Electronic Supplementary Information

Autocatalytic Cycle in Autoxidation of Triethylborane

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1. Kinetic simulation

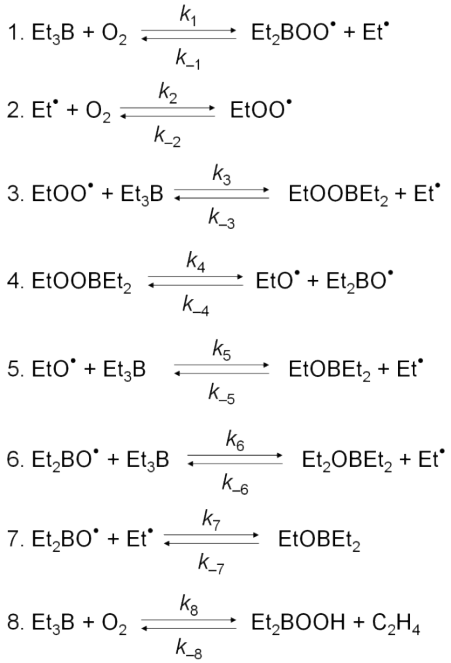

Fig. S1 Eight reaction steps considered in the kinetic simulations.

Rate equations for the 12 chemical species in Fig. S1 are described as bellow.

$$\frac{d[Et_3B]}{dt} = -(k_1[Et_3B][O_2] + k_3[Et_3B][EtOO] + k_5[Et_3B][EtO] + k_6[Et_3B][Et_2BO]) + k_{-1}[Et_2BOO][Et] + k_{-3}[Et][EtOOBEt_2] + k_{-5}[Et][EtOBEt_2] + k_{-6}[Et][Et_2BOBEt_2] \quad \text{(eq.1)}$$

$$\frac{d[O_2]}{dt} = -(k_1[Et_3B][O_2] + k_2[O_2][Et]) + k_{-1}[Et_2BOO][Et] + k_{-2}[EtOO] \quad \text{(eq.2)}$$

$$\frac{d[Et_2BOO]}{dt} = -k_{-1}[Et_2BOO][Et] + k_1[Et_3B][O_2] \quad \text{(eq.3)}$$

$$\frac{d[Et]}{dt} = -(k_{-1}[Et_2BOO][Et] + k_2[O_2][Et] + k_{-3}[Et][EtOOBEt_2] + k_{-5}[Et][EtOBEt_2] + k_{-6}[Et][Et_2BOBEt_2] + k_7[Et][Et_2BO]) + k_1[Et_3B][O_2] + k_{-2}[EtOO] + k_3[Et_3B][EtOO] + k_5[Et_3B][EtO] + k_6[Et_3B][Et_2BO] + k_{-7}[EtOBEt_2] \quad \text{(eq.4)}$$

$$\frac{d[EtOO]}{dt} = -(k_{-2}[EtOO] + k_3[Et_3B][EtOO]) + k_2[O_2][Et] + k_{-3}[Et][EtOOBEt_2] \quad \text{(eq.5)}$$

$$\frac{d[EtOOBEt_2]}{dt} = -(k_{-3}[Et][EtOOBEt_2] + k_4[EtOOBEt_2]) + k_3[Et_3B][EtOO] + k_{-4}[Et_2BO][EtO] \quad \text{(eq.6)}$$

$$\frac{d[Et_2BO]}{dt} = -(k_{-4}[Et_2BO][EtO] + k_6[Et_3B][Et_2BO] + k_7[Et][Et_2BO]) + k_4[EtOOBEt_2] + k_{-6}[Et][Et_2BOBEt_2] + k_{-7}[EtOBEt_2] \quad \text{(eq.7)}$$

$$\frac{d[EtO]}{dt} = -(k_{-4}[Et_2BO][EtO] + k_5[Et_3B][EtO]) + k_4[EtOOBEt_2] + k_{-5}[Et][EtOBEt_2] \quad \text{(eq.8)}$$

$$\frac{d[EtOBEt_2]}{dt} = -(k_{-5}[Et][EtOBEt_2] + k_{-7}[EtOBEt_2]) + k_5[Et_3B][EtO] + k_7[Et][Et_2BO] \quad \text{(eq.9)}$$

$$\frac{d[Et_2BOBEt_2]}{dt} = -k_{-6}[Et][Et_2BOBEt_2] + k_6[Et_3B][Et_2BO] \quad \text{(eq.10)}$$

$$\frac{d[Et_2BOOH]}{dt} = -k_{-8}[Et_2BOOH][C_2H_4] + k_8[Et_3B][O_2] \quad \text{(eq.11)}$$

$$\frac{d[C_2H_4]}{dt} = -k_{-8}[Et_2BOOH][C_2H_4] + k_8[Et_3B][O_2] \quad \text{(eq.12)}$$

The rate constants were estimated by the standard transition state theory using the free-energy difference between the transition state and the reactant, where the transmission coefficient was set to unity.

Table S1 Rate constants (k) at 25 °C and 1 atm of both forward and backward reactions for all the considered elementary steps

Step	k_i (forward)	k_{-i} (backward)
1	9.66×10^{-10}	5.51×10^{5}
2	3.66×10^{9}	3.33×10^{-8}
3	7.37×10^{7}	1.82×10^{-6}
4	6.25×10^{-4}	4.88×10^{4}
5	2.75×10^{6}	2.70×10^{-19}
6	4.41×10^{7}	3.11×10^{-15}
7	5.44×10^{8}	2.52×10^{-35}
8	7.30×10^{-9}	2.45×10^{-31}

Rate constants (k_1 and k_{-1}) for the initial S_H2 reaction (step1) were obtained as the sum of rate constants of the three elementary steps in Fig. 1.

$$k_1 = k_1^{MESX2} + k_1^{TS1} + k_1^{TS2} = 8.56\times10^{-10} + 8.55\times10^{-11} + 2.37\times10^{-11}$$

$$k_{-1} = k_{-1}^{MESX2} + k_{-1}^{TS1} + k_{-1}^{TS2} = 4.89\times10^{5} + 4.88\times10^{4} + 1.36\times10^{4}$$

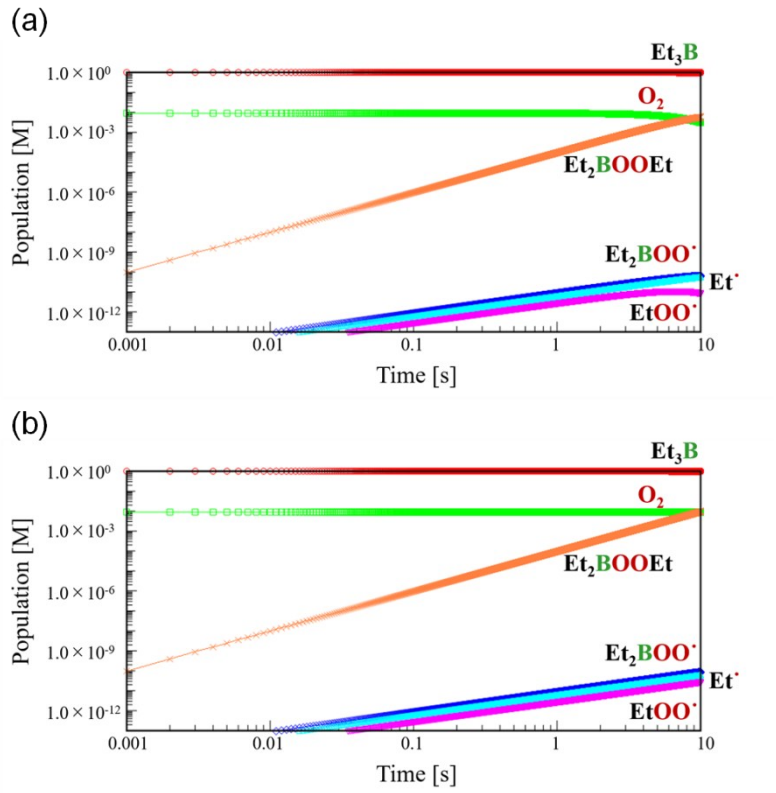

Fig. S2 Time evolution of concentration of reactants, intermediates, and radicals, involved in the autoxidation of Et_3B, (a) in the normal simulation and (b) in the simulation in which concentration of O_2 is kept fixed. In these simulations, the rate constant of the homolytic decomposition of $(EtOO)BEt_2$ was set to zero.

2. Cartesian coordinates

Geometry of EQ1 (Et_3B)

B	-0.000538514814	0.000086570281	0.002223337150
C	-1.471540180625	-0.581068068307	0.005503090204
H	-1.548298427806	-1.275279414941	-0.848360483669
H	-1.548060221296	-1.254817660455	0.876040878335
C	-2.657445914239	0.395863774898	-0.005207544049
H	-2.639975235336	1.036427162019	-0.894538999437
H	-3.619867819836	-0.128325266103	0.002126887599
H	-2.638205424992	1.058469112460	0.867753019341
C	0.232612735015	1.564663271643	0.002952272295
H	-0.317343567402	1.972202820213	0.868250939352
H	-0.324789911541	1.974834018334	-0.856218558800
C	1.671935432036	2.102158378585	-0.002924668771
H	1.700122737934	3.197729510695	-0.000359928301
H	2.231894613844	1.757821899893	0.874262721520
H	2.221922832162	1.762293447507	-0.888028776953
C	1.238443916618	-0.983002414719	0.001646759916
H	1.871833851330	-0.704548509779	-0.857525189239
H	1.866218034121	-0.709708007844	0.866823690233
C	0.986220562763	-2.498660187244	-0.003579805049
H	0.409082793050	-2.811664725179	0.874087810009
H	0.416888142697	-2.806352617444	-0.888211553771
H	1.921762734556	-3.069488721897	-0.001221055264

Geometry of EQ2 ($^3O_2$)

O	0.000000000000	0.000000000000	0.606267000000
O	0.000000000000	0.000000000000	-0.606267000000

Geometry of EQ3 ($Et_2BOO^{\cdot}$)

B	0.107406794867	-0.207998989332	0.275514341647
C	-1.251841661989	-0.903250056693	0.625159135850
H	-1.061856799443	-1.868488767730	1.110462192710
H	-1.824897983477	-0.285367044575	1.326816240294
C	-2.108598252871	-1.128238336299	-0.648246252217
H	-1.578953451130	-1.738818338522	-1.388905856980
H	-3.041777444093	-1.646099318762	-0.403442800825
H	-2.366359082016	-0.174187725538	-1.117742716112
C	1.495171304935	-0.933199924561	0.194335515476
H	1.344905636356	-1.846586313288	-0.403767737039
H	1.693040289579	-1.321871571858	1.207879590045
C	2.706090497587	-0.138713603460	-0.320660487364
H	3.615590803642	-0.748562754837	-0.316998685550
H	2.541854373012	0.212963559366	-1.344433628351
H	2.890721511861	0.746310050934	0.296265198888
O	-1.007912613811	1.841675044142	0.034170175112
O	0.163774579880	1.176115634423	-0.046569004375

Geometry of EQ4 ($Et^{\cdot}$)

C	-1.220083311286	-2.211666049697	-0.881734634088
H	-0.944468844007	-1.940215983805	-1.895838025634
H	-0.440203740817	-2.603161565047	-0.236311110751
C	-2.647672227835	-2.221137820983	-0.451705657648
H	-2.748354293526	-2.075344156498	0.630269542883
H	-3.230914505121	-1.442795562830	-0.957700635879
H	-3.140812175408	-3.181510516141	-0.684404887883

Geometry of EQ5 ($EtOO^{\cdot}$)

C	-1.740399976652	-2.835505309156	0.391038637546
H	-1.420952003017	-3.192892397184	-0.592010203454
H	-1.686688343461	-3.649071771575	1.119899109019
C	-3.105814464374	-2.172123819679	0.357146616050
H	-3.352814227313	-1.772509638953	1.344177621122
H	-3.124950101708	-1.356561988689	-0.371820290630
H	-3.866692066949	-2.907964132812	0.076650873834
O	-0.700936719300	-1.866958418996	0.751753948202
O	-0.767600047223	-1.540598721956	2.032583274311

Geometry of EQ6 (Et_2BOOEt)

B	0.993855152784	-0.027605652472	0.262976201306
C	1.414436147677	1.420648387792	0.721343669730
H	0.658637892158	1.828857296961	1.404133162816
H	2.363648821287	1.380456440324	1.270679472847
C	1.560748238197	2.375966309250	-0.488486111215
H	0.613208468149	2.466334466651	-1.027841897853
H	1.865360355963	3.378586447921	-0.167900993625
H	2.317618469804	2.014438838844	-1.194999316012
C	1.999569556694	-1.247132654458	0.191054168465
H	2.870555276139	-0.906057722427	-0.391414077476
H	2.398028795293	-1.384636769039	1.209242781379
C	1.476201191979	-2.581718766914	-0.361095754860
H	0.637148955476	-2.953517859165	0.236554012173
H	1.112253422390	-2.468160095739	-1.387775435902
H	2.254796285876	-3.352697305015	-0.363504422939
O	-1.205604248518	0.797680532649	-0.084642862910
O	-0.274079772494	-0.339699327600	-0.149555060843
C	-2.470286327307	0.277220702003	-0.494020058297
H	-3.072730487916	1.187381827150	-0.601256475857
H	-2.365945840482	-0.188500377743	-1.482805779392

C	-3.082818981783	-0.681884008306	0.518046910112
H	-4.075728471027	-1.000030148761	0.180713927321
H	-2.455958496746	-1.569989933749	0.632112552714
H	-3.184479175980	-0.197306015212	1.494224571776

Geometry of EQ7 (Et_2BO^-)

B	-0.003441458613	-0.465250360012	0.055808620972
C	-1.586352919274	-0.310404581793	0.425083514859
H	-2.097131717885	-1.254902460200	0.219379521229
H	-1.600017236993	-0.158710537792	1.513655374260
C	-2.267191278721	0.860482097296	-0.294582472107
H	-3.320661730620	0.930759493481	0.002136560395
H	-1.792474642118	1.817991914890	-0.057787731417
H	-2.241649320987	0.732719143021	-1.382338718959
C	0.918547358541	0.864414553858	0.051915731594
H	0.587987115048	1.431782219045	-0.830167430946
H	0.621056776741	1.461735027156	0.924290403309
C	2.431907623205	0.631887415390	0.020002451626
H	2.724393281021	0.057893417730	-0.864187513254
H	2.974240346520	1.584547695359	0.003378587172
H	2.765841657764	0.071170742152	0.898701944241
O	0.466658338490	-1.635625433329	-0.217184505734

Geometry of EQ8 (EtO^-)

C	1.270792798873	-0.221314998565	0.000003903861
H	1.362027916079	-0.848859913232	-0.891979207208
H	1.353245406193	-0.864943851041	0.881182893920
H	2.103119864298	0.491843248975	0.009471485879
C	-0.069863671452	0.510363108074	-0.000601228821
H	-0.168532600745	1.183969767811	0.877593968073
H	-0.160797812032	1.207881752754	-0.859274878793
O	-1.183834975890	-0.290568775424	-0.000622656840

Geometry of EQ9 ($EtOBEt_2$)

B	0.397825625154	-0.007109281003	-0.143388677588
C	0.519729137923	-1.594713455247	-0.208139687296
H	-0.276074294645	-2.050904604352	0.399767599109
H	0.285873620497	-1.905233464428	-1.240332039836
C	1.877712755924	-2.191233445721	0.200440653046
H	2.125454095183	-1.942746097259	1.238689219787
H	1.884853610884	-3.283513037863	0.112924489579
H	2.689842032945	-1.805471322334	-0.425438280725
C	1.645602533365	0.927250861191	0.130881574204
H	2.421941779954	0.681274571941	-0.611773866033
H	2.095780200312	0.613467241410	1.086635906308
C	1.379362260366	2.439546313666	0.140646020781
H	2.291155576915	3.014099502839	0.340835897701
H	0.973329925387	2.773321661505	-0.820130759272
H	0.639317221514	2.702494688480	0.903902454319
C	-2.814071914192	-0.194802703936	0.734924201913
H	-3.798775517351	-0.636825125540	0.545948752855
H	-2.269496816670	-0.848363535087	1.424315342481
H	-2.954558252348	0.775610572265	1.220784245818
C	-2.047304589318	-0.025723365270	-0.570873642645
H	-1.897261524427	-0.993660983977	-1.063812531763
H	-2.605284630437	0.616536768109	-1.260706852114
O	-0.795928650034	0.629088046864	-0.338985128028

Geometry of EQ10 (Et_2BOBEt_2)

B	-1.140260781911	-0.056470964484	0.048790796728
B	1.510754328594	0.068664485676	0.342592151257
C	-2.196221593858	-0.040690672609	1.229829169188
H	-2.117113155993	0.952856361751	1.702082788059
H	-1.862095854374	-0.741083588417	2.008850128472
C	-3.661246887276	-0.315428962811	0.853159406590
H	-4.324445280958	-0.255592973083	1.723273253044
H	-4.026472231762	0.404324271460	0.111824439259
H	-3.780161218846	-1.314817430581	0.418528042381
C	-1.539478441446	-0.009387130006	-1.484529479511
H	-2.200113749621	-0.866971257130	-1.686909163326
H	-2.193056957065	0.864735893095	-1.633649006210
C	-0.376223064491	0.017074915600	-2.486115723646
H	0.262519701163	-0.866405611796	-2.372561287888
H	-0.725353742014	0.041964358398	-3.524123799095
H	0.259643063529	0.896621610563	-2.331583676134
C	2.447607577011	-1.208187975978	0.394177991036
H	3.250865112939	-1.085071865527	-0.347641048572
H	2.973022329038	-1.186683542827	1.363207803119
C	1.747869085840	-2.563500241847	0.209409426247
H	1.266186001500	-2.628365930041	-0.773279288025
H	2.447502159959	-3.402758888651	0.290632739750
H	0.963559836059	-2.705819796459	0.960792623492
C	2.098145765153	1.540997541021	0.278883221942
H	2.852266542423	1.652584266121	1.072918807091
H	2.679613195929	1.617322874242	-0.654108003987
C	1.070905632998	2.680517457706	0.352611841286
H	0.339434577083	2.605977915037	-0.460597908192
H	0.509942470394	2.646643173176	1.293442916832
H	1.542672005313	3.666717208771	0.281458888735
O	0.170125019931	-0.103125027788	0.381339213860

Geometry of EQ11 (Et_2BOOH)

B	-0.861718208271	0.872479060605	-0.565389430175

H	1.117564749843	-0.792424827953	1.129693737631
C	-1.027961084609	2.168960195624	0.312638034842
H	-1.150106965106	1.892251268211	1.367363961639
H	-1.931980706608	2.712804017369	0.010732521977
C	0.201901987582	3.101178144245	0.180361323312
H	0.076212112326	4.008681326997	0.781234731491
H	1.111075968951	2.595199460752	0.518349611404
H	0.356714673084	3.415502590628	-0.858790409370
C	-1.589151354004	0.651977695690	-1.951859738446
H	-2.670616321792	0.690960728561	-1.743394373168
H	-1.401090067267	1.556371734817	-2.552448199476
C	-1.247549668398	-0.608810671501	-2.760456681505
H	-0.182112882106	-0.639711894092	-3.012147184125
H	-1.469041346278	-1.516436177099	-2.189183921896
H	-1.815052445675	-0.654033783737	-3.696569355825
O	0.634086093196	0.047133832968	1.077477621394
O	-0.034174089868	-0.162828667086	-0.212915680700

Geometry of EQ12 (CH_2CH_2)

C	1.013485713225	-3.169436664095	0.382436708430
H	1.167857383578	-3.954315566369	1.118615147292
H	-0.012029045011	-2.843864801257	0.226695209654
C	2.030215287719	-2.633030813210	-0.295374657417
H	3.055856127731	-2.958242658485	-0.140034510497
H	1.875294015758	-1.848138208584	-1.031495359462

Geometry of EQ13 ($^1O_2$)

O	0.000000000000	0.000000000000	0.606267000000
O	0.000000000000	0.000000000000	-0.606267000000

Geometry of MESX1

B	-0.441712913657	0.022885146844	-0.358088996359
C	-0.131572882970	-1.664285016484	-0.076646087020
H	-1.134148997742	-1.934211402432	0.281865250421
H	0.049907588370	-2.149308556733	-1.037496323166
C	0.957989229795	-1.949245726601	0.931198601184
H	0.666119040990	-1.662235335370	1.944837329944
H	1.212895451859	-3.018114757184	0.934763421908
H	1.886731844454	-1.412704473588	0.687718151046
C	-0.494358315012	0.865541308369	1.005391458517
H	0.405372430512	0.680484888676	1.605408126706
H	-1.340530680410	0.485295244627	1.596347259060
C	-0.654878205364	2.386039209998	0.805678927213
H	-0.665760477004	2.918232760949	1.764038670840
H	0.171354791256	2.797000721990	0.213224054450
H	-1.586756505178	2.626487724103	0.282907713502
C	-1.607882667578	0.220242429013	-1.449660338413
H	-2.556043603742	0.011871078027	-0.931358829790
H	-1.647944060928	1.289582417807	-1.702711241669
C	-1.536777936855	-0.599701076292	-2.747347200943
H	-0.582097802874	-0.444868238327	-3.264064571301
H	-1.633589385884	-1.674050525263	-2.554081459746
H	-2.336094130923	-0.323819647172	-3.444707610213
O	1.985913709308	0.588634644147	-0.516779557667
O	0.915323241221	0.301647177168	-1.126492433996

Path connection : (EQ1 + EQ2)-(EQ11 + EQ12)

Geometry of MESX2

B	-0.263417111354	-0.043513428555	-0.392076698858
C	0.003470461946	-1.582714064909	-0.013411814312
H	-0.987307174709	-2.045104259235	0.109237807291
H	0.431850015446	-2.055658079086	-0.910689393706
C	0.880265080793	-1.926104020631	1.199921865460
H	0.441328417189	-1.552120135071	2.132177623362
H	1.000403897278	-3.010134414049	1.310204624525
H	1.880832858988	-1.490088967973	1.110435030937
C	-0.485767343426	0.934880642446	1.064599043840
H	0.463723819583	0.786369091161	1.587271929696
H	-1.288693718265	0.358448095431	1.538237827456
C	-0.836497176911	2.390780430823	0.862928734689
H	-0.947449677403	2.886530887618	1.838361700978
H	-0.053824783957	2.922437919853	0.312653154658
H	-1.781285603612	2.513926953047	0.325850915201
C	-1.423907010786	0.301909213727	-1.454174064447
H	-2.393151036805	0.180352708207	-0.949542493616
H	-1.369762371744	1.356559244482	-1.753282477123
C	-1.394969551467	-0.586151648890	-2.714947896192
H	-0.444083890644	-0.479833848548	-3.249908465082
H	-1.514733767865	-1.645332289793	-2.463393720661
H	-2.199330703683	-0.318828730177	-3.410668697877
O	2.165970134578	0.480286825694	-0.399053313574
O	1.004907813738	0.680681202059	-0.894315131837

Path connection : (EQ1 + EQ2)-(EQ3 + EQ4)

Geometry of ^{3}TS1

B	-0.326303506586	-0.102016827709	0.299178455818
C	-1.448666258948	0.981442754341	-0.021269828930
H	-1.567638066471	1.080286899017	-1.108548168542
H	-2.417059408518	0.661691375147	0.381378761935
C	-1.099262692712	2.364211089024	0.580186193511
H	-0.169468039447	2.761702867114	0.159173145571
H	-1.892818858952	3.093358981536	0.380676995831
H	-0.972314650387	2.299733655648	1.666477173268

C	1.169206263224	0.076581160743	-0.227677379882
H	1.528926048089	0.992644576214	0.270193898003
H	1.141940120028	0.326856836722	-1.297079004620
C	2.178316388701	-1.052939441698	0.031581074256
H	3.195729449883	-0.757203832651	-0.247531167809
H	2.190964280325	-1.336271263301	1.089496876412
H	1.935623123823	-1.951196619014	-0.547840060282
C	-0.957076496250	-1.769901108877	-0.584285899184
H	-0.660642001660	-1.489379443710	-1.595494409303
H	-0.271934289847	-2.467864245160	-0.105686923010
C	-2.413365554142	-2.013871534808	-0.346157218049
H	-2.662456133879	-1.936651479585	0.717694566954
H	-3.046868730857	-1.324125430594	-0.908843203154
H	-2.665743887642	-3.039959638940	-0.660058254960
O	-1.424706813859	-0.713955998555	2.381724576628
O	-0.293476800414	-0.584090768410	1.713717004586

Path connection : (EQ1 + EQ2)-(EQ3 + EQ4)

Geometry of ¹TS2

B	-0.326303507000	-0.102016828000	0.299178456000
C	-1.462763328000	0.995051193000	-0.025294714000
H	-1.581735135000	1.093895337000	-1.112573054000
H	-2.431156477000	0.675299814000	0.377353876000
C	-1.113359762000	2.377819527000	0.576161308000
H	-0.183565108000	2.775311305000	0.155148260000
H	-1.906915928000	3.106967420000	0.376652110000
H	-0.986411719000	2.313342094000	1.662452288000
C	1.187954697000	0.078820151000	-0.234282299000
H	1.547674482000	0.994883567000	0.263588979000
H	1.160688554000	0.329095827000	-1.303683924000
C	2.197064822000	-1.050700451000	0.024976155000
H	3.214477883000	-0.754964842000	-0.254136087000
H	2.209712714000	-1.334032273000	1.082891957000
H	1.954371557000	-1.948957628000	-0.554444980000
C	-0.858816697000	-1.510083429000	-0.446662647000
H	-0.562382202000	-1.229561763000	-1.457871157000
H	-0.173674490000	-2.208046565000	0.031936329000
C	-2.315105755000	-1.754053855000	-0.208533966000
H	-2.564196334000	-1.676833799000	0.855317819000
H	-2.948608931000	-1.064307750000	-0.771219951000
H	-2.567484088000	-2.780141959000	-0.522435003000
O	-1.351759201000	-0.770586999000	2.530505907000
O	-0.289084610000	-0.648591933000	1.902981297000

Path connection : (EQ1 + EQ2)-(EQ3 + EQ4)

Geometry of VTS

C	-3.979807732038	-2.163612794855	-1.122271812381
H	-5.069539999356	-2.049496427510	-1.094279049713
H	-3.582115054254	-1.517209641257	-1.913262314912
H	-3.784882351671	-3.203835868387	-1.445462912660
C	-3.356770470000	-1.876404398000	0.195694649000
H	-2.322798652775	-1.554443622632	0.267325631264
H	-3.880107476119	-2.092745126158	1.121506502399
O	-2.343908256000	-5.320578624000	-0.072212128000
O	-2.882862406222	-5.427895891305	-1.160229523004

Path connection : (EQ2 + EQ4)-EQ5

Geometry of TS3

B	-1.076994883857	0.745542516287	0.510672720776
C	-0.421411388215	-0.123798345660	1.685976391376
H	-0.876630033362	0.268856286621	2.612671417709
H	0.644946087605	0.121244806754	1.789449702368
C	-0.602855942854	-1.647878967818	1.639256467860
H	-0.124249160549	-2.147551489513	2.490614046820
H	-1.662675419622	-1.925718290380	1.647304308098
H	-0.171247081555	-2.069368961200	0.723467734104
C	-2.313709091946	0.141915174036	-0.293045105042
H	-2.089744640972	-0.886350180414	-0.607161101411
H	-3.125704912149	0.030122133007	0.446727989014
C	-2.831658866532	0.946868955195	-1.495939393228
H	-2.043144409927	1.077215529944	-2.247427347604
H	-3.679254214090	0.455708012642	-1.989433049967
H	-3.160351709928	1.949145365831	-1.198675894271
C	-0.860055518505	2.326551813898	0.527442319080
H	-0.918274049103	2.719684567364	-0.496820166645
H	-1.751809588085	2.741303646802	1.029280984680
C	0.404581683150	2.864870502172	1.217285810801
H	0.445379840364	2.567307927337	2.271428791041
H	1.310114144688	2.474686741780	0.736973859373
H	0.460073947109	3.959715804969	1.182801841332
O	0.372702808725	-0.792632568436	-1.515445608615
O	0.508145041020	0.354087587737	-0.870121390609
C	1.643857844277	-1.202971090561	-2.121281364229
H	1.341611557880	-1.989845633807	-2.817223512444
H	2.029170491424	-0.340582615886	-2.671646591693
C	2.601716038610	-1.696252094656	-1.051264066249
H	3.539226900459	-2.014156323760	-1.518569541112
H	2.818126696898	-0.893964720607	-0.341180094787
H	2.175751885330	-2.544469092069	-0.508386935601

Path connection : (EQ1 + EQ5)-(EQ4 + EQ6)

Geometry of TS4

B	0.187961499588	-0.481950247000	-1.124321941284
C	-0.067018252222	-1.714889235368	-2.167033203938
H	-1.134368757814	-1.800894559624	-2.386438201035
H	0.453918733540	-1.434340422119	-3.091952913787
C	0.490796851380	-3.030060724732	-1.603481126518
H	0.355638425429	-3.844147418221	-2.326120943708
H	1.560659637701	-2.957831276093	-1.381549089996
H	-0.024778187473	-3.318656361453	-0.681417532580
C	1.713485099238	-0.053592706735	-0.792565576385
H	1.875981676851	-0.366366759280	0.246688617883
H	2.390539499835	-0.630767433151	-1.432891009907
C	1.958446542655	1.455008995777	-0.933125567141
H	1.321490269577	2.011663893271	-0.242044321643
H	3.004307402446	1.696913963213	-0.707457223671
H	1.752668373130	1.804313057817	-1.951500121034
O	-0.830694053350	0.093550812223	-0.582232019391
C	-1.113744103484	1.595473570435	3.698888212605
H	-0.621558103755	2.569917171509	3.748357211917
H	-0.556412082225	0.881976663300	4.310951009905
H	-2.132016680637	1.686748050239	4.089992508759
C	-1.199083460024	1.102320854701	2.228862466089
H	-1.705362311792	0.125544482950	2.206694990706
H	-1.772943863159	1.832241636479	1.638184824471
O	0.101105961519	1.004176825400	1.781897166915

Path connection : EQ6-(EQ7 + EQ8)

Geometry of TS5

B	-2.115253515424	-1.149058659312	0.358013829911
C	-2.903086070588	0.233133561244	0.388810458035
H	-2.282927203655	1.036529760571	0.804739461865
H	-3.026268059740	0.509702660289	-0.674006000107
C	-4.282826889012	0.236240406859	1.067177251454
H	-4.199291371110	-0.063645251008	2.119008891423
H	-4.755588875624	1.225352882127	1.040226588866
H	-4.968225341592	-0.469846594500	0.586263710798
C	-2.948787944168	-2.494977114902	0.183450447612
H	-3.496794990545	-2.388082035959	-0.769328868185
H	-3.737478866934	-2.534210557404	0.946953207725
C	-2.172666347469	-3.821496610338	0.180053051109
H	-2.835283865867	-4.686053705931	0.053335937647
H	-1.433770243245	-3.855020268340	-0.629192649796
H	-1.630200323911	-3.953342898016	1.122971119775
C	-0.561167310713	-1.160556589754	-0.041033655785
H	-0.037159675065	-1.981283534942	0.467020626542
H	-0.576913168704	-1.478301108945	-1.099587014296
C	0.240977103968	0.141945943355	0.080292532386
H	-0.206382958534	0.945219319091	-0.515275595641
H	0.279176285086	0.502773334684	1.115995268860
H	1.277446178249	0.019203454099	-0.256270418346
C	-1.475104336990	0.585272970472	3.704892565479
H	-0.888134587723	1.044561493112	4.507414485575
H	-1.406639142235	1.211996333090	2.813976623296
H	-2.521695877445	0.547315916656	4.020512178794
C	-0.957591511734	-0.826557989362	3.429618235930
H	0.087402576647	-0.784416162425	3.050147012138
H	-0.899209239445	-1.438578685907	4.346655174542
O	-1.628153791686	-1.528355869991	2.452009870524

Path connection : (EQ1 + EQ8)-(EQ4 + EQ9)

Geometry of TS6

B	-1.663124291071	0.132492159695	1.508477855602
B	-2.804213629914	-0.153449435141	4.411581209036
C	-0.213457374996	-0.612188086869	1.347519332132
H	-0.268268405793	-1.111870942348	0.370752782799
H	-0.127449948526	-1.381139744440	2.118383100352
C	0.958956794359	0.373351096635	1.401489337824
H	1.905668470921	-0.163773464842	1.266216518044
H	0.893151107101	1.132620449478	0.616023115708
H	1.006130423028	0.885434062905	2.367532651454
C	-1.987655630112	1.389883565897	0.548042547897
H	-1.386092512971	2.208523213738	0.968888444224
H	-1.559965848875	1.170140655983	-0.438393168215
C	-3.464921106457	1.781421506597	0.455903956164
H	-3.870284762067	2.025479956484	1.441066738746
H	-3.594838480676	2.653355687888	-0.195461485747
H	-4.067804382699	0.964804544036	0.046591580585
C	-1.334393674561	0.302241416030	4.863599253945
H	-1.304670621008	0.132289854379	5.953610662164
H	-0.582940253413	-0.390063136241	4.460681956856
C	-0.911284062603	1.750750033648	4.576415019543
H	-1.569059329687	2.468553562364	5.078476339416
H	0.114449561121	1.957379759000	4.905928928677
H	-0.959180748768	1.979633700799	3.503742076996
C	-3.944589991463	0.973936464201	4.348934996702
H	-3.574608523559	1.858065719811	3.812611943188
H	-4.061683859565	1.314783395996	5.392705789406
C	-5.314950034602	0.563637087021	3.789396742301
H	-6.023528552641	1.401190078598	3.778551193078
H	-5.220452975419	0.191727732541	2.762826897681
H	-5.766674967114	-0.239171002777	4.382301759588
C	-3.247007940181	-1.663805710458	4.677420529092
H	-3.688764626339	-1.676549428501	5.688918446451
H	-4.072354109083	-1.931225719717	4.005155192222

C	-2.151169043701	-2.738441330530	4.590583462888
H	-1.703249343277	-2.752802690424	3.589110757841
H	-1.341786123473	-2.552946765980	5.306308831915
H	-2.540213560804	-3.744316070674	4.790233635555
O	-2.486809936140	-0.311957111718	2.399372849273

Path connection : (EQ1 + EQ7)-(EQ4 + EQ10)

Geometry of TS7

B	-0.487445340725	-0.681271999969	0.402177305142
C	-1.570518982324	0.544476812656	0.376500423670
H	-1.039664261518	1.495278291571	0.277133277486
H	-2.198482397601	0.403019593785	-0.512449647521
C	-2.419938141922	0.526391221879	1.654794143030
H	-3.149157447210	1.345874021381	1.645333527897
H	-2.977595978754	-0.410465989284	1.761586246766
H	-1.796319646629	0.646024203387	2.546674802424
C	-1.030088981283	-2.139724324023	-0.037170983793
H	-2.013839121303	-2.280798289096	0.429431383832
H	-1.225292222098	-2.034643672702	-1.115145678195
C	-0.108461927682	-3.331558600912	0.233873723845
H	0.049815662574	-3.475369346835	1.306263216454
H	-0.536024328228	-4.258255232477	-0.167063262447
H	0.874181885785	-3.184947241254	-0.224581671827
O	0.726187266553	-0.427065309577	0.762458914460
C	1.099785255905	-2.044225224486	3.522984088765
H	1.272579918108	-3.126914013535	3.536599247836
H	1.810411639620	-1.563126314437	4.203886720814
H	1.354405227207	-1.691752154657	2.503771483522
C	-0.302418026365	-1.698673136596	3.849160390286
H	-0.553971062027	-0.751720255737	4.315126750623
H	-1.125449331046	-2.330309662236	3.528624417903

Path connection : (EQ4 + EQ7)-EQ9