Supporting Information Section.

Variable Scan Rate Cyclic Voltammetry and Theoretical Studies on Tocopherol (Vitamin E) Model Compounds.

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CONTENTS

(1) (CH_3)α-TO^+ (closed structure) **(**B3LYP/6-31G*)

Total energy = -695.14662
No. of imaginary frequencies = 0

Cartesian Coordinates

O	3.748269	-1.394560	0.090844
C	2.657942	-0.852488	0.030184
C	0.150176	0.358867	-0.049787
C	1.410651	-1.698702	-0.014148
C	2.555418	0.646834	-0.003214
C	1.323804	1.226453	-0.041488
C	0.192982	-1.092120	-0.070466
C	1.592836	-3.182562	-0.009237
C	3.844228	1.411379	0.025712
C	1.089782	2.714221	-0.055043
C	-1.109128	-1.856201	-0.139364
H	3.898155	2.053088	0.913537
H	3.931466	2.064585	-0.850440
H	4.694288	0.729326	0.039646
H	2.624457	-3.443580	0.227434
H	1.358415	-3.598157	-0.999855
H	0.919017	-3.664423	0.707437
H	2.031505	3.262628	-0.067551
H	0.521178	3.029021	0.827265
H	0.505707	3.012877	-0.932460
H	-1.369725	-2.227035	0.861052
H	-0.977999	-2.745238	-0.764052
C	-2.240298	-0.991201	-0.705539
C	-2.345538	0.358918	-0.003932
H	-3.198670	-1.510959	-0.607383
H	-2.079199	-0.821363	-1.776995
C	-2.717750	0.282233	1.475749
C	-3.217944	1.350845	-0.762160
O	-0.969804	1.005194	-0.036670
H	-3.200907	2.334200	-0.284130
H	-4.250928	0.988621	-0.762988
H	-2.891164	1.454575	-1.801097
H	-2.047350	-0.370909	2.041803
H	-3.735276	-0.111153	1.567357
H	-2.698595	1.276786	1.929977

(2) (CH_3)α-TO^+ (open structure) **(**B3LYP/6-31G*)

Total energy = -695.09745
No. of imaginary frequencies = 0

Cartesian Coordinates

O	3.209022	-2.365839	-0.239005
C	2.480162	-1.399870	-0.067639
C	0.737559	0.820093	0.262094
C	0.997880	-1.638729	0.100527
C	3.029297	-0.012181	-0.026695
C	2.197036	1.047729	0.137223
C	0.192307	-0.569395	0.289129
C	0.582159	-3.078316	0.050480
C	4.516532	0.131653	-0.176380
C	2.683014	2.470547	0.184968
C	-1.290340	-0.637712	0.549182
H	4.967076	0.485252	0.760450
H	4.765511	0.869116	-0.947803
H	4.972582	-0.824720	-0.434122
H	0.941059	-3.540239	-0.875211
H	-0.498228	-3.215897	0.117630
H	1.058152	-3.636099	0.865484
H	3.196118	2.741140	-0.746290
H	3.406157	2.608359	0.997563
H	1.852536	3.161201	0.334879
H	-1.528397	0.080539	1.337863
H	-1.619965	-1.622763	0.877587
C	-2.105813	-0.270121	-0.806265
C	-3.272845	0.434120	-0.298828
H	-2.351820	-1.207372	-1.311159
H	-1.477740	0.363938	-1.430913
C	-3.230004	1.898136	-0.201722
C	-4.450456	-0.308002	0.181190
O	-0.053398	1.766260	0.336040
H	-5.277180	-0.061452	-0.510703
H	-4.788280	0.062681	1.158281
H	-4.322169	-1.391677	0.191585
H	-4.064167	2.338752	0.345701
H	-3.199822	2.307141	-1.226311
H	-2.253535	2.193728	0.221188

(3) (CH_3)β-TO^+ (closed structure) **(**B3LYP/6-31G*)

Total energy = -655.82339
No. of imaginary frequencies = 0

Cartesian Coordinates

O	4.295728	0.582041	0.100966
C	3.077578	0.612960	0.044181
C	0.280413	0.691903	-0.042916
C	2.281203	-0.669042	-0.009399
C	2.356877	1.903650	0.019518
C	1.009928	1.969940	-0.024858
C	0.917669	-0.608337	-0.075527
C	3.048912	-1.949264	0.000468
C	0.230977	3.254727	-0.039823
C	0.042311	-1.838660	-0.163221
H	4.106318	-1.761056	0.188329
H	2.958800	-2.459163	-0.969540
H	2.659794	-2.639353	0.758118
H	0.910832	4.109025	-0.024255
H	-0.435424	3.323338	0.827070
H	-0.397748	3.325358	-0.934359
H	-0.036898	-2.304255	0.828019
H	0.523484	-2.581368	-0.806971
C	-1.346523	-1.502726	-0.720034
C	-1.996068	-0.324102	-0.002178
H	-2.008490	-2.369552	-0.630996
H	-1.271173	-1.269152	-1.788869
C	-2.298789	-0.562870	1.475718
C	-3.197064	0.235184	-0.753130
O	-1.001200	0.830762	-0.022788
H	-3.591509	1.127763	-0.259375
H	-3.987786	-0.521746	-0.772380
H	-2.939290	0.485136	-1.786510
H	-1.422001	-0.906489	2.032326
H	-3.076204	-1.329144	1.559162
H	-2.672738	0.350731	1.946023
H	2.978081	2.793764	0.047230

(4) (CH_3)β-TO^+ (open structure) **(**B3LYP/6-31G*)

Total energy = -655.77695
No. of imaginary frequencies = 0

Cartesian Coordinates

O	3.760723	-2.249171	-0.291782
C	2.995044	-1.312597	-0.122217
C	1.200979	0.877354	0.212186
C	1.517087	-1.582268	0.056183
C	3.482070	0.080196	-0.088617
C	2.660325	1.135980	0.071481
C	0.691212	-0.525830	0.249129
C	1.132251	-3.029684	0.015398
C	3.111831	2.565382	0.103353
C	-0.786200	-0.625486	0.531903
H	1.507374	-3.489482	-0.905158
H	0.055127	-3.193174	0.078528
H	1.618545	-3.570393	0.836117
H	2.628144	3.143728	-0.691959
H	4.194970	2.634768	-0.017173
H	2.828922	3.040932	1.049393
H	-1.026284	0.088718	1.323996
H	-1.090011	-1.616996	0.865687
C	-1.632898	-0.274750	-0.809297
C	-2.819013	0.374852	-0.275494
H	-1.846902	-1.215369	-1.322354
H	-1.038210	0.392422	-1.432400
C	-2.839131	1.839406	-0.165185
C	-3.957215	-0.417763	0.218835
O	0.402226	1.813697	0.287855
H	-4.828473	-0.153369	-0.407026
H	-4.243428	-0.102451	1.231885
H	-3.806113	-1.497354	0.171941
H	-3.660129	2.233130	0.436053
H	-2.911123	2.246021	-1.189786
H	-1.856870	2.192233	0.190232
H	4.555170	0.197318	-0.211707

(5) (CH_3)γ-TO^+ (closed structure) **(**B3LYP/6-31G*)

Total energy = -655.82150
No. of imaginary frequencies = 0

Cartesian Coordinates

O	3.580218	-2.346917	-0.017455
C	2.597092	-1.624637	-0.020905
C	0.305136	-0.023087	-0.009202
C	1.243340	-2.229612	-0.048339
C	2.730503	-0.124152	0.000539
C	1.599042	0.642737	0.001857
C	0.124826	-1.477178	-0.032874
C	1.604860	2.149753	0.012342
C	-1.277158	-2.033405	-0.041157
H	2.622282	2.537933	-0.003368
H	1.100069	2.539015	0.903436
H	1.070999	2.549986	-0.856780
H	-1.580563	-2.266343	0.987543
H	-1.290210	-2.981506	-0.586956
C	-2.252775	-1.035963	-0.675047
C	-2.173904	0.343894	-0.024510
H	-3.280792	-1.400084	-0.583906
H	-2.044204	-0.939772	-1.747605
C	-2.618316	0.388861	1.435623
C	-2.838822	1.428368	-0.861882
O	-0.707241	0.775214	-0.001606
H	-2.707751	2.413652	-0.405987
H	-3.911886	1.220078	-0.923727
H	-2.436054	1.449083	-1.878841
H	-2.091112	-0.340983	2.057120
H	-3.689734	0.169164	1.485880
H	-2.456235	1.385305	1.855280
C	4.122507	0.425039	0.013503
H	1.211835	-3.315422	-0.075262
H	4.850798	-0.385494	0.050064
H	4.279359	1.081475	0.877550
H	4.313891	1.024996	-0.885328

(6) (CH_3)γ-TO^+ (open structure) **(**B3LYP/6-31G*)

Total energy = -655.77530
No. of imaginary frequencies = 0

Cartesian Coordinates

O	3.166062	-2.807926	-0.156179
C	2.478224	-1.807580	-0.017272
C	0.791895	0.484736	0.262547
C	1.004558	-1.961774	0.142242
C	3.064591	-0.431886	-0.007688
C	2.259021	0.655840	0.128350
C	0.208857	-0.891425	0.285884
C	4.554230	-0.329678	-0.161431
C	2.790088	2.063567	0.139550
C	-1.276695	-0.978906	0.513162
H	4.999457	0.195450	0.692774
H	4.817765	0.243670	-1.059291
H	5.001712	-1.321495	-0.237547
H	3.286344	2.303052	-0.809152
H	3.537637	2.192969	0.930995
H	1.985331	2.781903	0.299192
H	-1.534760	-0.328563	1.354879
H	-1.587910	-1.995176	0.761853
C	-2.075739	-0.526580	-0.818780
C	-3.226428	0.191162	-0.283640
H	-2.352038	-1.430421	-1.367037
H	-1.432060	0.116156	-1.418539
C	-3.144225	1.646783	-0.128257
C	-4.426354	-0.539092	0.154110
O	0.027775	1.450606	0.348829
H	-5.222915	-0.274498	-0.567264
H	-4.795124	-0.173624	1.121016
H	-4.314750	-1.624784	0.152683
H	-3.966765	2.089018	0.435255
H	-3.098023	2.095132	-1.136385
H	-2.158680	1.898972	0.303482
H	0.638922	-2.985607	0.141661

(7) (CH_3)δ-TO^+ (closed structure) **(**B3LYP/6-31G*)

Total energy = -616.49696
No. of imaginary frequencies = 0

Cartesian Coordinates

O	4.331237	-1.719893	-0.049348
C	3.251436	-1.150818	-0.034203
C	0.757116	0.140407	-0.009911
C	1.984376	-1.927400	-0.044233
C	3.157167	0.328114	-0.004888
C	1.966628	0.971199	0.006527
C	0.775353	-1.321830	-0.021739
C	1.819109	2.467050	0.031197
C	-0.544266	-2.054028	-0.011116
H	2.800872	2.943911	0.050637
H	1.256406	2.794142	0.912322
H	1.274856	2.824922	-0.849544
H	-0.811772	-2.300643	1.024152
H	-0.437687	-3.006990	-0.537642
C	-1.642064	-1.203539	-0.660814
C	-1.748858	0.184739	-0.033845
H	-2.612729	-1.700179	-0.563563
H	-1.446086	-1.098366	-1.734640
C	-2.194237	0.197998	1.426233
C	-2.543360	1.162158	-0.888823
O	-0.343015	0.803791	-0.015041
H	-2.526181	2.166911	-0.457866
H	-3.584515	0.826285	-0.931110
H	-2.156873	1.204692	-1.911211
H	-1.580219	-0.449588	2.058768
H	-3.229532	-0.153940	1.480958
H	-2.160975	1.213269	1.830516
H	2.087460	-3.008970	-0.067118
H	4.100354	0.866597	0.005346

(8) (CH_3)δ-TO^+ (open structure) **(**B3LYP/6-31G*)

Total energy = -616.45424
No. of imaginary frequencies = 0

Cartesian Coordinates

O	3.622434	-2.943056	-0.245129
C	2.952235	-1.933319	-0.093548
C	1.342189	0.419808	0.218595
C	1.474428	-2.038451	0.090922
C	3.551947	-0.581383	-0.089286
C	2.818318	0.541978	0.059111
C	0.718335	-0.938745	0.248421
C	3.388869	1.929240	0.067158
C	-0.765782	-0.975783	0.502088
H	2.956740	2.531839	-0.739751
H	4.474338	1.906883	-0.051356
H	3.145310	2.443500	1.003569
H	-0.986432	-0.318282	1.349141
H	-1.106608	-1.981441	0.755535
C	-1.571652	-0.493511	-0.814308
C	-2.701879	0.241753	-0.259186
H	-1.871555	-1.385511	-1.369553
H	-0.922284	0.143728	-1.414133
C	-2.586251	1.693919	-0.087241
C	-3.914829	-0.467392	0.176047
O	0.625789	1.417342	0.318946
H	-4.706935	-0.181303	-0.542626
H	-4.275507	-0.102931	1.146322
H	-3.825266	-1.555128	0.164131
H	-3.385758	2.144522	0.502068
H	-2.564363	2.151092	-1.092522
H	-1.586273	1.926731	0.318842
H	1.070172	-3.047798	0.097044
H	4.630269	-0.548301	-0.219302

(9) $(CH_3)H_3$-TO^+ (closed structure) **(**B3LYP/6-31G*)

Total energy = -577.17351
No. of imaginary frequencies = 0

Cartesian Coordinates

O	4.725649	-0.432325	-0.046483
C	3.554917	-0.092735	-0.025891
C	0.839291	0.660757	0.010235
C	2.464530	-1.105499	-0.051608
C	3.164952	1.342824	0.024828
C	1.863914	1.691860	0.041140
C	1.154708	-0.765856	-0.024545
C	0.009902	-1.748009	-0.028703
H	-0.200595	-2.060283	1.002211
H	0.301880	-2.651690	-0.571614
C	-1.236648	-1.121287	-0.666225
C	-1.621719	0.213265	-0.026953
H	-2.090231	-1.799266	-0.568815
H	-1.071096	-0.970409	-1.739855
C	-2.072562	0.121813	1.428323
C	-2.584227	1.024202	-0.882900
O	-0.365444	1.101023	0.014136
H	-2.792381	1.996354	-0.427968
H	-3.528038	0.475545	-0.966488
H	-2.189318	1.178620	-1.891222
H	-1.348979	-0.401859	2.059600
H	-3.019443	-0.426256	1.467177
H	-2.239953	1.118822	1.844428
H	2.787016	-2.142857	-0.090394
H	3.969972	2.071066	0.044256
H	1.523903	2.722181	0.073328

(10) $(CH_3)H_3$-TO^+ (open structure) **(**B3LYP/6-31G*)

Total energy = -577.13076
No. of imaginary frequencies = 0

Cartesian Coordinates

O	4.496379	-1.800047	-0.256900
C	3.637051	-0.950282	-0.090677
C	1.577028	1.032306	0.248545
C	2.206030	-1.344860	0.072118
C	3.958793	0.499229	-0.044445
C	2.994880	1.422158	0.116535
C	1.239828	-0.425011	0.244122
C	-0.207260	-0.768303	0.482061
H	-0.555410	-0.198440	1.349605
H	-0.340075	-1.829798	0.698720
C	-1.091088	-0.411540	-0.822486
C	-2.348074	0.063129	-0.253441
H	-1.205907	-1.325412	-1.410792
H	-0.583872	0.364725	-1.394734
C	-2.536521	1.504518	-0.058840
C	-3.385621	-0.890145	0.169158
O	0.681348	1.871188	0.349522
H	-4.229529	-0.754673	-0.534394
H	-3.799393	-0.630367	1.151705
H	-3.074900	-1.935685	0.128216
H	-3.389993	1.769087	0.566830
H	-2.666726	1.954170	-1.060561
H	-1.594731	1.950647	0.302764
H	2.010772	-2.414306	0.053951
H	5.007332	0.759626	-0.154368
H	3.199659	2.488084	0.147784