Supporting Information

Silica Microspheres Containing High Density Surface Hydroxyl Groups as Efficient Epoxidation Catalysts

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S-1: Materials: Chemical: Tetraethyl orthosilicate (TEOS), cyclohexene, styrene, n-heptene, *cis*-cyclooctene, allylbenzene and 50 % H_2O_2 were purchased from Sigma-Aldrich chemical India, Absolute ethanol (99.9%), NH_3 (25%) solution, acetonitrile, *tert*-butanol, ethyl acetate were purchased from Thomas Bakar India Ltd. and KOH has purchased from Rankem India Ltd. Furthermore, all the chemicals were used as received unless stated otherwise.

S-2: Catalyst characterization

The synthesized catalysts were characterized by Scanning electron microscopy (SEM) measurements were performed on a FEI quanta 200 3D dual beam (ESEM) having thermionic emission tungsten filament in the 3 nm range at 30 kV and HRTEM experiment was performed with Tecnai FEI G2 microscope, using an accelerating voltage of 300 kV. For TEM analysis, a sample was deposited on a coated 200 mesh Cu grid. N_2 adsorption–desorption isotherms were recorded at 77 K by using an automated quantasorb instrument from quantachrome. Before each run, a known mass of sample (around 0.200 g) was heated at 200 °C under vacuum for 2.5 h. Specific surface areas were calculated from the linear part of the Brunauer–Emmett–Teller line. Pore-size distributions were obtained by applying the Barrett–Joyner–Halenda (BJH) equation to the desorption branch of the isotherm. The total pore volume was estimated from the N_2 uptake at a P/P_0 value of 0.991. FTIR spectra were obtained using a Thermo-Nicolet 670 spectrometer with samples loaded onto a KBr disk in the range of 4000–400 cm^{-1} region with 4 cm^{-1} resolution. Solid-state ^{29}Si NMR spectra was obtained using a 300 MHz Bruker Advance NMR spectrometer. For ^{29}Si MAS NMR experiments, 8.0 kHz spin rate, 5 s recycle delay, 10 ms contact time, $\pi/2$ pulse width of 5.6 μs, and 10000-20000 scans using TPPM 1H decoupling was employed.

S-3: Catalyst surface area analysis by BET method

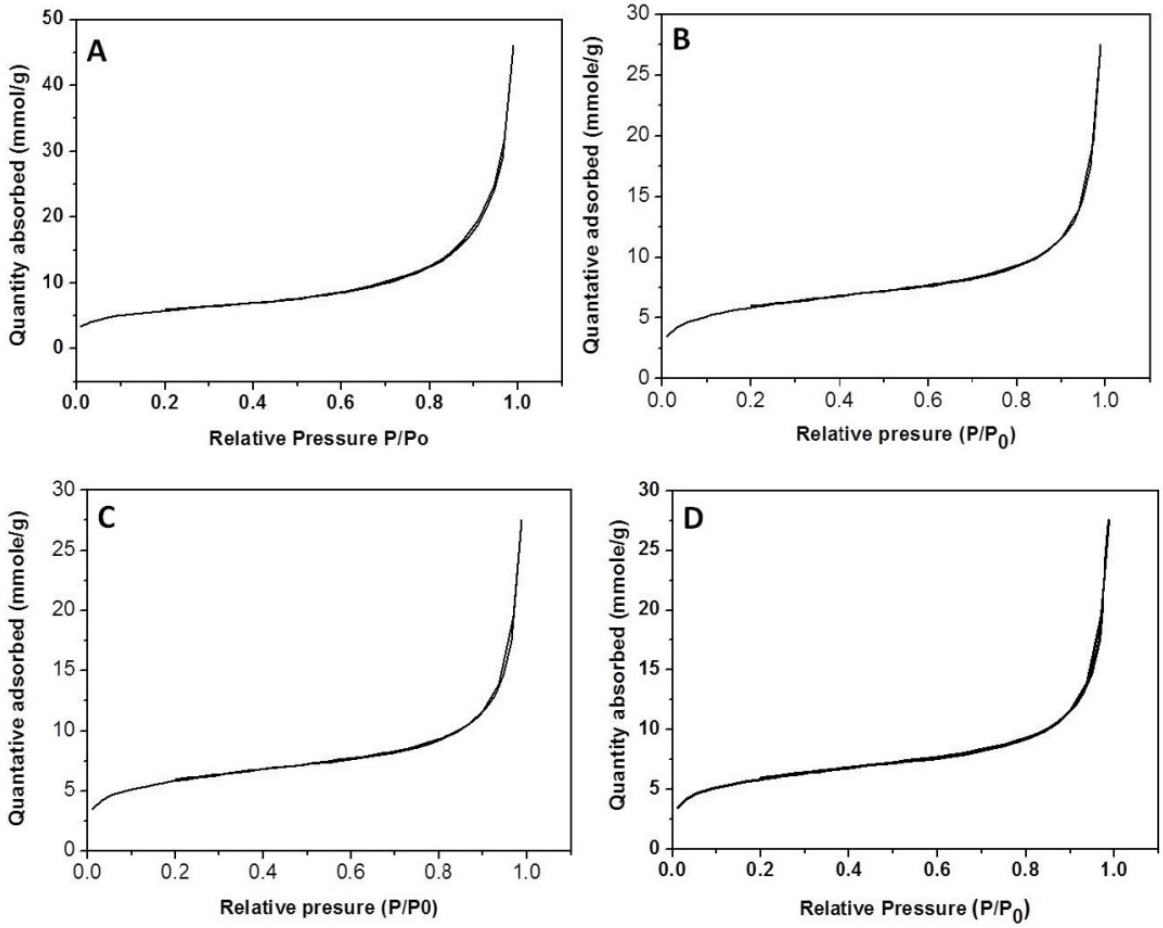


Figure-S1: Nitrogen adsorption-desorption isotherms for (A) silica microspheres (B) after etching for 2 h., (c) after etching for 3 h., and (d) after etching for 4 h.

S-4: FTIR analysis of silica microspheres

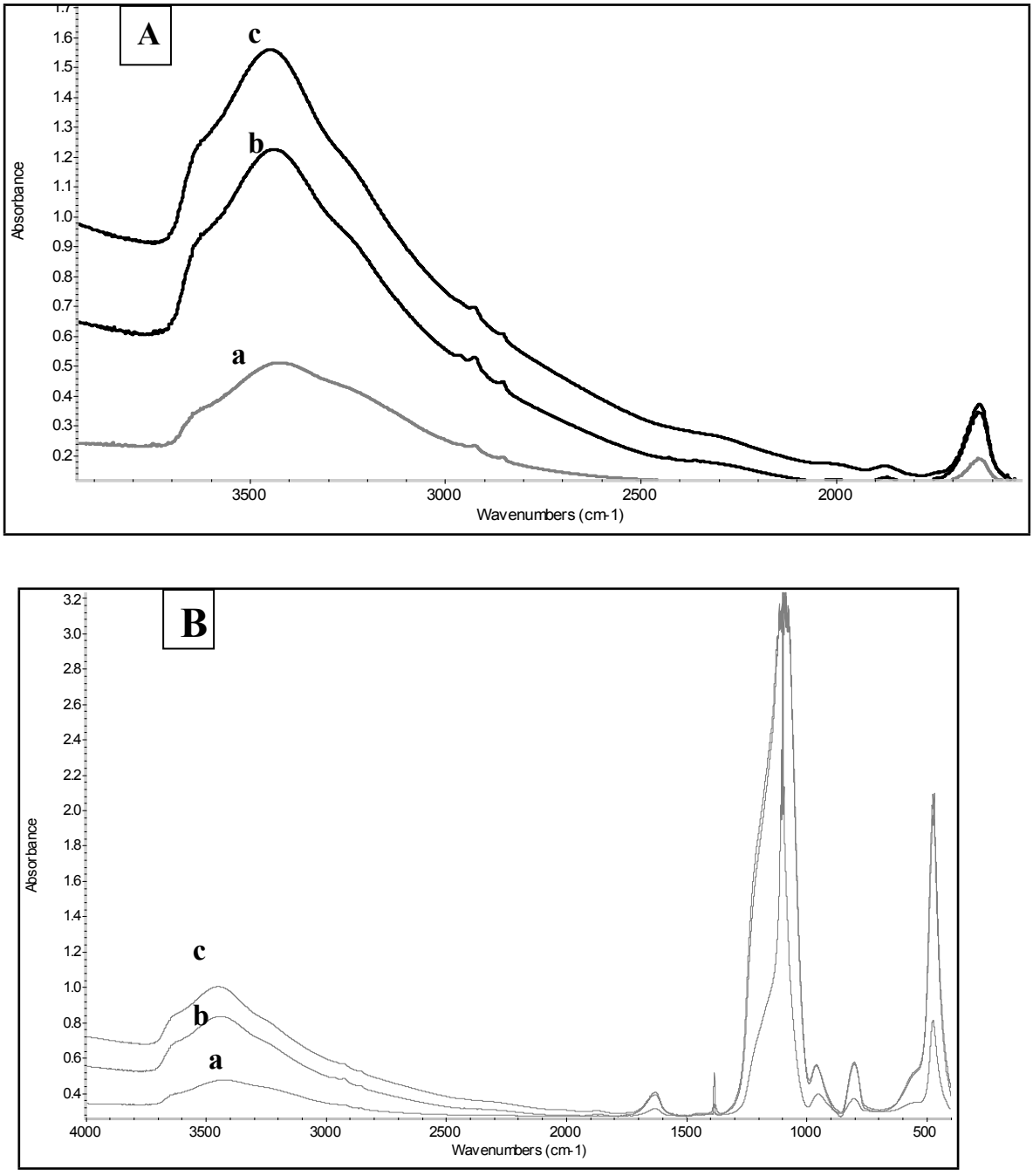


Figure-S2: FT-IR spectra of (a) Silica microspheres, (b) 3h and (4) 4h silica in (A) 1800-4000 cm^{-1} and (B) 400 – 4000 cm^{-1}

S-5: SEM analysis of the catalysts

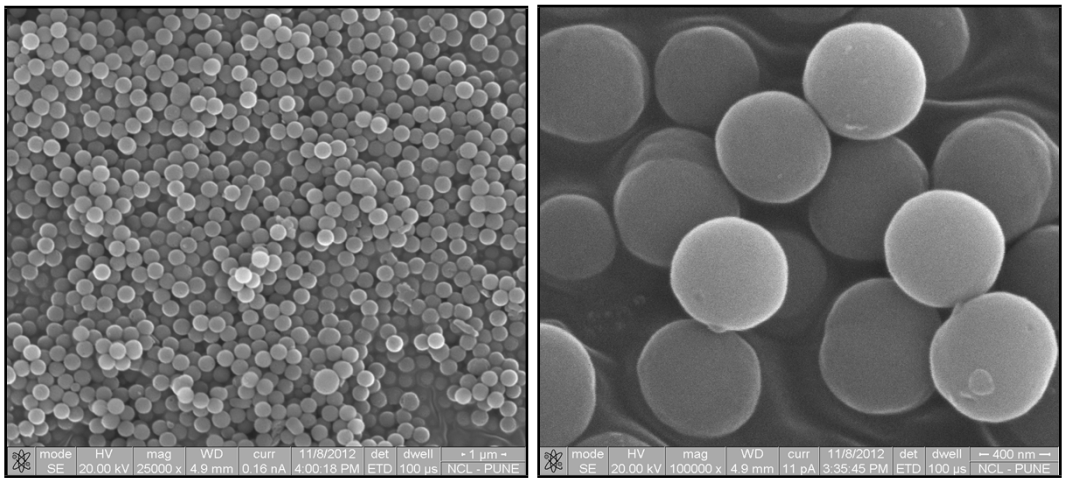


Figure-S3: SEM images of silica spheres A) 1 µm B) 400 nm

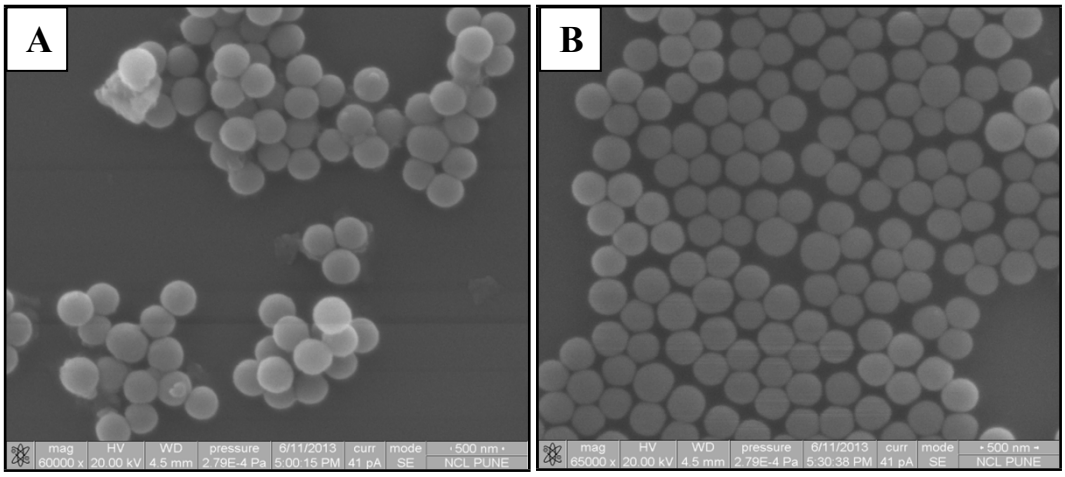


Figure-S4: SEM image of A) 3 h and B) 4 h silica

S-6: TEM analysis of the catalysts

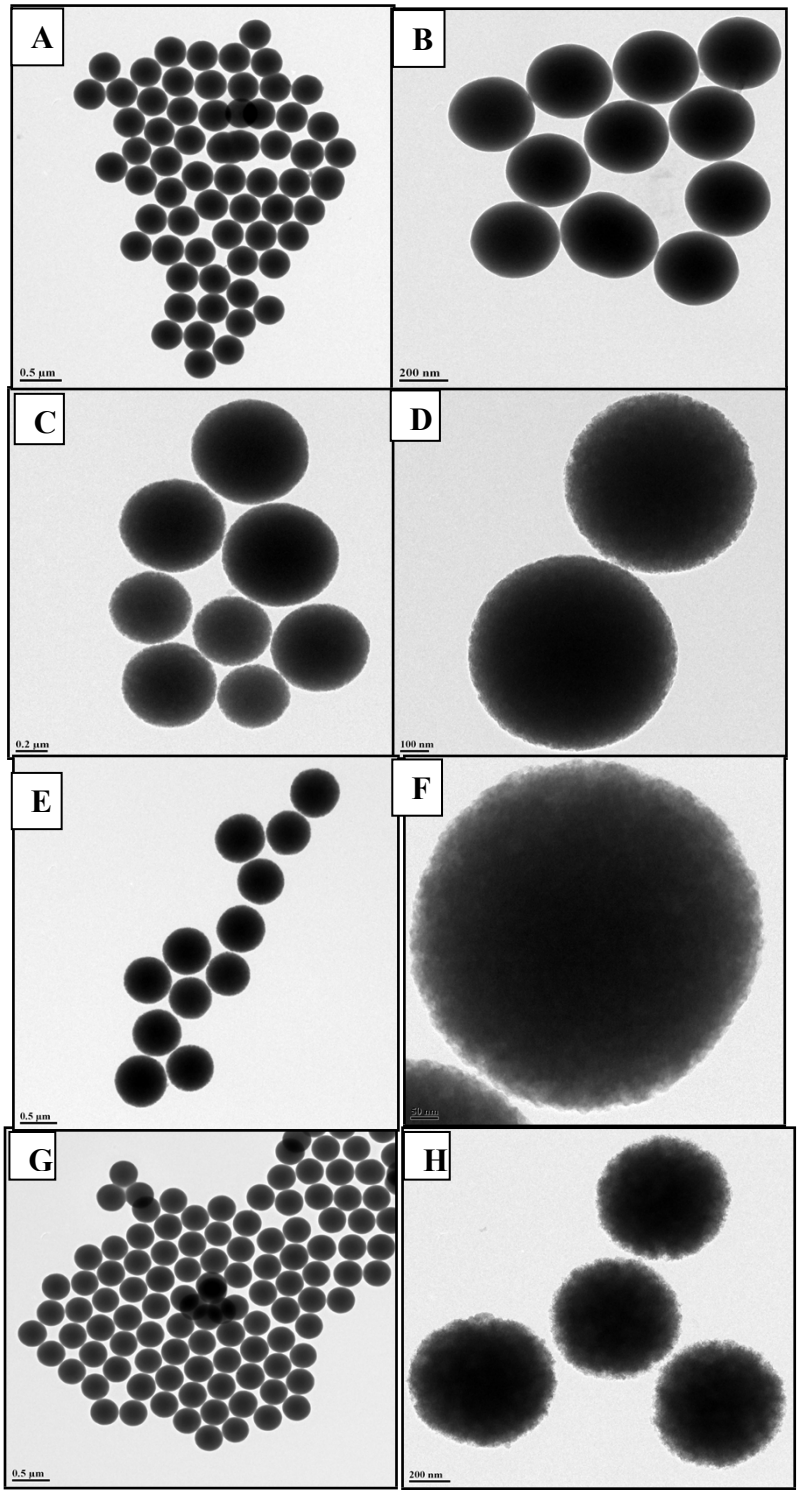


Figure-S5: HRTEM images of silica A) silica spheres; D) magnified image of silica spheres; C) 2h silica spheres; D) magnified image of 2h silica spheres; E) 3h silica spheres; F) magnified image of 3h silica spheres; G) 4h silica spheres and H) magnified image of 4h silica spheres.

S-7: Catalytic activity

Table ST1: Control experiments carried out using 4h etched SiO_2

Entry	Catalyst	% Conv.	% Sel.			
		1	2	3	4	5
1.	Etched SiO_2- 500 ^oC calcined	25.1	62	-	38	-
2.	Hot filteration[a]	30.0	93	-	7	-
3.	Hot filteration [b]	42.0	85	-	15	-

[a]**Reaction condition:** Cyclohexene: 0.825 g (0.01 mol); 50% H_2O_2: 2.76 g (0.04 mol); Temperature: 80 °C; Solvent: Acetonitrile (10 g); Catalyst: 0.08 g; time-24h; [b]: catalyst 4h etched silica.[a] Reaction up to 10 h with catalyst; [b] Reaction without catalyst.

Table ST2: results of epoxidation of cyclohexene using different oxidant molar ratios[a]

Entry	Oxidant molar ratio	% Conv. 1	% Selectivity		
			2	3	4
1.	1:2	25.2	92.8	--	7.2
2.	1:4	72.3	90.4	4.1	5.5
3.	1:6	95.0	89	8.4	2.1

[a]**Reaction condition:** Cyclohexene: 0.82 g (0.01 mol); Solvent: Acetonitrile (10 g); Catalyst (4h etched silica sphere): 0.08 g; Temperature: 80 °C; Time-24 h.

S-8: Computational analysis

S8-S15: Mechanistic studies for olefin epoxidation silica microspheres synthesized by hydrolysis-condensation (HC)

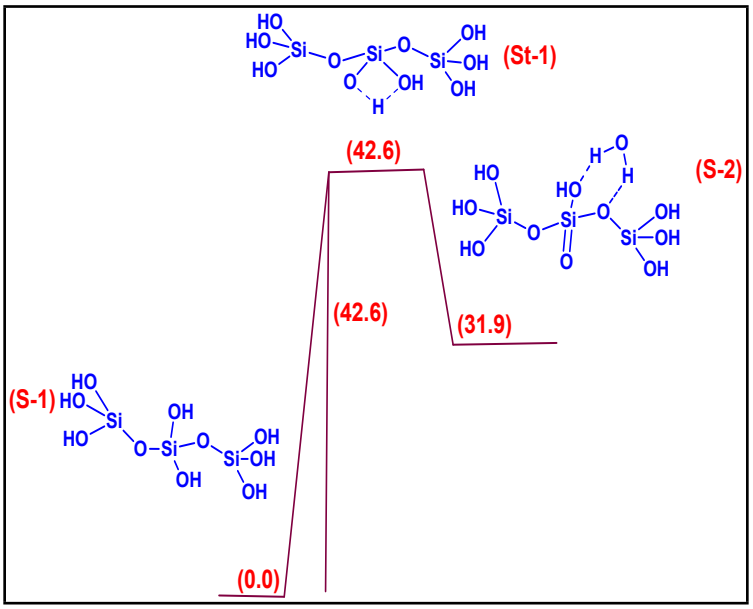


Figure-S8: The potential energy surface for the conversion of the germinal diols to Si=O species; energy values (ΔG) are in kcalmol^{-1}.

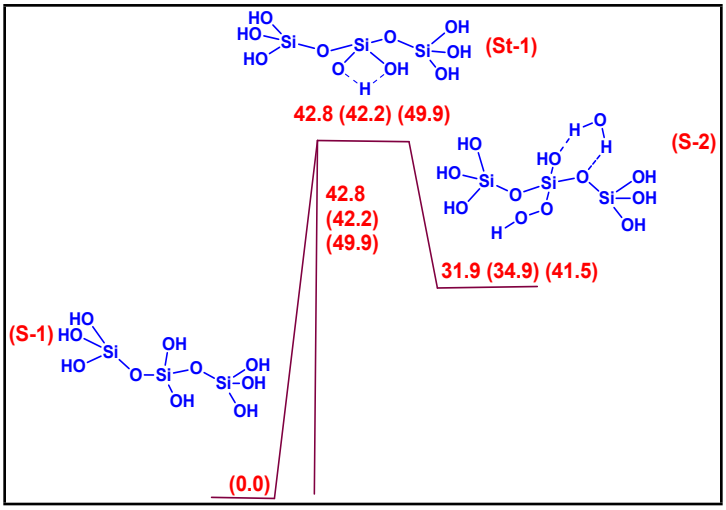


Figure-S9: The potential energy surface for the conversion of the germinal diols to Si=O species; the values shown in the figure are the electronic energies calculated using the BP-86, PBE and B3LYP functionals respectively – the BP-86 values are shown outside the parenthesis, while the PBE and the B3LYP energies are shown (in that order), inside the parenthesis.

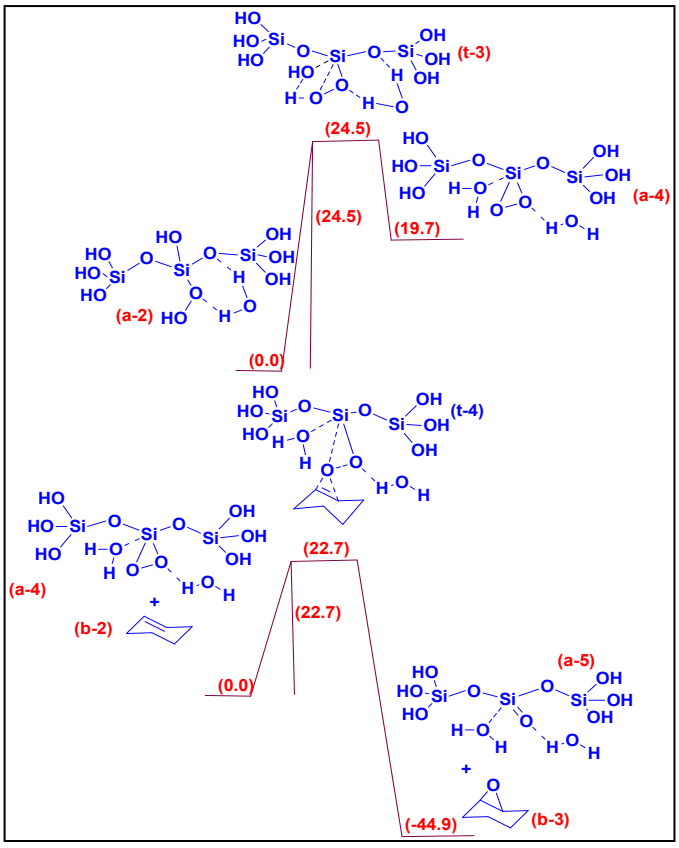


Figure-S10: The potential energy surface for olefin epoxidation catalyzed by secondary salinols present on the synthesized silica microspheres; energy values (ΔG) are in kcalmol^{-1}.

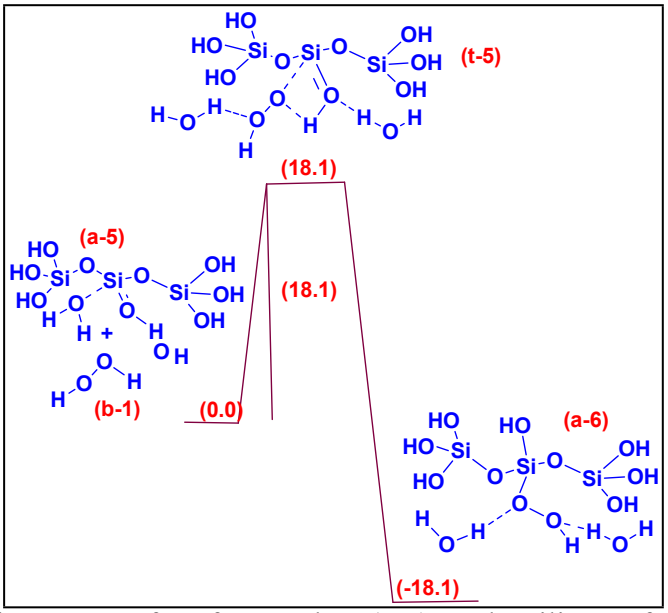


Figure-S11: The potential energy surface for attack at (a-4) on the silica surface by H_2O_2 to fom (a-5); energy values (ΔG) are in kcalmol^{-1}.

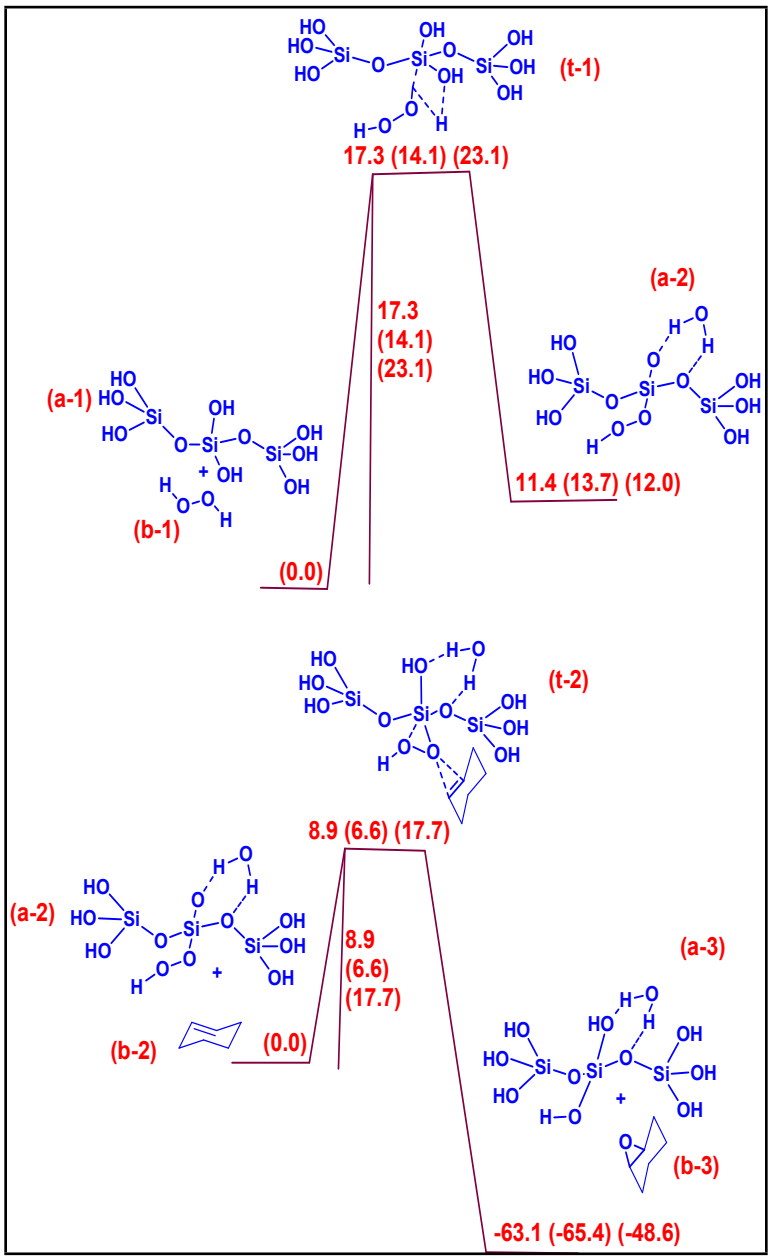


Figure-S12: The potential energy surface for olefin epoxidation catalyzed by secondary salinols present on the synthesized silica microspheres; the values shown in the figure are the electronic energies calculated using the BP-86, PBE and B3LYP functionals respectively – the BP-86 values are shown outside the parenthesis, while the PBE and the B3LYP energies are shown (in that order), inside the parenthesis.

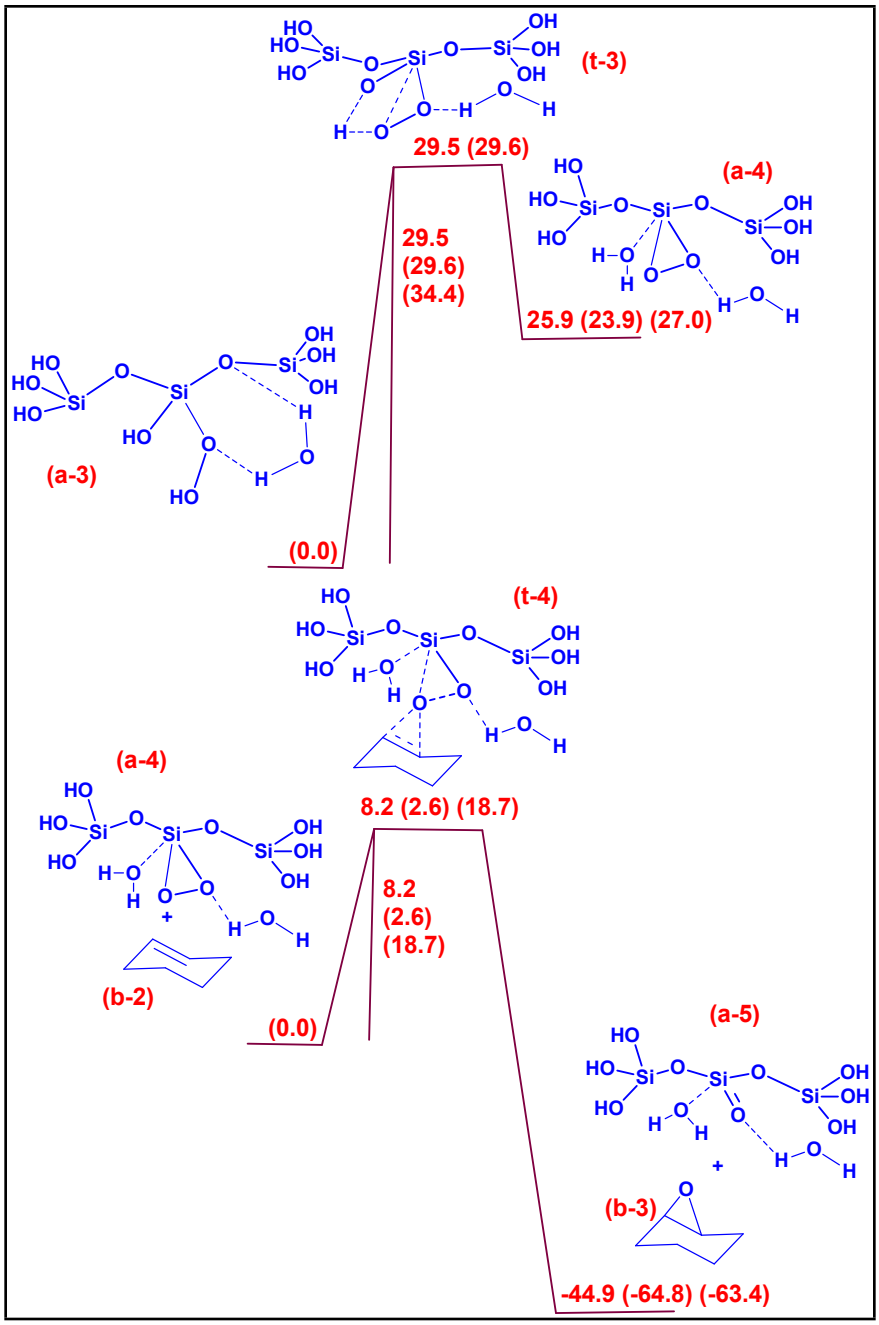


Figure-S13: The potential energy surface alternative pathway for olefin epoxidation catalyzed by secondary salinols present on the synthesized silica microspheres; the values shown in the figure are the electronic energies calculated using the BP-86, PBE and B3LYP functionals respectively – the BP-86 values are shown outside the parenthesis, while the PBE and the B3LYP energies are shown (in that order), inside the parenthesis.

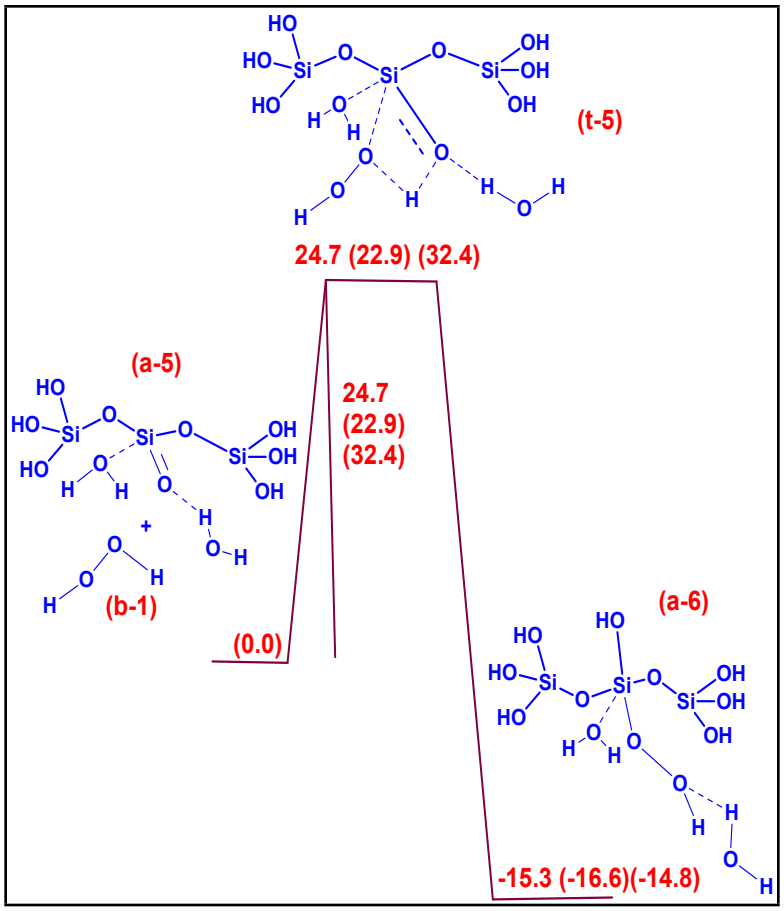


Figure-S14: The potential energy surface for double bond activation of secondary salinols by hydrogen peroxide present on the synthesized silica microspheres; the values shown in the figure are the electronic energies calculated using the BP-86, PBE and B3LYP functional respectively – the BP-86 values are shown outside the parenthesis, while the PBE and the B3LYP energies are shown (in that order), inside the parenthesis.

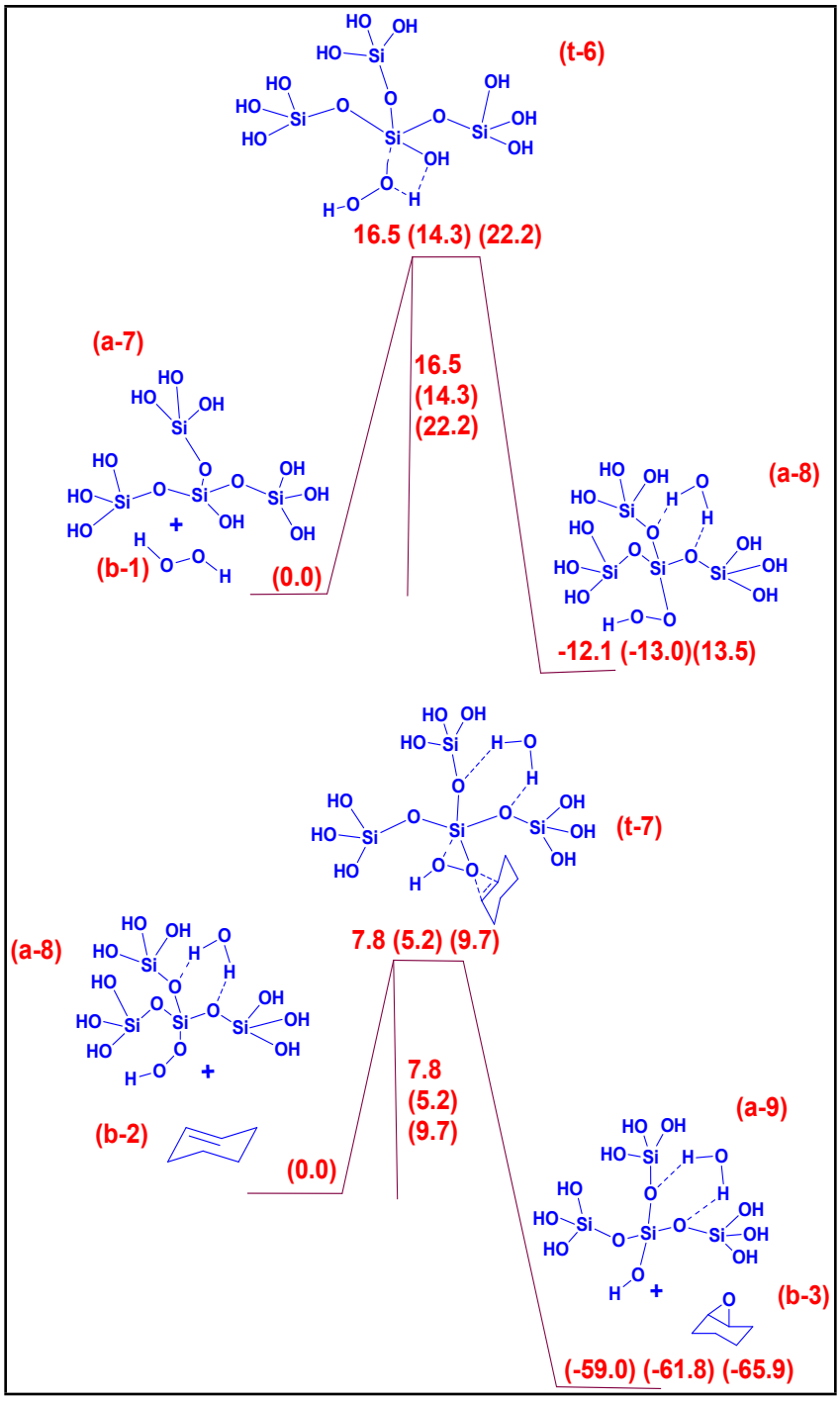
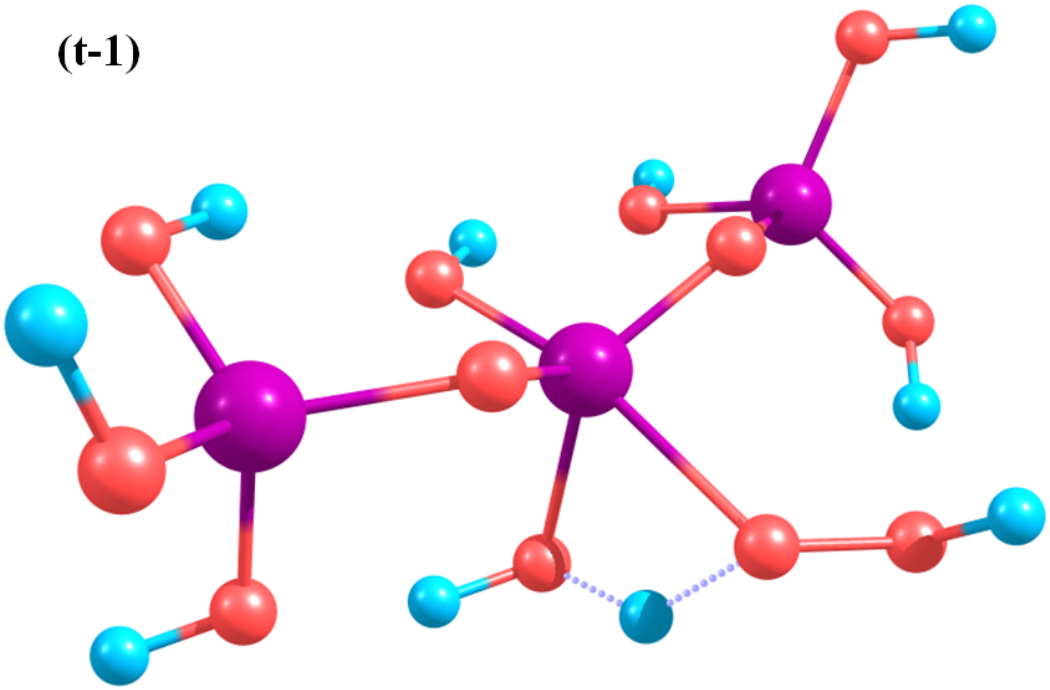


Figure S15: The potential energy surface for olefin epoxidation catalyzed by secondary salinols present on silica microspheres; the values shown in the figure are the electronic energies calculated using the BP-86, PBE and B3LYP functionals respectively – the BP-86 values are shown outside the parenthesis, while the PBE and the B3LYP energies are shown (in that order), inside the parenthesis.

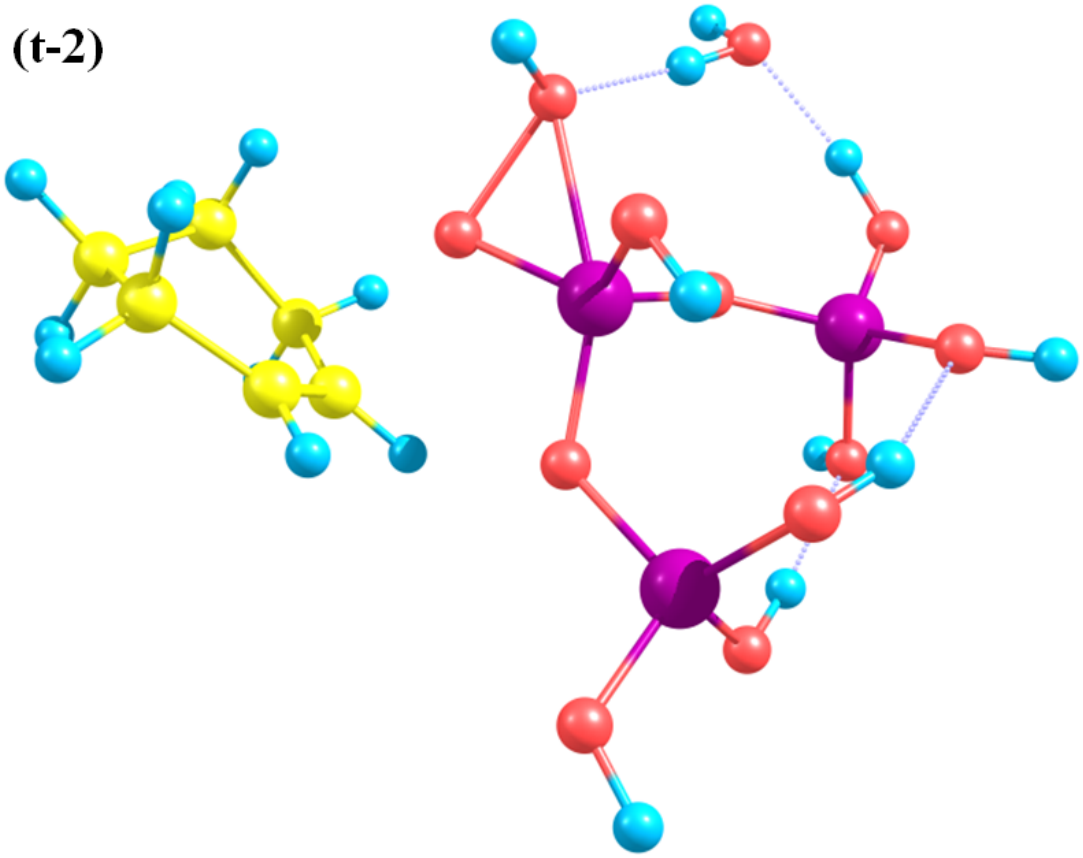
Table ST3: ΔH, ΔG and single imaginary vibrational frequencies for various transition states for silica catalyzed olefin epoxidation

Entry	Transition state	Δ H (298)	Δ G (298)	Imaginary Vibrational frequency (cm^{-1})
1	(t-1)	32.0	39.0	-554.55
2	(t-2)	20.5	23.7	-228.94
3	(t-3)	27.3	24.5	-405.95
4	(t-4)	19.6	22.7	-220.02
5	(t-5)	10.7	18.1	-874.78
6	(t-6)	28.4	32.6	-613.32
7	(t-7)	17.0	23.3	-223.02
8	(St-1)	42.6	42.6	-879.71

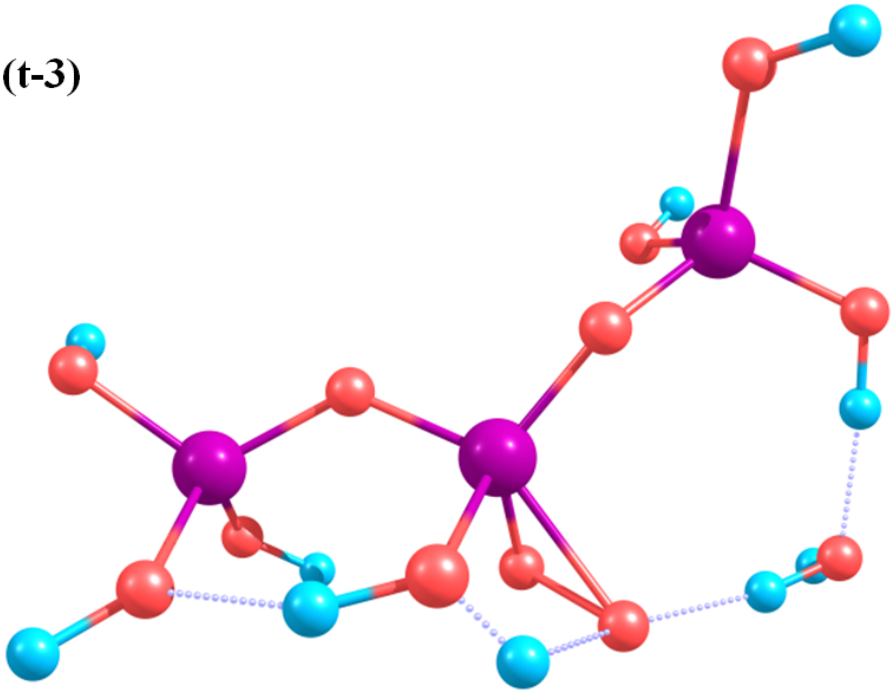
S-16- Optimized structures for various transition states involved during the silica catalyzed olefin epoxidation. (Nomenclature of each transition state t-1 to t-7 is according to as mentiond in the text)



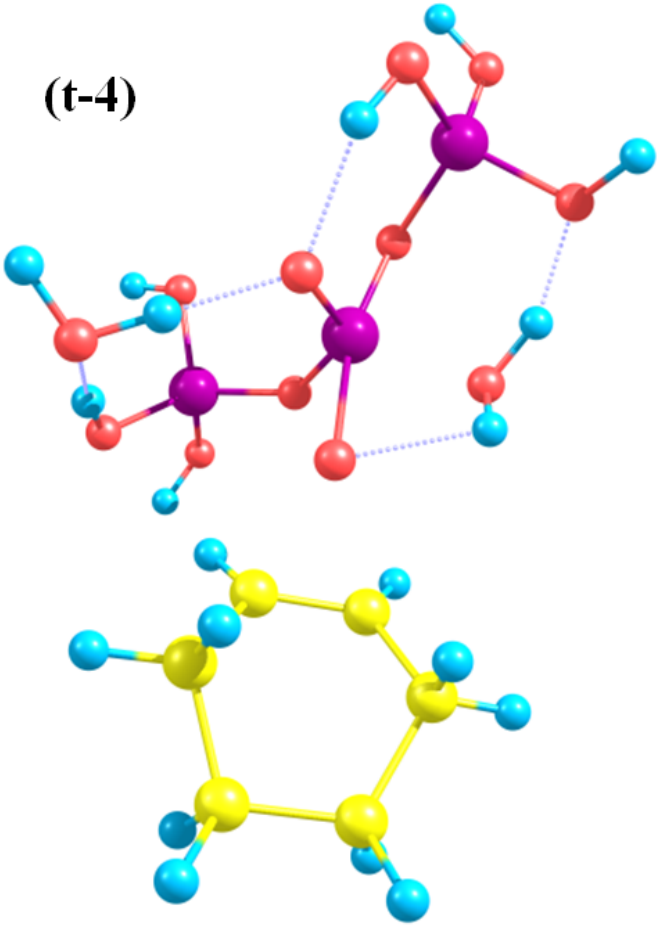
(t-2)



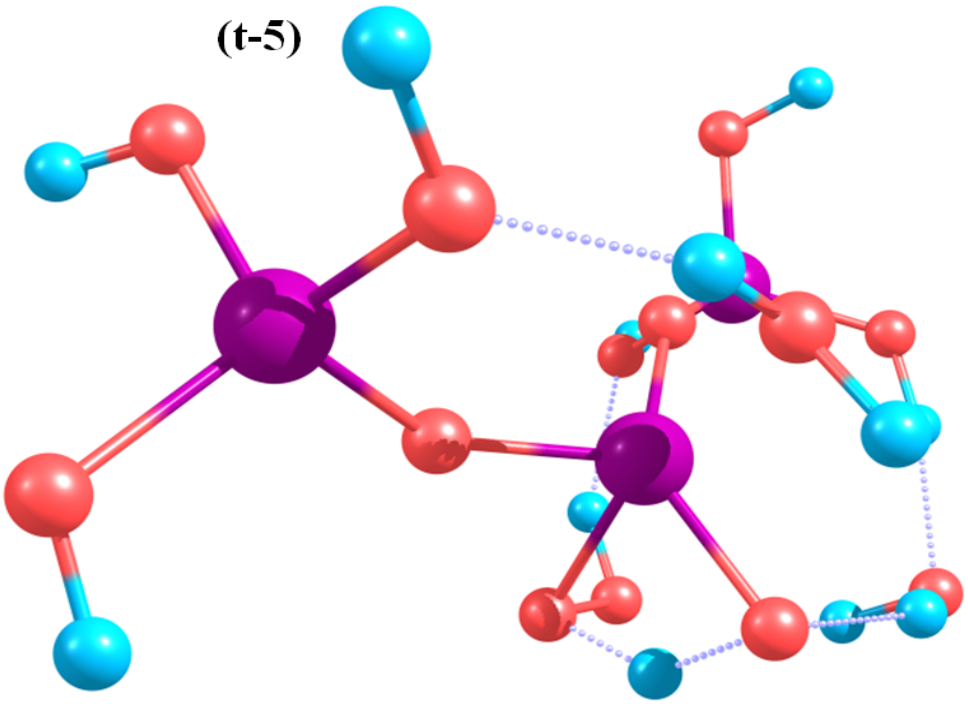
(t-3)



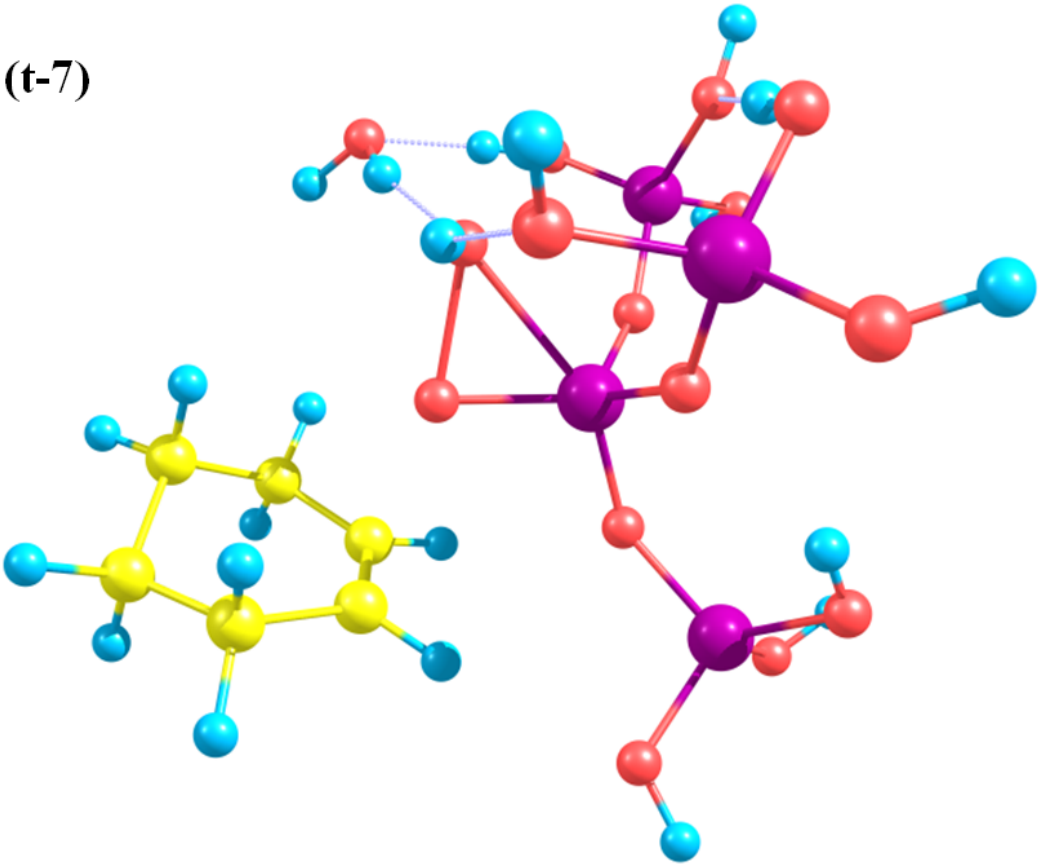
(t-4)



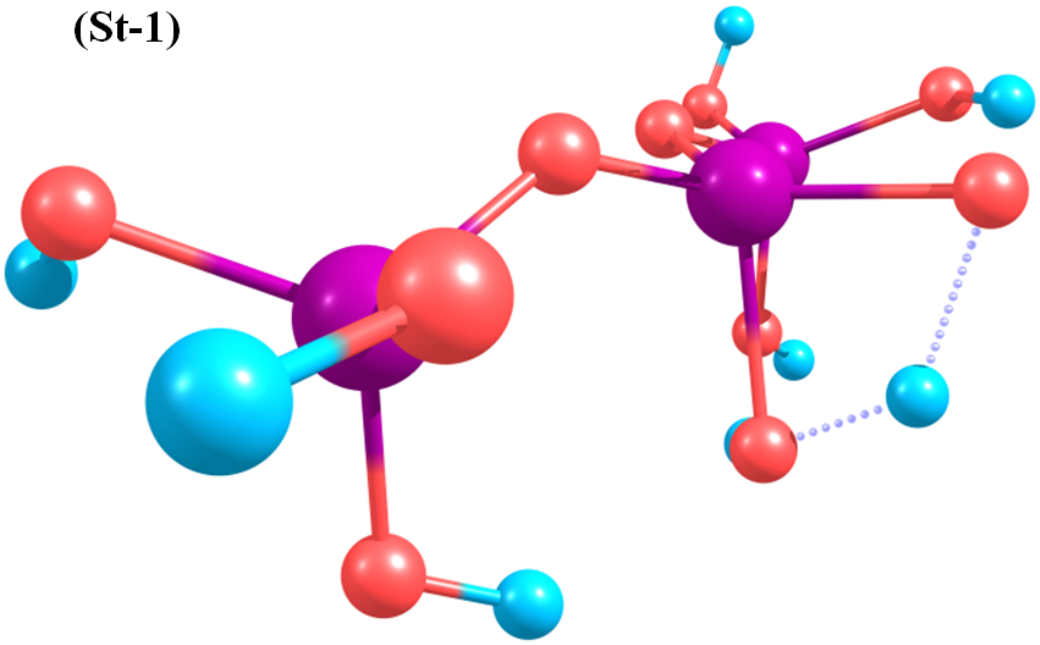
(t-5)



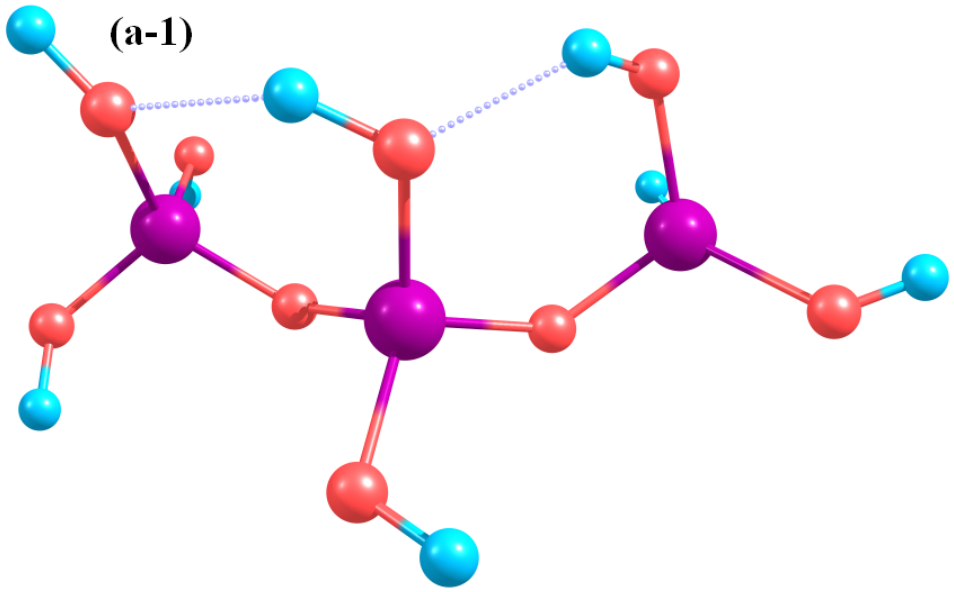
(t-7)

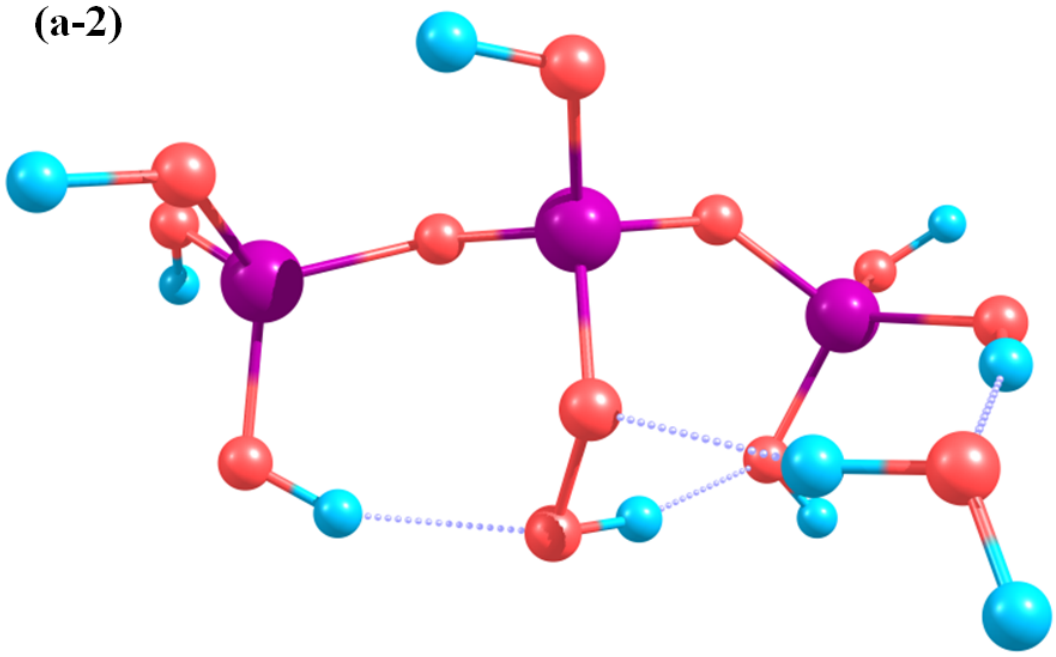


(St-1)

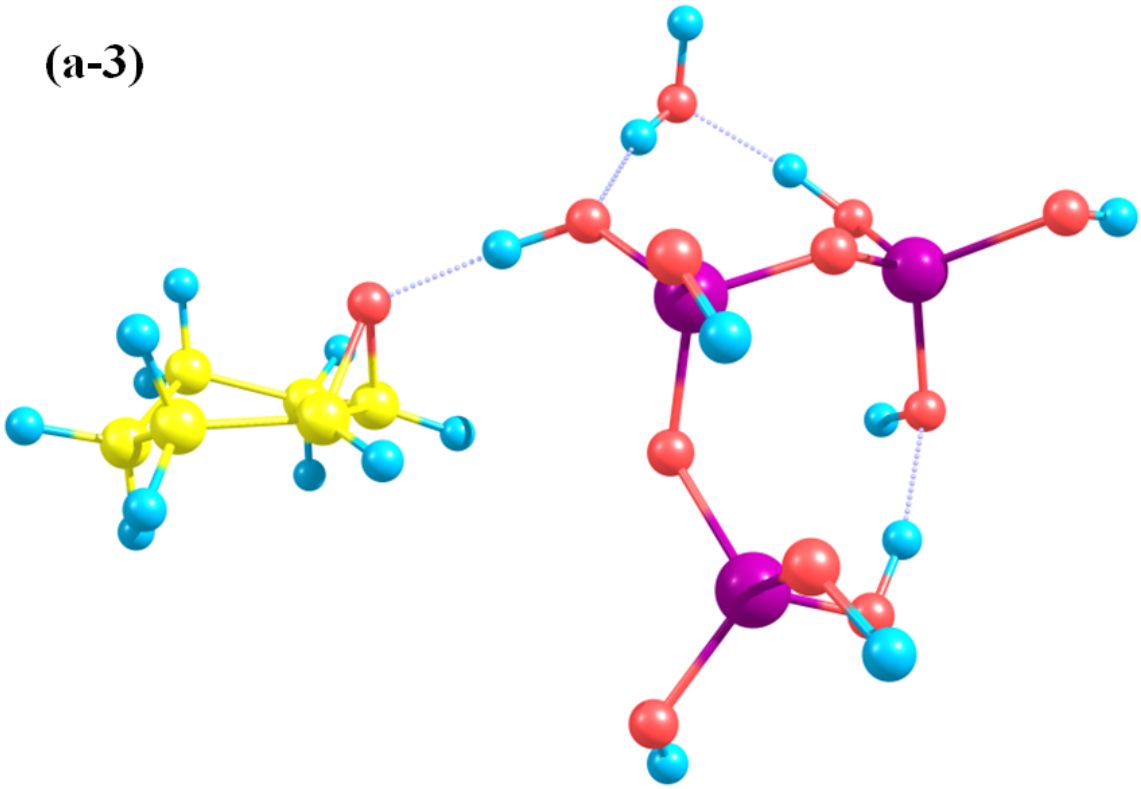


S17- Optimized structures for various reactants, produts and intermedates involved during the silica catalyzed olefin epoxidation. (Nomenclature of each reactant, products and intermediates 1-1 to a-9 is according to as mentiond in the text)

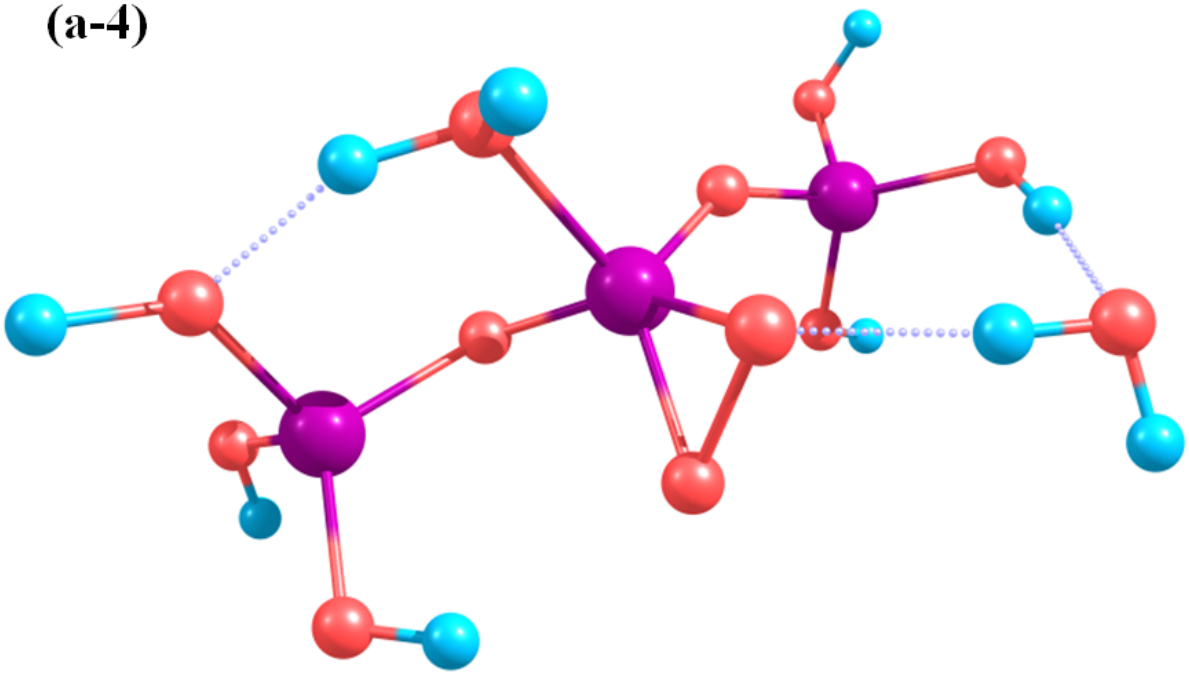




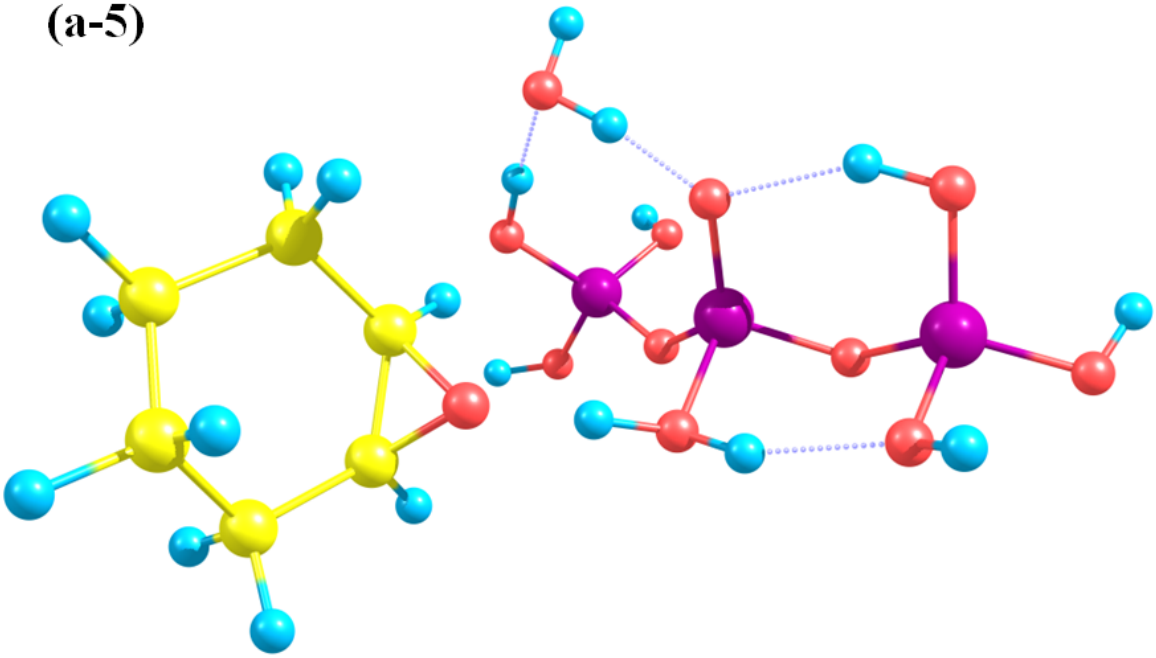
(a-3)



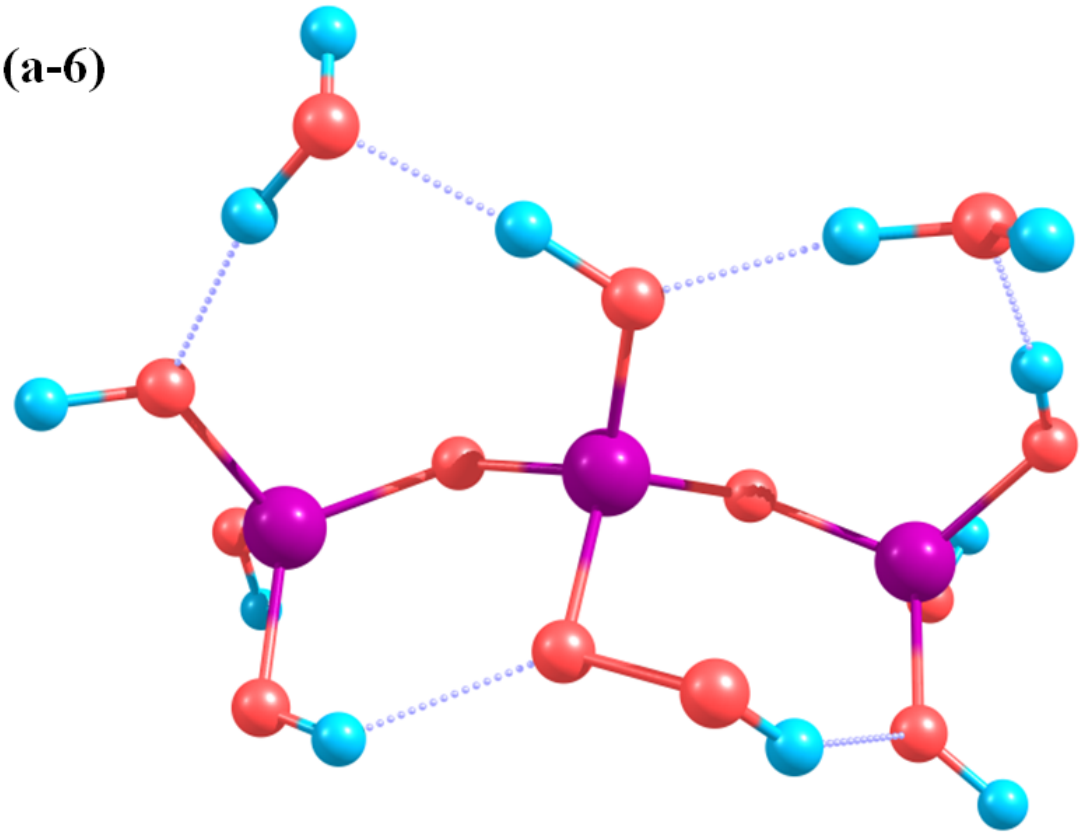
(a-4)



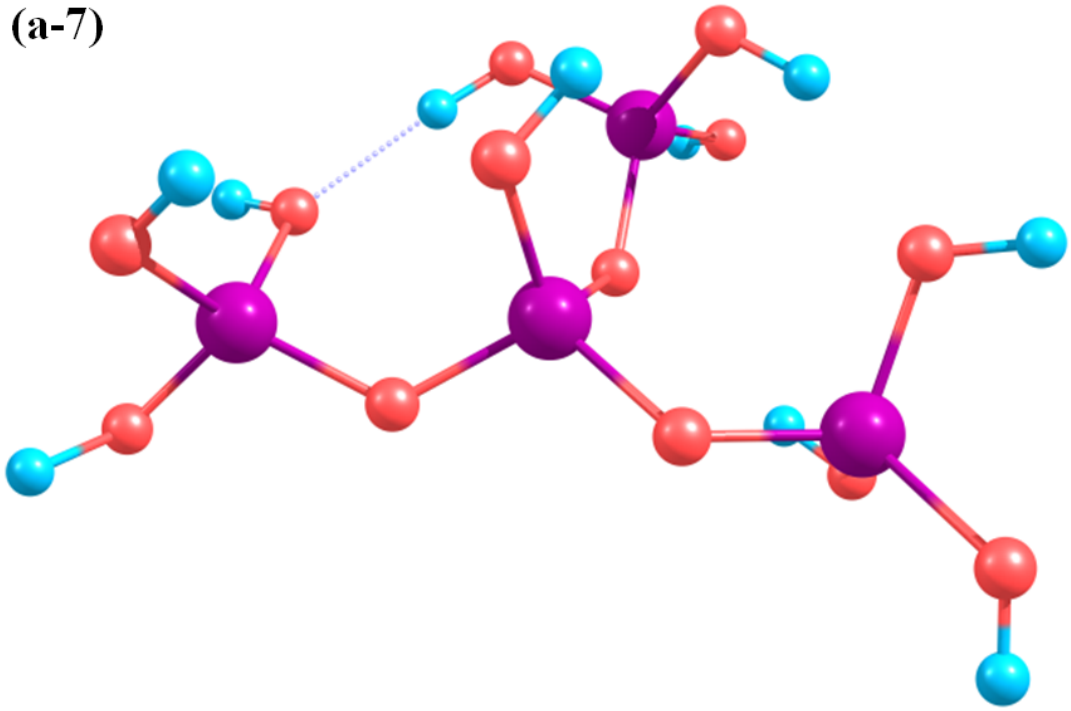
(a-5)



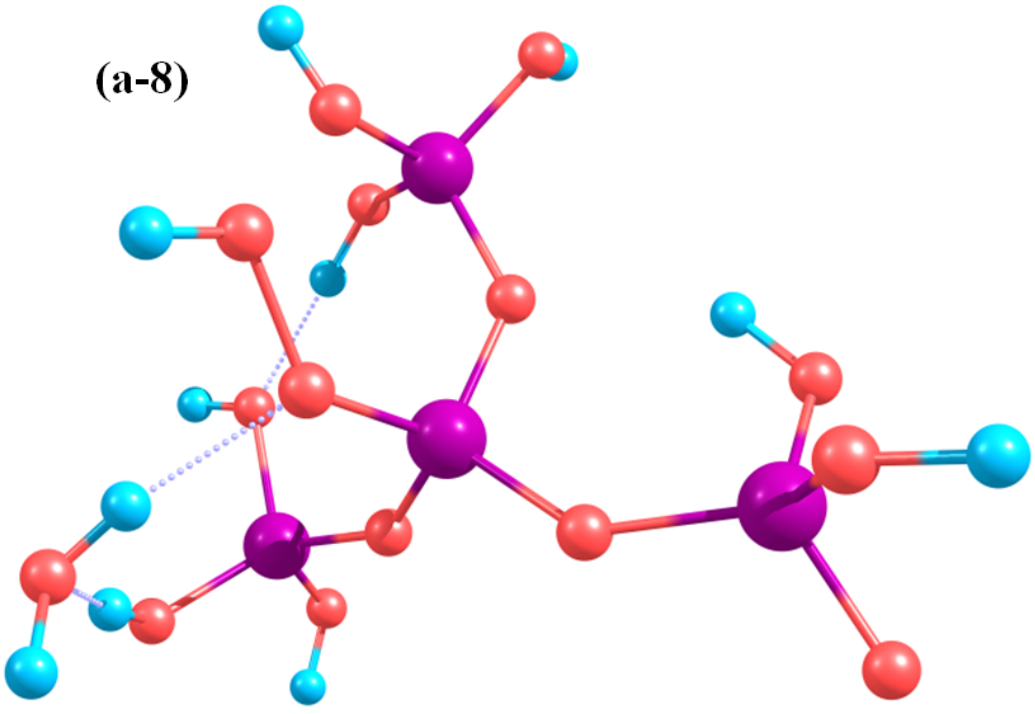
(a-6)

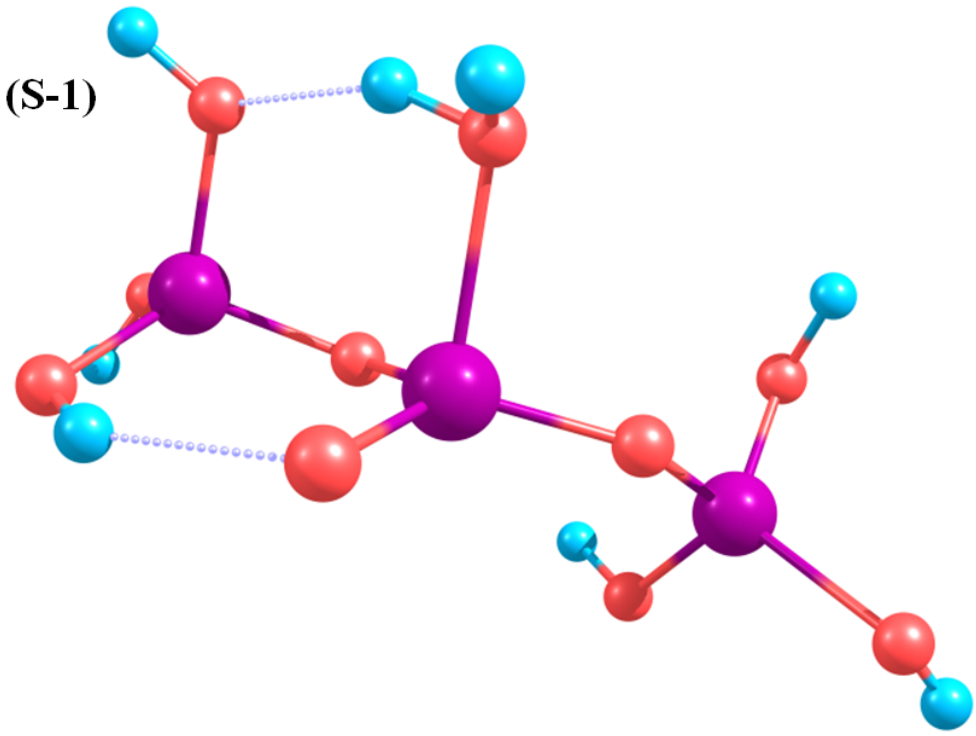


(a-7)



(a-8)





Xyz coordints :

Silica trimer (a-1)

Si	-0.188	0.286	0.066
O	0.840	0.515	1.347
H	1.534	1.177	1.200
O	0.261	-0.888	-1.002
Si	-0.393	-2.320	-1.537
O	-1.453	-2.911	-0.375
O	-1.116	-1.931	-2.982
H	-1.333	-2.689	-3.550
O	0.748	-3.485	-1.753
Si	1.084	-4.951	-1.024
O	2.707	-5.181	-0.736
H	3.004	-4.842	0.123
O	0.294	-5.032	0.438
H	-0.504	-4.461	0.454
O	0.624	-6.075	-2.162
H	0.945	-6.974	-1.988
H	-1.854	-2.188	0.154
O	-0.305	1.753	-0.710
H	-0.577	1.706	-1.641
O	-1.632	-0.294	0.706
H	-1.968	0.170	1.490

TS_for_silica_to_oxo_formation (St-1)

O	0.658	1.494	0.146
Si	-0.335	0.357	-0.524
O	-1.491	-0.072	0.636
O	0.406	-1.131	-0.765
Si	-0.481	-2.315	-1.515
O	0.378	-3.694	-1.559
Si	0.252	-5.289	-1.063
O	-0.194	-6.115	-2.427
O	-0.975	0.929	-1.938
O	-1.973	-2.622	-0.375
O	-1.584	-1.820	-2.575
O	1.702	-5.905	-0.544
O	-0.802	-5.365	0.223
H	1.110	2.068	-0.492
H	1.910	-5.722	0.386
H	-1.533	-4.720	0.203
H	-0.089	-7.079	-2.379
H	-2.023	-1.860	0.264
H	-1.331	0.176	-2.476
H	-2.017	0.654	1.008
H	-2.346	-2.229	-1.375

Optimized_geometry_after_silica_oxo_formation (S-2)

O	0.856	0.858	0.530
Si	-0.208	0.051	-0.441
O	-0.543	0.903	-1.810
O	-1.596	-0.263	0.518
O	0.211	-1.531	-0.787
Si	-0.779	-2.305	-1.906
O	-1.377	-1.417	-3.051
O	-0.343	-3.876	-2.022
Si	0.179	-5.135	-1.062
O	-0.513	-5.003	0.452
O	-2.298	-2.479	-0.655
O	-0.252	-6.480	-1.930
O	1.820	-5.184	-0.816
H	1.486	1.422	0.053
H	2.136	-4.628	-0.086
H	-1.429	-4.678	0.466
H	0.187	-7.299	-1.650
H	-2.215	-1.646	-0.061
H	-0.893	0.256	-2.500
H	-2.079	0.506	0.861
H	-3.090	-2.345	-1.215

TS_Slica_trimer_H_2O_2_activation (t-1)

O	-0.279	0.584	1.670
Si	-0.647	0.239	0.088
O	-2.280	-0.145	0.047
O	0.081	-1.125	-0.506
Si	-0.334	-2.263	-1.651
O	0.458	-3.726	-1.784
Si	-0.322	-5.136	-2.213
O	-1.051	-4.697	-3.680
O	-0.188	1.522	-0.862
O	-1.809	-2.827	-0.985
O	-1.067	-1.949	-3.324
O	0.712	-6.391	-2.524
O	-1.410	-5.616	-1.056

H	0.478	1.181	1.779
H	-1.347	-2.831	-3.691
H	0.912	-6.947	-1.753
H	-1.856	-4.809	-0.707
H	-1.600	-5.382	-4.093
H	-2.331	-2.116	-0.562
H	0.266	1.191	-1.669
H	-2.885	0.471	0.487
O	1.105	-1.505	-2.869
H	-0.002	-1.659	-3.601
O	1.361	-0.050	-2.783
H	2.282	-0.078	-2.458

Silica_trimer_product_H_2O_2_activation (a-2)

O	0.506	0.672	1.961
Si	-0.069	0.228	0.472
O	0.924	0.872	-0.687
O	-1.683	0.683	0.388
O	-0.172	-1.428	0.264
Si	-1.124	-2.213	-0.830
O	-0.913	-1.489	-2.393
O	0.515	-1.193	-2.678
O	-0.708	-3.799	-0.927
Si	-0.056	-4.792	-2.093
O	-1.122	-5.255	-3.256
O	-2.742	-2.061	-0.551
O	-2.129	-3.020	-4.422
O	1.208	-3.827	-2.694
O	0.615	-6.148	-1.422
H	1.471	0.772	2.001
H	-1.933	-2.758	-5.337
H	0.059	-6.941	-1.485
H	-1.568	-4.510	-3.753
H	1.794	-4.269	-3.330
H	-2.962	-1.160	-0.242
H	0.947	0.317	-1.500
H	-1.868	1.632	0.472
H	-1.771	-2.300	-3.849
H	0.898	-2.116	-2.775

Cyclohexene_epoxidation_by_secondary_salinol (t-2)

C	-1.813	0.091	1.578
C	-2.266	-0.797	0.458
C	-3.209	-1.767	0.612
C	-3.901	-2.035	1.914
C	-3.704	-0.903	2.936
C	-2.244	-0.429	2.958
O	-0.905	-2.693	0.924
Si	-0.503	-3.529	-0.511
O	-1.527	-2.960	-1.714
Si	-1.537	-3.471	-3.305
O	-0.922	-5.040	-3.316
O	1.023	-3.113	-1.042
Si	2.205	-3.272	-2.168
O	3.687	-3.097	-1.485
O	2.022	-2.145	-3.411
O	1.907	-4.738	-2.945
O	-0.752	-5.171	-0.357
O	0.410	-3.624	1.519
O	-3.131	-3.496	-3.757
O	-0.704	-2.456	-4.319
O	3.250	-3.469	1.158
H	2.433	-1.281	-3.240
H	-0.109	-4.321	1.967
H	0.236	-2.268	-4.103
H	0.059	-5.086	-3.382
H	-3.279	-3.580	-4.712
H	3.658	-3.238	-0.491
H	2.597	-5.020	-3.568
H	3.554	-2.824	1.817
H	2.267	-3.488	1.250
H	-3.493	-2.361	-0.258
H	-1.862	-0.615	-0.539
H	-4.974	-2.209	1.724
H	-3.521	-2.991	2.320
H	-4.358	-0.056	2.668
H	-4.019	-1.238	3.936

Alternate_mechanism_peroxo_formation_TS (t-3)

O	1.131	-0.052	1.898
Si	0.098	-0.044	0.610
O	-0.273	-1.539	0.008
Si	-1.563	-1.984	-0.965
O	-2.933	-1.323	0.025
O	0.730	0.977	-0.536
O	-1.409	0.470	1.200
O	-1.502	-0.952	-2.284
O	-1.623	-3.597	-1.016
Si	-1.217	-4.965	-1.906
O	-1.154	-6.286	-0.896
O	-2.328	-5.286	-3.071
O	0.328	-4.603	-2.424
O	-3.167	-3.136	-4.403
H	2.075	0.003	1.679
H	-2.627	-2.812	-5.141
H	-1.966	-6.818	-0.920
H	-2.653	-4.514	-3.632
H	0.769	-5.324	-2.900
H	-2.615	-0.546	0.583
H	0.339	0.896	-1.423
H	-1.439	1.296	1.709
H	-3.132	-2.417	-3.706
O	-2.971	-1.439	-2.322
H	-3.381	-1.056	-0.916

Optimized_geometry_for_peroxo_formation (a-4)

O	1.229	0.070	1.700
Si	0.035	-0.034	0.565
O	-1.410	0.381	1.372
O	-0.356	-1.554	0.058
Si	-1.554	-1.959	-1.064
O	-2.618	-1.356	-2.342
O	-1.078	-1.026	-2.413
O	0.385	0.983	-0.697
O	-2.898	-1.378	0.182
O	-1.666	-3.582	-1.030
Si	-1.275	-4.970	-1.882
O	0.300	-4.684	-2.354
O	-1.306	-6.290	-0.868
O	-2.356	-5.269	-3.089
O	-2.976	-3.041	-4.470
H	2.130	0.170	1.351
H	-2.352	-2.787	-5.170
H	-2.127	-6.803	-0.949
H	-2.610	-4.489	-3.668
H	0.721	-5.435	-2.802
H	-2.512	-0.678	0.816
H	-0.043	0.703	-1.533
H	-1.440	1.195	1.897
H	-2.882	-2.340	-3.769
H	-3.611	-0.965	-0.346

TS_for_sharpless_epoxidation_mechanism (t-4)

O	2.443	-0.846	0.222
Si	1.019	-0.871	-0.623
O	0.217	0.577	-0.209
O	-0.105	-1.970	-0.132
Si	-1.610	-2.220	-0.890
O	-2.726	-1.824	-2.199
O	-1.072	-2.529	-2.469
O	1.340	-1.003	-2.247
O	-2.169	-0.530	-0.065
O	-2.349	-3.334	0.063
Si	-2.889	-4.907	0.073
O	-1.508	-5.811	0.326
O	-3.936	-5.147	1.351
O	-3.742	-5.280	-1.296
O	-2.316	-4.727	-3.527
H	3.139	-1.413	-0.145
H	-1.625	-5.371	-3.752
H	-4.864	-5.189	1.069
H	-3.256	-5.133	-2.163
H	-1.685	-6.739	0.546
H	-1.372	0.086	0.022
H	0.591	-1.467	-2.696
H	0.705	1.413	-0.270
H	-1.824	-3.899	-3.260
H	-2.804	-0.144	-0.705
C	-4.909	-0.688	-1.679

C	-4.868	-1.948	-2.213
C	-5.076	0.480	-2.606
C	-6.227	0.240	-3.629
C	-6.343	-1.236	-4.087
C	-5.115	-2.090	-3.688
H	-4.908	-0.548	-0.593
H	-4.866	-2.835	-1.579
H	-4.138	0.613	-3.174
H	-5.243	1.415	-2.053
H	-6.061	0.901	-4.492
H	-7.176	0.559	-3.172
H	-6.482	-1.289	-5.177
H	-7.239	-1.692	-3.639
H	-4.222	-1.737	-4.230
H	-5.255	-3.142	-3.965

Optimized_geometry_after_sharpless_Mechanism (a-5)

C	-5.133	-1.886	-3.993
C	-4.762	-1.763	-2.532
C	-5.337	-0.704	-1.675
C	-6.330	0.287	-2.226
C	-6.293	0.372	-3.761
C	-6.348	-1.026	-4.387
O	-3.961	-0.557	-2.181
Si	-1.228	-2.490	-0.547
O	-2.244	-3.364	0.398
Si	-3.057	-4.824	0.284
O	-3.918	-4.928	-1.123
O	0.131	-1.998	0.297
Si	1.222	-1.058	-0.547
O	1.612	-1.753	-1.997
O	2.588	-0.660	0.296
O	0.308	0.372	-0.713
O	-0.924	-2.904	-2.055
O	-2.071	-0.863	-0.542
O	-1.861	-5.965	0.503
O	-4.163	-4.943	1.528
O	-2.513	-4.506	-3.303
H	3.323	-1.284	0.186
H	-2.005	-5.234	-3.695
H	-5.078	-4.836	1.225
H	-3.391	-4.874	-1.992
H	-2.192	-6.858	0.685
H	-1.361	-0.159	-0.652
H	0.815	-2.275	-2.307
H	0.697	1.065	-1.270
H	-1.819	-3.868	-2.889
H	-2.851	-0.735	-1.244
H	-5.369	-0.882	-0.595
H	-4.386	-2.666	-2.041
H	-6.156	1.273	-1.766
H	-7.329	-0.041	-1.891
H	-5.373	0.888	-4.079
H	-7.139	0.984	-4.109
H	-6.408	-0.956	-5.483
H	-7.273	-1.529	-4.056
H	-4.247	-1.610	-4.587
H	-5.318	-2.948	-4.207

TS_for_conversion of Si=O to Si-(O-H) (OOH) species (t-5)

O	1.084	-0.263	1.095
Si	-0.442	-0.516	0.511
O	-1.472	-0.592	1.809
O	-0.313	-1.965	-0.368
O	-1.033	0.535	-0.599
Si	-1.227	0.846	-2.230
O	0.150	1.459	-2.873
Si	0.855	2.444	-4.013
O	0.194	2.276	-5.507
O	-2.691	0.684	-2.948
O	-0.806	-1.013	-2.763
O	0.662	3.959	-3.291
O	2.490	2.166	-4.132
O	-2.475	2.243	-5.286
H	1.153	0.340	1.852
H	-2.582	3.025	-4.704
H	2.728	1.630	-4.906
H	-0.815	2.237	-5.535
H	1.114	4.694	-3.737
H	-0.572	-1.586	-1.966
H	-2.389	-0.328	1.627
H	0.310	-2.621	-0.016
H	-2.678	1.506	-4.654
H	-1.675	-1.298	-3.116
O	-2.209	2.626	-1.755
H	-2.870	1.853	-2.368
O	-2.046	3.727	-2.734
H	-1.078	3.937	-2.663

Optimized_geometry_for_OH_OOH_formation (a-6)

O	0.923	-1.449	0.971
Si	-0.323	-0.644	0.235
O	0.037	-0.122	-1.299
Si	-0.603	1.040	-2.292
O	-1.334	2.069	-1.141
O	-2.049	3.137	-1.885
O	-0.796	0.608	1.212
O	-1.521	-1.806	-0.023
O	0.565	1.842	-3.115
Si	0.912	3.294	-3.852
O	2.539	3.630	-3.853
O	-1.652	0.392	-3.393
O	-2.741	-1.852	-2.507
O	0.364	3.338	-5.398
O	0.209	4.414	-2.796
O	-1.878	1.890	-5.691
H	1.544	-0.879	1.453
H	-2.711	2.385	-5.627
H	2.983	3.391	-4.683
H	-0.480	2.823	-5.581
H	0.479	5.337	-2.929
H	-2.370	-1.951	-1.592
H	-1.195	1.357	0.718
H	-1.824	-2.270	0.773
H	-1.889	1.264	-4.920
H	-2.446	-2.639	-2.994
H	-2.129	-0.453	-3.105
H	-1.305	3.788	-2.012

Optimized_geometry_after_second_TS_(a-3)

C	-2.983	-0.028	3.319
C	-2.112	0.307	2.099
C	-1.933	-0.871	1.172
C	-2.862	-2.020	1.213
C	-4.019	-2.067	2.192
C	-4.283	-0.719	2.887
O	-1.521	-2.121	1.812
O	0.444	-3.365	0.509
Si	0.083	-4.085	-0.942
O	-0.703	-5.521	-0.696
O	-0.881	-3.058	-1.851
Si	-1.559	-3.311	-3.350
O	-0.598	-2.759	-4.576
O	1.523	-4.321	-1.722
Si	2.725	-3.557	-2.560
O	3.542	-4.802	-3.296
O	-1.827	-4.973	-3.344
O	-3.035	-2.555	-3.503
O	3.643	-2.540	-1.648
O	2.049	-2.577	-3.780
O	3.072	-2.745	0.952
H	2.224	-1.638	-3.597
H	-0.317	-2.960	1.026
H	0.376	-2.750	-4.385
H	-2.158	-5.354	-4.174
H	-2.987	-1.725	-4.004
H	3.529	-2.607	-0.649
H	4.305	-4.526	-3.827
H	3.482	-3.471	1.451
H	2.102	-2.965	0.914
H	-2.955	-2.622	0.304
H	-1.404	-0.680	0.232
H	-4.920	-2.401	1.653
H	-3.798	-2.848	2.938
H	-4.827	-0.053	2.195
H	-4.945	-0.875	3.752
H	-3.206	0.895	3.874

Tertary_salinol_model_optimized (a-7)

O	-0.580	1.211	1.123

Si	-0.890	0.045	-0.009
O	-2.440	-0.543	0.312
O	0.108	-1.284	0.134
Si	-0.056	-2.663	-0.760
O	1.377	-3.479	-0.889
Si	1.549	-5.134	-0.962
O	0.470	-5.641	-2.157
O	-0.734	0.733	-1.513
O	-1.115	-3.731	-0.030
O	-0.642	-2.130	-2.236
O	3.062	-5.597	-1.450
O	1.273	-5.835	0.520
H	0.085	1.867	0.862
H	-1.194	-2.799	-2.700
H	3.708	-5.711	-0.734
H	0.449	-5.541	0.948
H	0.672	-6.524	-2.513
Si	-2.589	-4.213	-0.696
H	-0.708	0.052	-2.216
H	-3.093	0.155	0.486
O	-3.093	-5.611	0.042
O	-3.711	-3.014	-0.526
O	-2.260	-4.520	-2.312
H	-3.333	-2.143	-0.259
H	-3.763	-5.483	0.732
H	-1.484	-5.117	-2.415

Tertary_salinol_H_2O_2_activiation (t-6)

O	-1.755	-0.002	2.177
Si	-1.420	-0.263	0.571
O	-0.836	1.141	-0.090
O	-2.878	-0.782	-0.104
O	-0.318	-1.468	0.303
Si	0.027	-2.595	-0.860
O	-0.495	-2.260	-2.559
O	1.268	-3.696	-0.681
Si	1.167	-5.358	-0.677
O	0.319	-5.941	0.626
O	-1.274	-3.694	-0.544
Si	-2.541	-4.175	-1.503
O	-1.853	-4.410	-3.044
O	0.506	-5.781	-2.179
O	2.666	-6.070	-0.638
O	-3.125	-5.625	-0.937
O	-3.725	-3.031	-1.613
H	-1.173	0.647	2.602
H	-0.939	-3.033	-3.059
H	2.991	-6.280	0.251
H	-0.537	-5.487	0.739
H	0.767	-6.674	-2.463
H	-0.105	0.929	-0.717
H	-3.628	-0.205	0.118
H	-3.488	-2.203	-1.129
H	-4.067	-5.616	-0.706
H	-1.140	-5.092	-2.974
O	1.426	-1.449	-1.733
O	1.341	0.015	-1.548
H	2.194	0.159	-1.094
H	0.484	-1.779	-2.720

Optimized_geometry_after_tertary_salinol_activation (a-8)

O	3.676	-0.804	-1.975
Si	5.107	0.031	-1.915
O	5.091	0.968	-0.515
O	6.343	-1.047	-2.023
O	5.151	1.197	-3.115
Si	6.173	2.459	-3.489
O	7.577	1.953	-4.171
Si	9.069	1.255	-3.945
O	10.202	2.310	-3.405
O	5.381	3.475	-4.490
Si	3.852	3.625	-5.153
O	3.149	4.874	-4.321
O	6.710	3.183	-2.042
O	3.077	2.152	-5.071
O	3.897	4.064	-6.757
O	8.736	-0.013	-2.873
O	9.618	0.558	-5.347
O	9.274	4.143	-1.688
H	3.732	-1.658	-2.433
H	7.223	-0.703	-2.333
O	5.513	3.604	-1.270
H	3.372	1.586	-4.332
H	3.960	3.315	-7.371
H	2.370	5.258	-4.754
H	9.524	-0.502	-2.580
H	10.211	1.128	-5.863
H	9.918	3.017	-2.750
H	8.303	3.957	-1.667
H	9.356	5.078	-1.938
H	5.035	0.485	0.324
H	5.352	2.764	-0.759

TS_for_cyclohexene_epoxidation_by_tertary_salinol (t-7)

O	-1.934	0.428	2.009
Si	-1.487	0.009	0.460
O	-2.861	-0.674	-0.258
O	-0.390	-1.225	0.483
Si	0.340	-2.518	-0.232
O	-0.720	-3.791	-0.510
Si	-2.009	-4.128	-1.512
O	-2.475	-5.716	-1.340
O	-0.953	1.381	-0.269
O	1.358	-2.144	-1.562
O	0.108	0.989	-2.703
O	-0.195	-1.651	-2.218
O	1.352	-3.121	0.942
Si	1.434	-4.428	1.960
O	2.803	-5.240	1.454
O	1.699	-4.026	3.555
O	0.021	-5.306	1.889
O	-3.325	-3.184	-1.218
O	-1.348	-3.978	-3.059
H	-1.486	1.226	2.333
H	-0.341	-2.403	-2.847
H	0.888	-3.825	4.050
H	-0.451	-5.163	1.044
H	3.137	-5.896	2.085
H	-0.541	1.310	-1.182
H	-3.634	-0.085	-0.261
H	-3.159	-2.260	-0.885
H	-3.267	-5.829	-0.790
H	-1.922	-4.273	-3.784
H	1.036	1.236	-2.849
H	0.091	-0.006	-2.689
C	3.528	-3.246	-1.340
C	3.585	-1.956	-0.897
C	3.876	-3.639	-2.743
C	4.639	-2.539	-3.500
C	4.004	-1.163	-3.261
C	4.004	-0.809	-1.766
H	3.262	-4.034	-0.632
H	3.394	-1.758	0.159
H	4.456	-4.577	-2.721
H	2.939	-3.893	-3.272
H	5.686	-2.521	-3.154
H	4.668	-2.772	-4.575
H	4.535	-0.387	-3.833
H	2.964	-1.178	-3.626
H	5.015	-0.490	-1.447

Optimized_geometry_after_tertary_salinol_catalyzed_epoxidation (a-9)

C	5.063	0.058	-1.974
C	3.732	-0.653	-1.912
C	3.575	-2.020	-2.454
C	4.733	-2.750	-3.106
C	6.093	-2.072	-2.863
C	6.012	-0.548	-3.020
O	3.056	-0.858	-3.189
O	-0.485	-3.087	-1.721
Si	-0.520	-3.090	-0.046
O	0.819	-3.794	0.588
Si	1.153	-5.144	1.508
O	-0.222	-5.629	2.313
O	-0.582	-1.541	0.501
Si	-1.269	-0.051	0.224
O	-0.518	0.807	-0.948
O	-1.289	0.850	1.620
O	-2.885	-0.435	-0.125
O	-1.854	-3.975	0.450
Si	-3.386	-4.096	-0.213
O	-3.011	-4.333	-1.839
O	-4.175	-5.442	0.347

O	-4.318	-2.777	0.108
O	1.783	-6.234	0.422
O	2.319	-4.867	2.661
O	0.299	-0.663	-2.954
H	-0.563	1.493	1.673
H	-1.233	-3.603	-2.102
H	1.966	-4.518	3.496
H	-1.049	-5.390	1.851
H	2.174	-7.026	0.826
H	-0.185	0.292	-1.764
H	-3.409	0.330	-0.415
H	-3.849	-1.901	0.069
H	-4.815	-5.261	1.054
H	-3.760	-4.452	-2.446
H	1.277	-0.687	-3.124
H	0.055	-1.579	-2.685
H	2.776	-2.643	-2.038
H	3.052	-0.337	-1.113
H	4.751	-3.785	-2.731
H	4.524	-2.814	-4.187
H	6.439	-2.308	-1.842
H	6.843	-2.491	-3.551
H	7.010	-0.098	-2.910
H	5.656	-0.295	-4.030
H	5.517	-0.011	-0.970
H	4.892	1.129	-2.168