	13.389531
O	-5.482039	2.858767	14.420851
O	-7.605268	1.620621	11.091701
O	-6.028162	4.639514	8.754320
O	-8.906195	7.343739	10.019922
O	-11.605922	5.993216	7.160482
N	-3.834401	1.608320	15.400640
N	-6.522140	0.749312	12.909704
N	-5.341939	2.870343	10.033235
N	-7.251807	6.005765	10.862417
N	-10.407193	5.239939	8.959616
C	-1.276724	-2.333990	12.616534
H	-1.582167	-1.485501	12.002442
H	-2.156876	-2.940480	12.852074
H	-0.585688	-2.951519	12.034073
C	0.614227	-0.958254	13.632667
H	0.332052	-0.101916	13.018535
H	1.388882	-1.523630	13.105043
H	1.039929	-0.598417	14.574477
C	-0.162555	-3.079527	14.753073
H	-1.026975	-3.708492	14.985590
H	0.293470	-2.749052	15.690986
H	0.567985	-3.683311	14.207006
C	-0.577100	-1.880594	13.899481
C	-2.199081	-0.065986	14.432059
C	-3.168802	0.320558	15.556966
H	-3.884860	-0.500610	15.668439
H	-2.600430	0.328098	16.485797
C	-3.519593	2.716402	16.357522
H	-4.307002	3.443938	16.158471
C	-3.709108	2.234890	17.806329
H	-3.735288	3.091394	18.483774
H	-2.916123	1.568100	18.157760
H	-4.663565	1.708511	17.901783
C	-2.174753	3.472757	16.072701
C	-2.158768	3.953526	14.607361
H	-3.011214	4.609127	14.399308
H	-2.194448	3.112140	13.910395
H	-1.241791	4.520196	14.409769
C	-2.131244	4.717680	16.989722
H	-3.042872	5.318805	16.891896
H	-1.282283	5.351462	16.711489
H	-2.009443	4.451077	18.043934
C	-0.908676	2.632668	16.342519
H	-0.885997	2.230492	17.360760
H	-0.021263	3.264562	16.224424

H	-0.799097	1.802927	15.639506
C	-4.879187	1.785954	14.532139
C	-5.282690	0.574559	13.662191
H	-4.447914	0.338274	12.997367
H	-5.409797	-0.298677	14.299981
C	-7.715727	-0.082807	13.258279
H	-8.390910	0.093918	12.420619
C	-7.346985	-1.576518	13.228520
H	-6.746779	-1.901460	14.083702
H	-6.787526	-1.802342	12.315702
H	-8.253300	-2.186012	13.219309
C	-8.505851	0.386995	14.529866
C	-7.743056	0.189395	15.856867
H	-7.399885	-0.842140	15.989659
H	-8.408615	0.419147	16.696571
H	-6.881979	0.856694	15.945462
C	-9.816625	-0.431741	14.600675
H	-9.636809	-1.484261	14.840673
H	-10.368189	-0.386177	13.654181
H	-10.464492	-0.022996	15.383783
C	-8.877022	1.876437	14.378076
H	-7.984200	2.502819	14.307546
H	-9.459728	2.207224	15.245483
H	-9.486239	2.039873	13.482248
C	-6.576228	1.501066	11.767252
C	-5.278388	2.222162	11.340773
H	-5.015015	2.935457	12.125199
H	-4.462884	1.501154	11.310130
C	-4.495677	2.355475	8.912990
H	-4.567431	3.148000	8.167452
C	-3.021860	2.284713	9.350011
H	-2.802391	1.457824	10.031647
H	-2.735232	3.217501	9.845024
H	-2.377911	2.163393	8.475930
C	-5.042412	1.068546	8.200411
C	-6.501297	1.308689	7.761181
H	-7.147928	1.493774	8.622774
H	-6.881137	0.428941	7.228824
H	-6.572209	2.167376	7.084516
C	-4.188336	0.831350	6.932738
H	-3.164677	0.526899	7.171901
H	-4.139344	1.731727	6.308806
H	-4.635696	0.032756	6.330763
C	-4.979332	-0.205158	9.069146
H	-5.666292	-0.162869	9.918180
H	-3.969874	-0.399668	9.446638
H	-5.272551	-1.072312	8.466576
C	-5.996623	4.057025	9.844987
C	-6.714641	4.663307	11.070886
H	-7.497578	3.968993	11.384059

H	-6.015203	4.712824	11.904400
C	-6.651505	7.163458	11.594213
H	-7.378945	7.959810	11.433459
C	-6.624544	6.879773	13.106463
H	-5.856942	6.160764	13.407008
H	-7.596018	6.492830	13.428806
H	-6.437348	7.803866	13.658277
C	-5.308386	7.707846	10.992506
C	-4.960754	9.025486	11.724677
H	-4.670971	8.857267	12.766573
H	-5.805404	9.724735	11.713839
H	-4.117286	9.514535	11.224856
C	-5.512677	8.027559	9.497314
H	-5.788623	7.131048	8.936448
H	-4.586548	8.429661	9.070311
H	-6.299142	8.777969	9.360029
C	-4.113659	6.743587	11.145714
H	-3.951726	6.445987	12.187115
H	-3.197998	7.240786	10.805717
H	-4.229001	5.841938	10.539578
C	-8.413301	6.219599	10.168696
C	-9.101279	4.978877	9.556757
H	-8.417863	4.545116	8.823532
H	-9.231730	4.222438	10.329618
C	-11.637534	4.671130	9.581811
H	-12.395674	4.830792	8.814000
C	-11.491060	3.148559	9.757444
H	-10.822543	2.860957	10.574263
H	-11.107387	2.703673	8.834029
H	-12.465034	2.697337	9.961307
C	-12.167403	5.437764	10.844549
C	-13.556264	4.859300	11.203974
H	-13.493871	3.837248	11.590542
H	-14.225297	4.854445	10.335033
H	-14.023711	5.475234	11.980269
C	-11.257337	5.311372	12.084499
H	-10.304848	5.831027	11.953889
H	-11.051155	4.267335	12.343006
H	-11.752779	5.767467	12.949376
C	-12.342979	6.930040	10.496017
H	-11.388579	7.382917	10.216160
H	-12.743030	7.472646	11.360682
H	-13.044381	7.059056	9.663979
C	-10.509027	5.802572	7.713723
C	-9.227979	6.170160	6.985238
H	-8.635251	5.277356	6.758207
H	-8.605268	6.848186	7.571585
H	-9.503686	6.653212	6.048001

Cartesian coordinates for *Left*- Ac-(stbe)$_6$-COOtBu - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -3049.858896 hartree

C	-3.946434	1.434965	-3.790779
C	-5.198141	2.302751	-3.569934
C	-5.721555	2.353173	-2.091306
C	-4.707961	2.935845	-1.084268
N	-5.027264	3.632125	-4.231483
C	-3.848284	4.441185	-3.930559
C	-4.141918	5.749914	-3.163959
O	-5.309669	6.105655	-2.963563
C	-5.887505	3.958609	-5.246158
O	-6.872286	3.269228	-5.535893
C	-5.578524	5.250266	-6.034815
N	-6.430476	5.470743	-7.199326
C	-5.856064	5.381605	-8.573506
C	-4.627200	6.300112	-8.699397
C	-7.696961	5.974834	-7.055052
C	-8.192912	6.277596	-5.651711
O	-8.429292	6.216830	-8.030098
C	-5.655870	3.926462	-9.126129
C	-6.985028	3.151972	-9.014629
C	-4.545048	3.130260	-8.409811
C	-5.283383	4.032533	-10.623590
N	-3.062499	6.470107	-2.731295
C	-1.691870	6.011411	-2.944423
C	-1.167801	6.203546	-4.385004
O	-1.936040	6.576543	-5.280088
C	-3.316854	7.644766	-1.841411
C	-2.662937	7.420360	-0.466853
C	-3.040476	9.045854	-2.491597
C	-3.574677	10.129459	-1.525525
C	-1.547786	9.333377	-2.758198
C	-3.820453	9.156353	-3.817721
N	0.156558	5.942496	-4.604359
C	1.052698	5.535042	-3.525127
C	0.911628	4.058174	-3.095009
O	-0.029081	3.375825	-3.518418
C	0.724397	6.284829	-5.945373
C	1.828850	7.346170	-5.798054
C	1.096270	5.055070	-6.846272
C	1.418392	5.586548	-8.262793
C	-0.119881	4.112352	-6.949883
C	2.316408	4.253026	-6.345539
N	1.857488	3.565973	-2.237597
C	2.982226	4.376058	-1.778634
C	2.623348	5.416815	-0.693915
O	1.442134	5.615187	-0.390843
C	1.839678	2.099247	-1.940890
C	1.419279	1.719888	-0.477594

C	0.064447	2.379228	-0.148162
C	3.140188	1.444233	-2.438750
N	3.662842	6.091309	-0.109886
C	5.052434	5.809945	-0.448615
C	5.537952	6.386770	-1.785695
O	6.851936	6.181025	-1.886727
C	7.654808	6.565351	-3.088649
C	7.143456	5.797986	-4.309458
C	3.355136	6.980635	1.054671
C	3.495322	8.516858	0.768970
C	2.659381	8.883485	-0.474287
C	4.082393	6.476995	2.313310
O	4.822482	6.921761	-2.612967
C	-7.020321	3.183392	-2.037343
C	-6.055756	0.906369	-1.657910
C	2.450116	2.120446	0.598981
C	1.236089	0.184856	-0.422049
C	9.061387	6.107940	-2.701418
C	7.602485	8.082997	-3.276210
C	4.949030	8.990007	0.557298
C	2.913420	9.277281	1.983697
H	0.916320	6.158720	-2.638516
H	2.072197	5.718866	-3.859963
H	-5.644517	6.090857	-5.340640
H	-4.544088	5.223071	-6.375458
H	-3.300709	4.694615	-4.841029
H	-3.169118	3.828656	-3.339377
H	-1.579320	4.957860	-2.678342
H	-1.051257	6.560004	-2.255635
H	3.460658	4.894365	-2.613688
H	3.734310	3.694740	-1.383344
H	5.260478	4.734592	-0.461329
H	5.695187	6.214700	0.331735
H	3.946620	5.396000	2.415061
H	3.657117	6.947248	3.202702
H	5.155873	6.687551	2.317574
H	-4.858667	7.287928	-8.288996
H	-4.363007	6.432614	-9.751284
H	-3.738415	5.920582	-8.186578
H	-6.005850	1.845188	-4.142347
H	-6.569743	0.919896	-0.690452
H	-5.159533	0.288655	-1.543243
H	-6.718555	0.415360	-2.380512
H	-4.535179	4.003210	-1.241748
H	-3.743805	2.417585	-1.117947
H	-5.099975	2.824107	-0.066868
H	-7.411702	3.200026	-1.013417
H	-7.790845	2.750133	-2.684575
H	-6.842108	4.214301	-2.353407
H	-3.655924	1.463998	-4.845359

H	-4.162071	0.394828	-3.535636
H	-3.083591	1.743742	-3.193568
H	-4.396021	7.608648	-1.689311
H	-2.899324	6.415899	-0.102993
H	-3.058777	8.136052	0.257351
H	-1.574912	7.531772	-0.471935
H	-4.895643	9.023654	-3.653939
H	-3.485380	8.404212	-4.536337
H	-3.667423	10.147365	-4.260726
H	-3.540764	11.109103	-2.014851
H	-2.978821	10.200142	-0.610287
H	-4.615723	9.934644	-1.241569
H	-1.133044	8.691397	-3.539514
H	-0.936215	9.223420	-1.856446
H	-1.431987	10.367312	-3.102721
H	-0.113173	6.766775	-6.450763
H	1.481896	8.155710	-5.148830
H	2.062044	7.781478	-6.772454
H	2.763433	6.956256	-5.384534
H	2.115828	3.732529	-5.405652
H	3.200904	4.884584	-6.211164
H	2.575341	3.485853	-7.084003
H	1.534304	4.744803	-8.954366
H	2.348585	6.162470	-8.289048
H	0.611398	6.222946	-8.644880
H	0.115164	3.267918	-7.608111
H	-0.986643	4.634609	-7.369365
H	-0.397147	3.716610	-5.969542
H	1.034135	1.730208	-2.576449
H	0.792048	-0.098741	0.538427
H	2.186290	-0.350241	-0.514227
H	0.566913	-0.167534	-1.215913
H	0.135151	3.469270	-0.185767
H	-0.256741	2.091216	0.859514
H	-0.710948	2.058145	-0.852428
H	2.525328	3.204064	0.720241
H	3.448415	1.722795	0.387449
H	2.139904	1.714525	1.568485
H	3.360412	1.780351	-3.456374
H	3.025012	0.358399	-2.467281
H	4.010680	1.661294	-1.812489
H	9.082659	5.029209	-2.520392
H	9.758104	6.336558	-3.513084
H	9.401475	6.622759	-1.798011
H	6.603346	8.421178	-3.554679
H	7.910934	8.594078	-2.358944
H	8.298475	8.365831	-4.072281
H	7.136452	4.721574	-4.111443
H	6.139096	6.115435	-4.593614
H	7.816325	5.983425	-5.152611

H	-8.100702	5.418254	-4.985736
H	-7.628900	7.108337	-5.213123
H	-9.240832	6.568735	-5.722771
H	5.385236	8.602893	-0.367234
H	4.967637	10.082903	0.479737
H	5.602202	8.714719	1.391999
H	1.902770	8.929011	2.227228
H	3.536115	9.169548	2.877055
H	2.851197	10.346571	1.754300
H	2.724320	9.960673	-0.664788
H	3.017213	8.358937	-1.364298
H	1.603904	8.631083	-0.326644
H	2.289508	6.813922	1.214749
H	-6.641103	5.815566	-9.194245
H	-3.585831	3.658567	-8.416619
H	-4.805276	2.896098	-7.374777
H	-4.391560	2.174414	-8.924000
H	-5.291533	3.035418	-11.077862
H	-6.001540	4.654368	-11.171518
H	-4.284225	4.452962	-10.774580
H	-7.307154	3.073344	-7.973312
H	-7.777235	3.647348	-9.587036
H	-6.863526	2.139038	-9.416605

Cartesian coordinates for Ac-tBu(-)-(stbe)$_4$-tBu(-)-*COOtBu* - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2892.596699 hartree

C	1.949768	3.839026	10.971754
N	2.322102	2.736526	10.249108
C	3.306592	1.738871	10.832863
C	4.656210	2.440778	11.093118
C	1.674031	2.467090	8.969010
C	0.362757	1.660003	9.096515
N	-0.152859	1.104913	7.956554
C	-1.469608	0.408021	8.041446
C	-2.464722	1.003060	7.034006
C	0.468860	1.314770	6.652742
C	0.286276	2.742622	6.084021
N	0.811937	2.983944	4.845025
C	0.625205	4.338386	4.244340
C	-0.509037	4.383113	3.155678
C	-0.211257	3.510060	1.920255
C	1.706743	2.026543	4.202317
C	3.119793	1.972725	4.836411
N	4.065211	1.221497	4.195763
C	5.438836	1.159263	4.781392
C	6.475767	2.074109	4.032154
C	5.976242	3.533349	4.033141
C	3.713739	0.325412	3.098568
C	2.968186	-0.953102	3.555731
N	2.833856	-1.964850	2.646555
C	2.079979	-3.189826	3.053178
C	0.939726	-3.485017	2.066106
C	3.232175	-1.810344	1.252357
C	2.279665	-0.901497	0.426607
N	2.503364	-0.811657	-0.919773
C	1.626279	0.098022	-1.774862
C	1.747591	1.555242	-1.283985
C	3.646801	-1.486501	-1.522323
C	4.945007	-0.668090	-1.503957
O	2.417026	4.094042	12.094302
O	-0.185755	1.553872	10.200415
O	-0.339628	3.592365	6.727229
O	3.353975	2.609257	5.870140
O	2.525415	-1.022500	4.708054
O	1.370307	-0.302410	1.007814
O	5.123864	0.311486	-0.803412
C	0.167935	-0.398903	-1.711180
C	2.071334	0.059190	-3.248886
C	2.735834	1.127509	12.130050
C	3.568558	0.586042	9.845528
C	-1.365840	-1.162495	8.027709
C	-0.341612	-1.626208	9.083300

C	-2.748792	-1.732132	8.420728
C	-0.965518	-1.755507	6.660384
C	1.969343	4.937880	3.803715
C	-1.842238	3.915483	3.774722
C	-0.683776	5.848924	2.696753
C	5.886731	-0.295888	4.983822
C	6.737085	1.648711	2.572751
C	7.812503	2.025310	4.807345
C	3.005774	-4.416142	3.386974
C	3.782485	-4.967079	2.172181
C	2.116661	-5.547351	3.953240
C	4.021164	-4.017981	4.477487
H	4.629997	0.055281	2.578186
H	3.090534	0.838528	2.362648
H	2.377566	1.976846	8.301875
H	1.427256	3.405899	8.474437
H	0.026566	0.609361	5.950577
H	1.529802	1.065207	6.692832
H	1.797182	2.300011	3.152940
H	1.275263	1.024065	4.218461
H	3.257608	-2.803896	0.811117
H	4.251958	-1.422723	1.183097
H	3.425309	-1.766305	-2.549151
H	3.856485	-2.430826	-1.016909
H	0.102048	-1.434808	-2.060564
H	-0.453597	0.220129	-2.366449
H	-0.231805	-0.341958	-0.699124
H	3.104825	0.389122	-3.389812
H	1.433824	0.753823	-3.802130
H	1.943842	-0.927311	-3.704512
H	1.404899	1.660657	-0.255202
H	1.134344	2.201031	-1.921007
H	2.785373	1.895519	-1.348797
H	2.548102	1.894947	12.881252
H	3.454275	0.408457	12.538573
H	1.799977	0.601343	11.921033
H	2.660247	0.032154	9.592744
H	4.252534	-0.116674	10.329449
H	4.049884	0.923493	8.922877
H	5.046420	2.871812	10.164643
H	5.382476	1.706072	11.457060
H	4.558769	3.232478	11.835463
H	-1.828444	0.663300	9.039656
H	-2.677455	-2.816423	8.560205
H	-3.505714	-1.550642	7.651727
H	-3.107195	-1.297388	9.361388
H	0.059956	-1.498189	6.378773
H	-1.637275	-1.435492	5.856730
H	-1.017668	-2.849403	6.708902
H	-0.309987	-2.721066	9.117546

H	-0.602969	-1.260761	10.081450
H	0.666146	-1.271853	8.845801
H	-2.505188	2.088164	7.152313
H	-3.465736	0.604491	7.213477
H	-2.208849	0.787110	5.992409
H	0.260081	4.944314	5.075550
H	2.701829	4.841870	4.608177
H	1.848371	6.001559	3.588230
H	2.384120	4.469358	2.905678
H	-2.129347	4.542741	4.624772
H	-1.784327	2.879865	4.122653
H	-2.640719	3.970311	3.026165
H	-1.573372	5.935610	2.063223
H	0.170386	6.204888	2.112925
H	-0.817290	6.522390	3.551875
H	-0.207956	2.443499	2.165174
H	0.746380	3.763287	1.453184
H	-0.990463	3.664134	1.165230
H	5.319921	1.600052	5.772656
H	5.105444	-0.859923	5.498128
H	6.782283	-0.325158	5.607823
H	6.124489	-0.812952	4.049266
H	5.855952	1.791955	1.939997
H	7.057415	0.604248	2.493116
H	7.538802	2.265127	2.150435
H	8.499909	2.778355	4.406668
H	8.306034	1.052504	4.721460
H	7.666045	2.240908	5.872491
H	6.710793	4.179262	3.539107
H	5.828630	3.903791	5.052636
H	5.029217	3.635222	3.495136
H	1.620344	-2.905910	4.000889
H	2.747483	-6.350454	4.349597
H	1.468395	-5.987563	3.189546
H	1.483348	-5.186632	4.772396
H	4.683281	-3.215402	4.139398
H	4.647515	-4.878919	4.736958
H	3.515829	-3.678752	5.387475
H	4.547934	-4.267769	1.820353
H	3.123635	-5.215027	1.332938
H	4.301410	-5.888656	2.459057
H	0.358367	-2.577638	1.887839
H	0.267358	-4.235341	2.487361
H	1.285183	-3.864357	1.099498
O	5.827471	-1.221069	-2.338536
C	7.221999	-0.710509	-2.510152
C	7.800509	-1.677533	-3.543540
H	7.230626	-1.634971	-4.476495
H	8.838124	-1.406719	-3.759392
H	7.781994	-2.704717	-3.167288

C	7.970280	-0.814819	-1.179641
H	7.561444	-0.132196	-0.433269
H	7.924503	-1.837680	-0.792704
H	9.022485	-0.560626	-1.341900
C	7.178926	0.717615	-3.058033
H	6.574638	0.760334	-3.969590
H	6.771508	1.417525	-2.327109
H	8.196396	1.032326	-3.310734
C	0.942959	4.805121	10.359441
H	1.348340	5.296379	9.468186
H	0.009844	4.310781	10.079365
H	0.731114	5.568705	11.107839

Cartesian coordinates for Ac-tBu(-)-(stbe)$_4$-tBu(+)-*COOtBu* - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2892.596846 hartree

C	-7.272531	5.273445	-6.587172
N	-5.907034	5.242191	-6.692729
C	-5.229549	5.691974	-7.975265
C	-5.670403	4.775521	-9.136021
C	-5.109279	4.875402	-5.526511
C	-4.782528	6.067358	-4.598227
N	-3.856584	5.858725	-3.611437
C	-3.557633	6.975847	-2.666713
C	-3.729736	6.522816	-1.208548
C	-3.303407	4.532493	-3.354298
C	-4.302335	3.548388	-2.697094
N	-3.828350	2.305859	-2.379716
C	-4.755471	1.336396	-1.722720
C	-4.527440	1.218516	-0.171297
C	-3.130948	0.682254	0.204490
C	-2.523749	1.850223	-2.850209
C	-2.490004	1.519929	-4.363680
N	-1.358139	0.929351	-4.851744
C	-1.300508	0.598478	-6.307505
C	-1.533040	-0.927161	-6.611494
C	-2.877822	-1.376115	-6.004520
C	-0.152672	0.789620	-4.041362
C	0.618599	2.115032	-3.826277
N	1.888326	2.030475	-3.326748
C	2.633838	3.298646	-3.058881
C	3.153478	3.331613	-1.613236
C	2.460666	0.764364	-2.883168
C	1.880459	0.249418	-1.536636
N	2.462793	-0.858646	-0.986552
C	1.973744	-1.385182	0.358450
C	0.504088	-1.832149	0.226988
C	3.588693	-1.502544	-1.653165
C	4.966358	-0.958944	-1.249446
O	-8.010598	5.621642	-7.524079
O	-5.351899	7.152445	-4.764850
O	-5.459659	3.908834	-2.455277
O	-3.469188	1.781778	-5.071626
O	0.077065	3.190707	-4.105622
O	0.918137	0.835832	-1.032826
O	5.139757	0.060192	-0.606833
C	2.138316	-0.291740	1.433976
C	2.800195	-2.606905	0.802021
C	-5.574777	7.167375	-8.266975
C	-3.697845	5.582573	-7.854606
C	-2.203895	7.713521	-2.975627
C	-2.215998	8.236825	-4.426284

C	-2.091325	8.931230	-2.029428
C	-0.955635	6.827173	-2.785966
C	-4.778632	-0.002166	-2.476401
C	-4.713694	2.600312	0.488353
C	-5.596575	0.264142	0.407603
C	-0.051161	1.209507	-6.958937
C	-0.420134	-1.849037	-6.070149
C	-1.615639	-1.105705	-8.145187
C	3.705463	3.639692	-4.158777
C	4.853739	2.613177	-4.249883
C	4.309224	5.024336	-3.829622
C	3.022297	3.731518	-5.538394
H	0.491738	0.062513	-4.529525
H	-0.389906	0.371597	-3.060440
H	-4.198203	4.380674	-5.853097
H	-5.639308	4.128810	-4.936952
H	-2.445293	4.646261	-2.693361
H	-2.913659	4.097626	-4.275499
H	-2.248505	0.963904	-2.281506
H	-1.754652	2.595643	-2.639669
H	3.534240	0.901401	-2.782315
H	2.325258	0.000594	-3.654418
H	3.507287	-1.409762	-2.737527
H	3.574933	-2.574514	-1.468094
H	3.191198	-0.011265	1.532112
H	1.794853	-0.681663	2.397697
H	1.556184	0.597492	1.193897
H	2.669989	-3.470499	0.143145
H	2.442609	-2.902659	1.791889
H	3.866945	-2.384966	0.898206
H	-0.148373	-0.996503	-0.024427
H	0.170229	-2.261177	1.177455
H	0.407961	-2.603317	-0.544882
H	-6.648218	7.303311	-8.398453
H	-5.067991	7.483731	-9.185131
H	-5.235281	7.804352	-7.445441
H	-3.294121	6.192004	-7.041279
H	-3.263780	5.956389	-8.786115
H	-3.357046	4.550193	-7.731360
H	-5.414072	3.733238	-8.916888
H	-5.143770	5.068784	-10.050547
H	-6.743256	4.845385	-9.313866
H	-4.342943	7.705364	-2.872590
H	-1.241835	9.555389	-2.328097
H	-1.928852	8.633542	-0.989095
H	-2.992870	9.554412	-2.068878
H	-0.908778	6.017753	-3.520566
H	-0.904831	6.388774	-1.783387
H	-0.053028	7.434685	-2.918605
H	-1.288031	8.781067	-4.635076

H	-3.056365	8.916828	-4.598599
H	-2.289568	7.417433	-5.147489
H	-4.679373	5.995664	-1.094291
H	-3.744808	7.392040	-0.547489
H	-2.929827	5.862173	-0.860158
H	-5.740371	1.791324	-1.844063
H	-4.910769	0.174124	-3.546119
H	-5.619319	-0.607915	-2.131896
H	-3.870218	-0.595896	-2.336168
H	-5.717265	2.997010	0.304426
H	-3.988010	3.328087	0.113646
H	-4.573220	2.517623	1.571983
H	-5.566531	0.294777	1.502312
H	-5.431440	-0.774039	0.104232
H	-6.605977	0.555647	0.093601
H	-2.337770	1.385348	-0.067882
H	-2.915205	-0.284785	-0.262690
H	-3.073434	0.536324	1.289124
H	-2.166306	1.114304	-6.725730
H	0.024287	2.267901	-6.698823
H	-0.125259	1.139671	-8.046095
H	0.880637	0.717806	-6.663256
H	-0.410172	-1.880867	-4.975999
H	0.574391	-1.552974	-6.421003
H	-0.593865	-2.873762	-6.417517
H	-1.941349	-2.124577	-8.381628
H	-0.649073	-0.949421	-8.633490
H	-2.339349	-0.412920	-8.590834
H	-3.062060	-2.429618	-6.243003
H	-3.710771	-0.786503	-6.400534
H	-2.880219	-1.276306	-4.915130
H	1.869222	4.072296	-3.145746
H	4.929326	5.365505	-4.665791
H	4.944954	4.996966	-2.939642
H	3.526257	5.774618	-3.667593
H	2.570016	2.778605	-5.828270
H	3.761064	3.995981	-6.303407
H	2.237616	4.494693	-5.545065
H	4.508345	1.643590	-4.623221
H	5.354220	2.459822	-3.287920
H	5.611039	2.975096	-4.954539
H	2.344202	3.084817	-0.922127
H	3.505815	4.336077	-1.369461
H	3.980680	2.639595	-1.429876
O	5.913336	-1.763553	-1.737049
C	7.375881	-1.503923	-1.569111
C	8.005482	-2.686781	-2.305590
H	7.707205	-2.691863	-3.358239
H	9.095681	-2.612378	-2.255173
H	7.702005	-3.634122	-1.850188

C	7.730664	-1.531113	-0.080868
H	7.291013	-0.687887	0.454038
H	7.388283	-2.463887	0.378028
H	8.818802	-1.479769	0.025663
C	7.741755	-0.179782	-2.242580
H	7.415680	-0.177114	-3.287296
H	7.294224	0.671022	-1.726900
H	8.829866	-0.061705	-2.226583
C	-7.909953	4.835021	-5.274681
H	-7.754635	3.765608	-5.094185
H	-7.517947	5.381483	-4.414053
H	-8.981241	5.018329	-5.357328

Cartesian coordinates for Ac-tBu(+)-(stbe)$_4$-tBu(-)-*COOtBu* - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2892.596194 hartree

C	-5.135925	6.056012	-7.730337
N	-5.648452	5.345986	-6.677135
C	-7.135804	5.041692	-6.614993
C	-7.942920	6.356278	-6.575535
C	-4.768286	4.975726	-5.571677
C	-4.600602	6.087153	-4.509740
N	-3.777000	5.812729	-3.451534
C	-3.540805	6.878550	-2.433879
C	-3.836456	6.365514	-1.016588
C	-3.260858	4.466548	-3.225625
C	-4.309128	3.478824	-2.654797
N	-3.873629	2.210145	-2.384309
C	-4.831551	1.242626	-1.770378
C	-4.614391	1.062931	-0.223476
C	-3.230081	0.486258	0.136537
C	-2.587157	1.736269	-2.884510
C	-2.582613	1.473100	-4.412828
N	-1.460058	0.903436	-4.945898
C	-1.445108	0.595418	-6.408123
C	-1.678086	-0.927918	-6.720969
C	-3.015520	-1.384313	-6.103384
C	-0.223326	0.802821	-4.177665
C	0.503537	2.159252	-4.000226
N	1.789960	2.130883	-3.539564
C	2.502013	3.429808	-3.335207
C	3.044112	3.538938	-1.901530
C	2.411409	0.904371	-3.053770
C	1.880842	0.441117	-1.668835
N	2.543242	-0.583260	-1.049478
C	2.044435	-1.101694	0.295654
C	0.612027	-1.653192	0.145029
C	3.637990	-1.266370	-1.728864
C	3.197114	-2.418120	-2.642408
O	-5.833999	6.449854	-8.679411
O	-5.155856	7.180823	-4.663902
O	-5.460913	3.859896	-2.423405
O	-3.580861	1.751323	-5.086237
O	-0.086377	3.208682	-4.281465
O	0.894082	1.004721	-1.186716
O	2.044661	-2.624180	-2.976213
C	2.105315	0.037374	1.333490
C	2.940109	-2.245226	0.807760
C	-7.531898	4.179010	-7.831905
C	-7.477397	4.238586	-5.347119
C	-2.154967	7.606388	-2.596877
C	-2.029238	8.175129	-4.024956

C	-2.115195	8.792895	-1.606340
C	-0.937573	6.698522	-2.323353
C	-4.887609	-0.069301	-2.568290
C	-4.774684	2.423431	0.485507
C	-5.705260	0.110627	0.316652
C	-0.219745	1.217916	-7.093264
C	-0.556909	-1.845628	-6.192036
C	-1.775480	-1.099395	-8.254327
C	3.544524	3.756550	-4.467152
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C	4.101917	5.175943	-4.212099
C	2.836211	3.761007	-5.836958
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H	-0.414186	0.384786	-3.186933
H	-3.783201	4.717907	-5.963580
H	-5.131384	4.064347	-5.105440
H	-2.437051	4.532461	-2.515840
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H	-2.338277	0.811930	-2.365430
H	-1.794087	2.444681	-2.639424
H	3.480959	1.087523	-2.994463
H	2.284285	0.092081	-3.774965
H	4.351834	-1.653595	-1.005753
H	4.216413	-0.572606	-2.340854
H	3.128745	0.416930	1.423207
H	1.801153	-0.350504	2.311076
H	1.445361	0.862091	1.066572
H	2.960774	-3.106015	0.132935
H	2.520485	-2.590827	1.756268
H	3.965701	-1.920697	1.008382
H	-0.080056	-0.880858	-0.189639
H	0.268177	-2.030585	1.113669
H	0.595229	-2.479171	-0.571961
H	-7.366013	4.707886	-8.770059
H	-8.593089	3.917268	-7.760164
H	-6.953737	3.248517	-7.842688
H	-7.017694	3.245445	-5.345670
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H	-7.196843	4.755753	-4.426279
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H	-9.012465	6.123210	-6.531681
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H	-4.295643	7.631296	-2.668337
H	-1.235465	9.413889	-1.807855
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H	-3.002818	9.428834	-1.707505
H	-0.833727	5.908724	-3.073484
H	-0.980046	6.233391	-1.332516
H	-0.020438	7.297752	-2.359599
H	-1.081228	8.714667	-4.129888

H	-2.843313	8.871055	-4.251058
H	-2.041802	7.380287	-4.776937
H	-4.811402	5.874669	-0.996546
H	-3.862672	7.202147	-0.314989
H	-3.091090	5.654084	-0.647982
H	-5.802938	1.728570	-1.880116
H	-4.996497	0.145259	-3.633368
H	-5.753730	-0.656240	-2.255497
H	-4.002221	-0.698243	-2.432879
H	-5.766550	2.851203	0.307099
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H	-4.647062	2.298583	1.566728
H	-5.678461	0.099677	1.411832
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H	-2.422627	1.181082	-0.114507
H	-3.033230	-0.470273	-0.359707
H	-3.176629	0.306319	1.216252
H	-2.325621	1.112726	-6.793040
H	-0.128057	2.269002	-6.810861
H	-0.339356	1.175619	-8.177780
H	0.720584	0.713914	-6.849473
H	-0.530741	-1.869719	-5.098209
H	0.431746	-1.549353	-6.558716
H	-0.733492	-2.872575	-6.531263
H	-2.101785	-2.117767	-8.492242
H	-0.814109	-0.938952	-8.751459
H	-2.504970	-0.405862	-8.689452
H	-3.198478	-2.437326	-6.345183
H	-3.854085	-0.795757	-6.489283
H	-3.008272	-1.290077	-5.013636
H	1.713870	4.176968	-3.439449
H	4.701178	5.497747	-5.070802
H	4.746853	5.215617	-3.329147
H	3.293491	5.904464	-4.078189
H	2.414406	2.780365	-6.075146
H	3.551871	4.016459	-6.626472
H	2.024503	4.495116	-5.864034
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H	5.250454	2.676617	-3.573949
H	5.460856	3.126393	-5.265396
H	2.256883	3.290809	-1.186036
H	3.364505	4.563703	-1.703051
H	3.901306	2.886620	-1.707656
O	4.270739	-3.117637	-3.015259
C	4.204865	-4.287100	-3.944008
C	5.671842	-4.704382	-4.051008
H	6.070193	-4.978340	-3.069551
H	5.759692	-5.570052	-4.713978
H	6.278062	-3.891259	-4.461314

C	3.661962	-3.834478	-5.301056
H	2.614746	-3.535588	-5.237186
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H	3.742282	-4.663967	-6.010721
C	3.363636	-5.395299	-3.306753
H	3.746345	-5.643031	-2.311717
H	2.314440	-5.107697	-3.223876
H	3.429216	-6.293681	-3.928650
C	-3.640754	6.350836	-7.750674
H	-3.305380	6.878550	-6.854497
H	-3.051162	5.432260	-7.843827
H	-3.445621	6.976026	-8.621833

Cartesian coordinates for Ac-tBu(+)-(stbe)$_4$-tBu(+)-*COOtBu* - B3LYP/6-31+G(d,p), acetonitrile.
Energy = -2892.596262 hartree

C	-5.095563	5.963270	-7.819648
N	-5.625557	5.286607	-6.753430
C	-7.110305	4.966086	-6.716355
C	-7.933043	6.271000	-6.755763
C	-4.763506	4.948013	-5.623963
C	-4.619930	6.084171	-4.584790
N	-3.801280	5.842951	-3.514239
C	-3.591717	6.931081	-2.514168
C	-3.888472	6.438815	-1.089723
C	-3.272079	4.507632	-3.255794
C	-4.314722	3.521331	-2.671928
N	-3.868776	2.264546	-2.365087
C	-4.824397	1.301462	-1.740764
C	-4.621696	1.154243	-0.188313
C	-3.239808	0.588596	0.198359
C	-2.571919	1.791269	-2.838043
C	-2.547189	1.484131	-4.357278
N	-1.423692	0.887687	-4.857844
C	-1.385335	0.550957	-6.312872
C	-1.618149	-0.977164	-6.604429
C	-2.956553	-1.424163	-5.982318
C	-0.205450	0.766364	-4.064055
C	0.556860	2.102958	-3.884079
N	1.837373	2.039140	-3.410224
C	2.582003	3.318111	-3.194254
C	3.127964	3.398471	-1.760421
C	2.416785	0.790339	-2.928560
C	1.859936	0.336477	-1.550007
N	2.463514	-0.733352	-0.950277
C	2.020085	-1.174940	0.440284
C	0.555502	-1.652450	0.382895
C	3.551209	-1.435374	-1.621605
C	4.953773	-0.899765	-1.302981
O	-5.774442	6.311547	-8.800016
O	-5.189611	7.166232	-4.765427
O	-5.473236	3.894941	-2.463387
O	-3.529591	1.759760	-5.054844
O	-0.001278	3.167415	-4.173274
O	0.900669	0.940447	-1.061272
O	5.173265	0.167616	-0.760267
C	2.197026	-0.007782	1.433309
C	2.881829	-2.348869	0.942961
C	-7.463583	4.045679	-7.903909
C	-7.477322	4.216777	-5.422941
C	-2.217221	7.679325	-2.680330
C	-2.097351	8.237744	-4.112900

C	-2.196909	8.874264	-1.699577
C	-0.987402	6.791269	-2.398248
C	-4.862254	-0.025685	-2.513916
C	-4.793670	2.528349	0.490792
C	-5.715323	0.209603	0.359895
C	-0.147017	1.159368	-6.987115
C	-0.498668	-1.892350	-6.065506
C	-1.714048	-1.167352	-8.135847
C	3.631957	3.626915	-4.323798
C	4.782376	2.601764	-4.401437
C	4.235625	5.024156	-4.052327
C	2.923555	3.670833	-5.692851
H	0.437003	0.036536	-4.550774
H	-0.425506	0.362482	-3.073239
H	-3.771109	4.684385	-5.992564
H	-5.131440	4.046919	-5.141677
H	-2.453109	4.597217	-2.542918
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H	-2.316238	0.888585	-2.285712
H	-1.788913	2.517067	-2.611561
H	3.492635	0.927633	-2.852831
H	2.264054	-0.003689	-3.665059
H	3.428721	-1.399631	-2.705507
H	3.523425	-2.495447	-1.378246
H	3.247976	0.292743	1.482143
H	1.886590	-0.335246	2.430849
H	1.595018	0.855221	1.150845
H	2.741955	-3.261670	0.356932
H	2.565669	-2.573478	1.965053
H	3.947537	-2.105573	0.981694
H	-0.117348	-0.847777	0.087485
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H	0.452226	-2.481002	-0.326151
H	-7.273794	4.533435	-8.859790
H	-8.524379	3.777643	-7.851937
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H	-4.357850	7.666162	-2.767661
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H	-0.872794	5.998189	-3.143275
H	-1.024329	6.332334	-1.404308
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H	-2.920916	8.919966	-4.346225
H	-2.097489	7.436339	-4.857880
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H	-5.798681	1.776839	-1.869355
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H	-4.674731	2.426163	1.575337
H	-5.701002	0.222475	1.455286
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H	-6.714777	0.523563	0.035768
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H	-3.199064	0.427425	1.281594
H	-2.258150	1.062875	-6.721370
H	-0.065820	2.218346	-6.731822
H	-0.240008	1.086099	-8.072587
H	0.789057	0.667044	-6.706265
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H	0.491937	-1.597541	-6.428278
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H	-2.040695	-2.188344	-8.361683
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H	1.812870	4.086031	-3.291500
H	4.840923	5.338173	-4.909728
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H	3.959561	2.713466	-1.570737
O	5.864151	-1.773036	-1.738924
C	7.337573	-1.542707	-1.635751
C	7.911996	-2.813261	-2.263221
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H	9.004807	-2.767485	-2.250131
H	7.596005	-3.699094	-1.704160

C	7.735981	-1.429601	-0.162618
H	7.341316	-0.520403	0.293276
H	7.376886	-2.297117	0.399772
H	8.828026	-1.407509	-0.091103
C	7.720175	-0.305497	-2.450405
H	7.364527	-0.399043	-3.481205
H	7.311751	0.606882	-2.013288
H	8.811136	-0.219318	-2.474600
C	-3.604773	6.279459	-7.813076
H	-3.297376	6.833213	-6.922701
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