Electronic Supplementary Material (ESI) for RSC Advances.

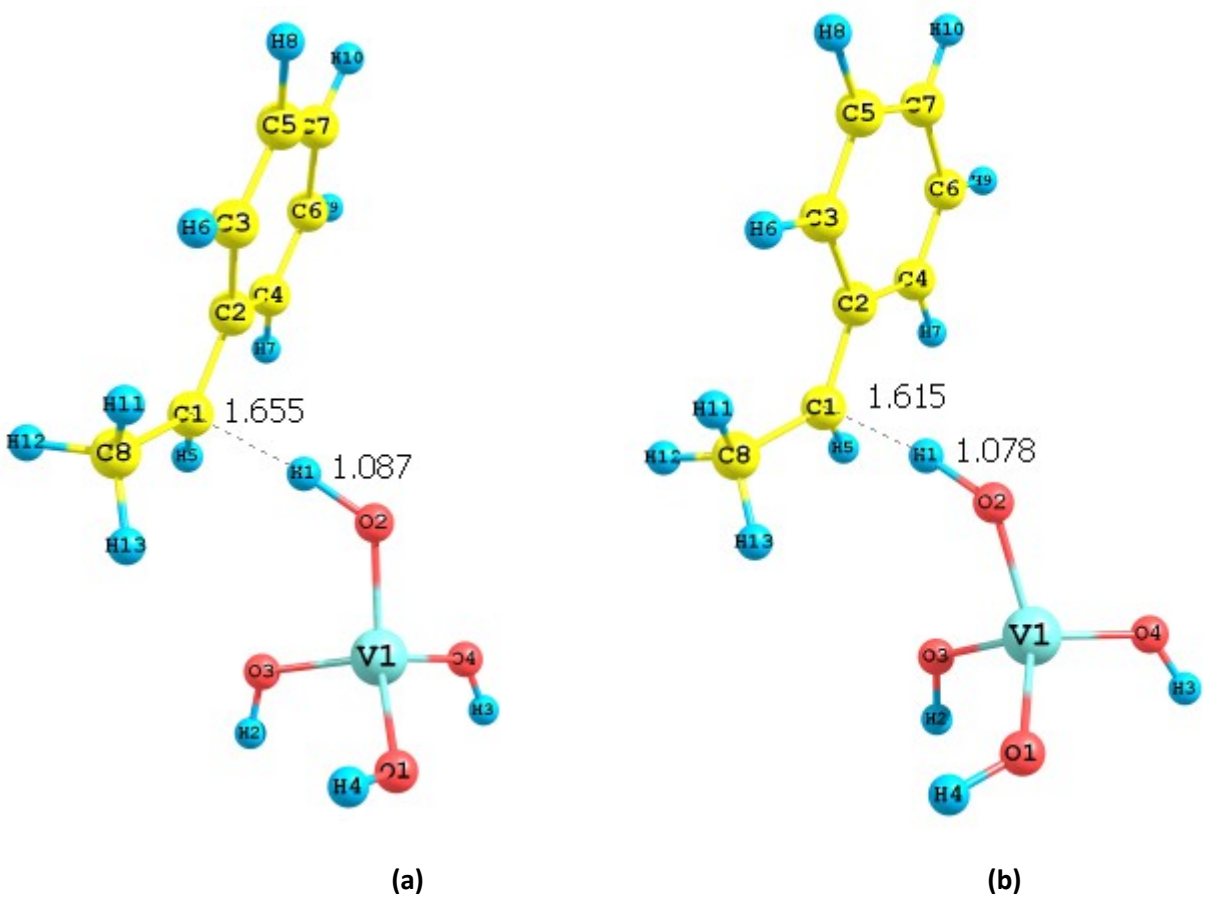

Figure: 1. TS structure modeled for calculation of closed shell vs open shell correction term. (a) The TS structure as closed shell calculation; (b) TS structure as open shell calculation.

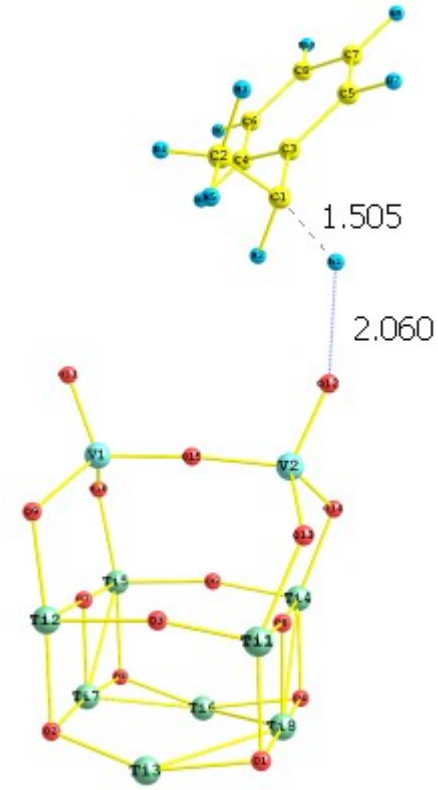

Figure 2. The Transition State (TS) structures for first hydrogen atom abstraction

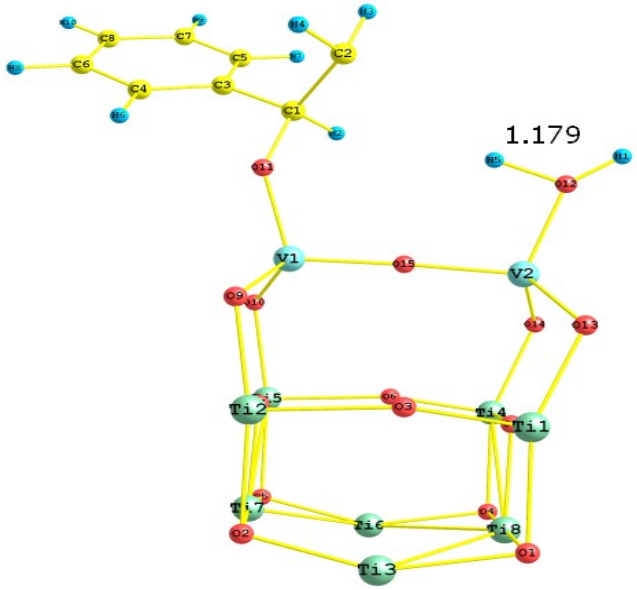

Figure 3. The TS structure for methyl H removal by V-OH.

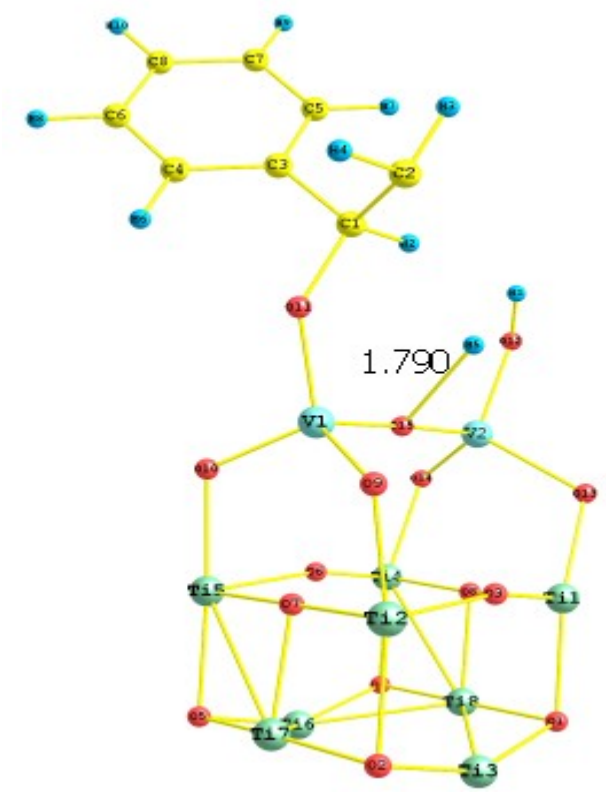

Figure 4. TS structure for methyl H removal by O2.

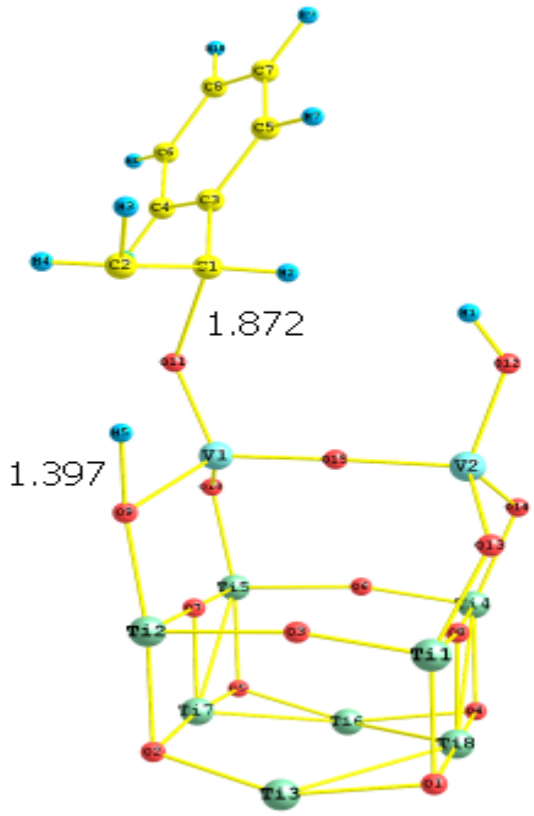

Figure 5. TS structure for methyl H removal by O3.

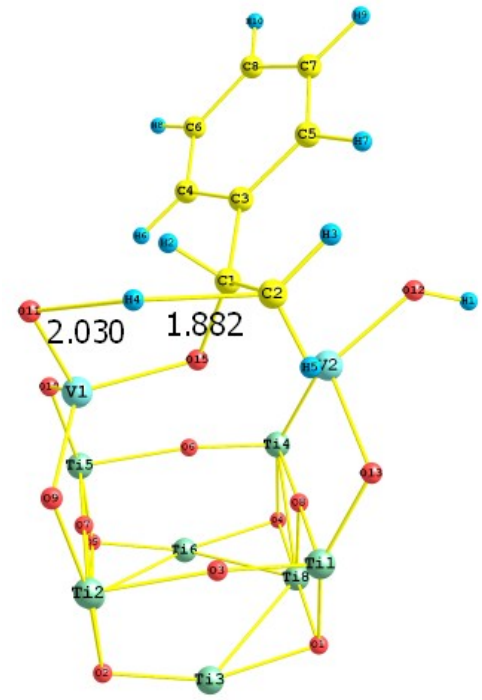

Figure 6(a). TS structure for methyl H removal by O1 site (Radical adsorb on O2 site).

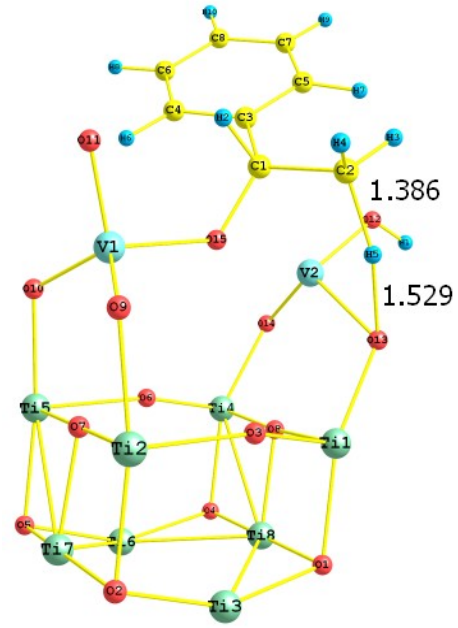

Figure 6(b). TS structure for methyl H atom removal by O3 (Radical adsorb on O2 site).

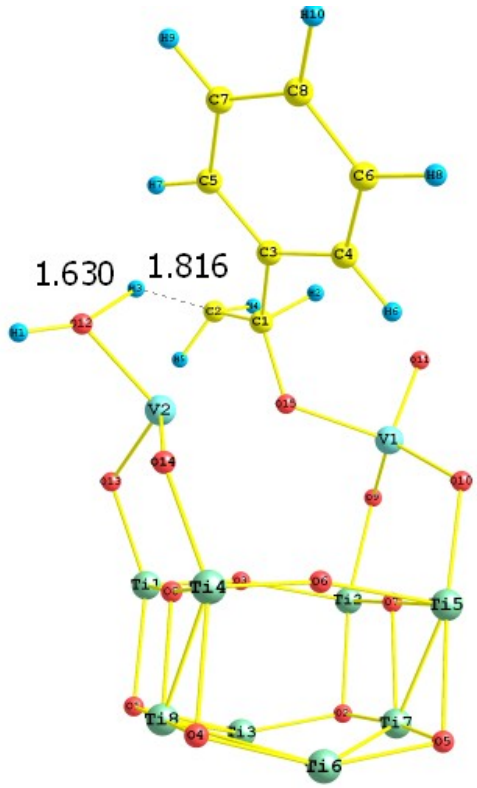

Figure 6(c). TS structure for methyl H removal by VOH (Radical adsorb on O2 site).

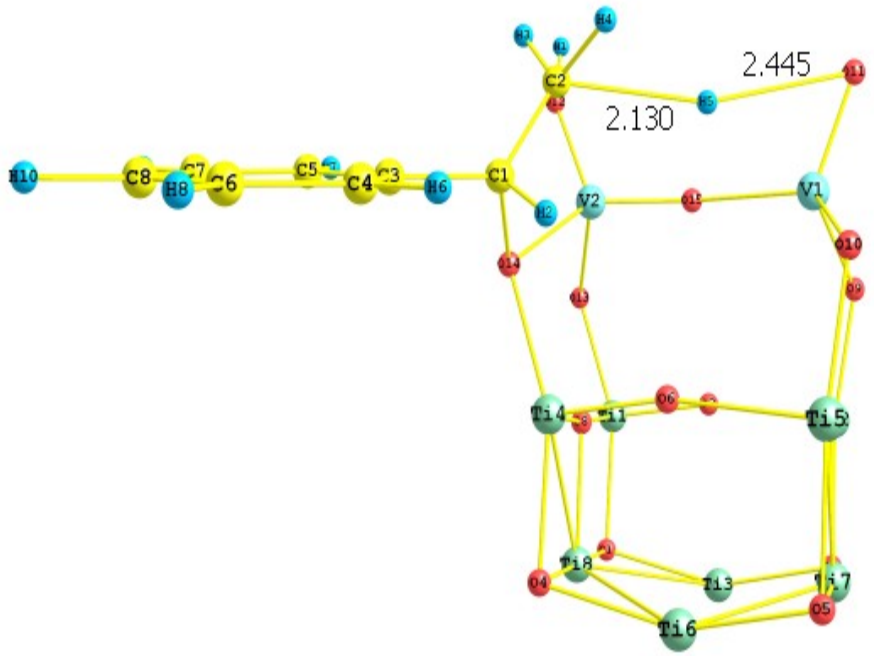

Figure 7(a). TS structure for methyl H removal by O1 (Radical adsorb on O3 site).

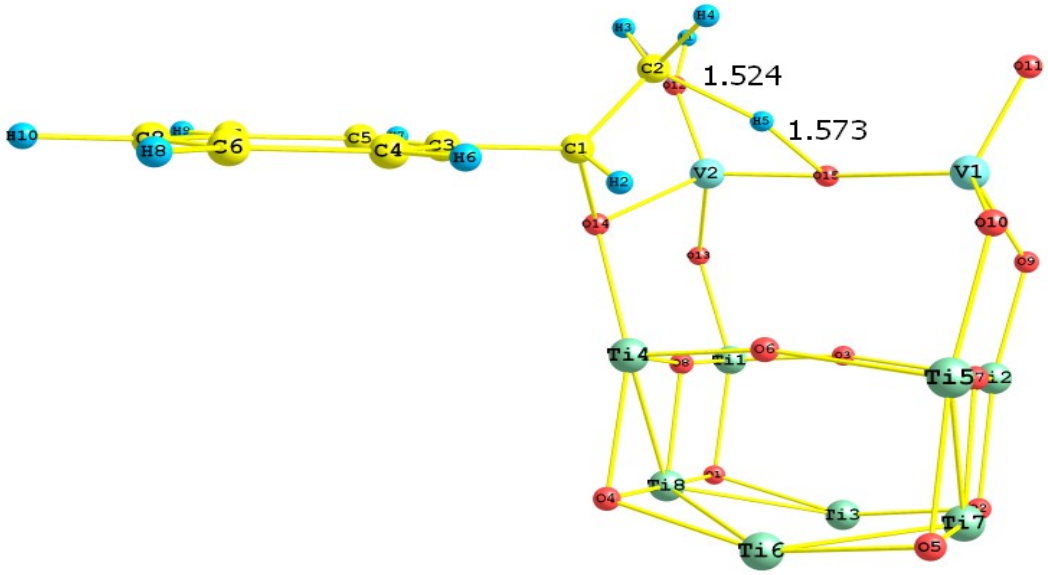

Figure 7(b). TS structure for methyl H removal by O2 (Radical adsorb on O3 site).

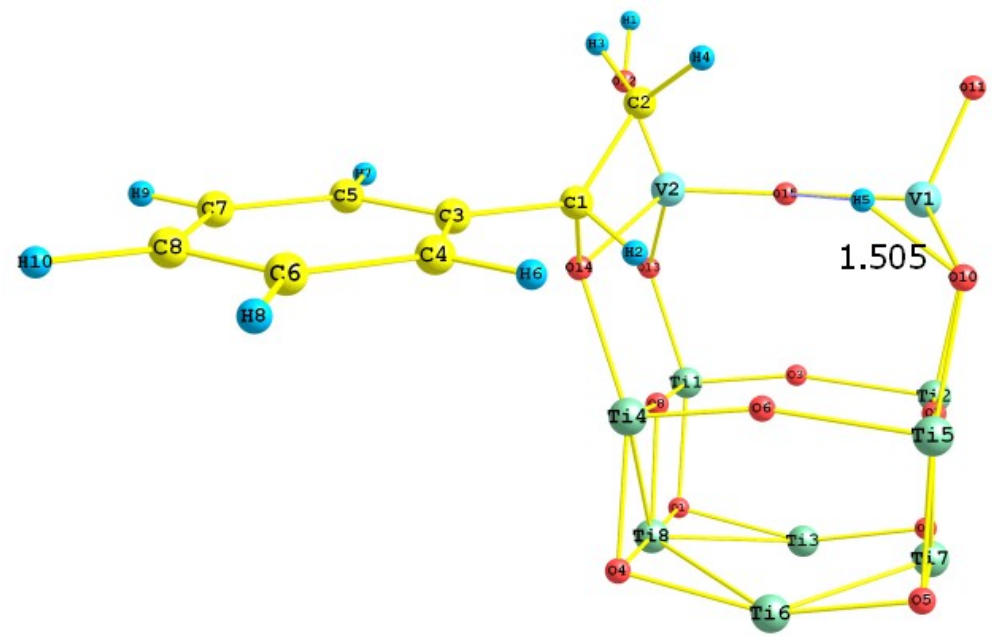

Figure 7(c). TS structure for methyl H removal by O3 site (Radical adsorbs on O3 site).

List of Cartesian Coordinate

S1. Cartesian coordinate for TS structure as closed shell calculation. Fig. 1.(a)

V	2.569804000	-0.306235000	-0.202809000
O	3.588502000	0.749686000	-1.174049000
O	0.854521261	-0.336512391	-0.619214576
H	0.057936685	0.188759359	-0.098935739
O	2.588334000	0.326030000	1.461289000
H	3.437649000	0.408770000	1.914535000
O	3.081644000	-1.995986000	-0.135136000
H	3.934652000	-2.384647000	0.074801000
H	3.374046543	1.741578793	-1.449707033
C	-1.004439630	1.065987315	0.818360946
H	-0.515901261	0.636490315	1.684361576
C	-2.194157000	0.402102370	0.366897315
C	-3.057053685	0.902378370	-0.633573315
C	-2.536501315	-0.845756946	0.947037685
C	-4.166491315	0.186310685	-1.048541000
H	-2.847874370	1.860228054	-1.101727315
C	-3.648653630	-1.554514630	0.532065685
H	-1.901831315	-1.248833261	1.727042685
C	-4.472187946	-1.050646000	-0.479507685
H	-4.807508000	0.592982000	-1.825174000
H	-3.882993630	-2.509100630	0.996144370
H	-5.343075261	-1.604831685	-0.809756370
C	-0.652131793	2.492270054	0.492520370

H	-1.091369478	2.835096739	-0.444817946
H	-1.012181957	3.175247946	1.282601424
H	0.429327522	2.638611587	0.435587793

S2. Cartesian coordinate for TS structure as open shell calculation. Fig. 1.(b)

V	2.569804000	-0.306235000	-0.202809000
O	3.588502000	0.749686000	-1.174049000
O	0.874496000	-0.136765000	-0.644183000
H	0.052943000	0.273652000	-0.078961000
O	2.588334000	0.326030000	1.461289000
H	3.437649000	0.408770000	1.914535000
O	3.081644000	-1.995986000	-0.135136000
H	3.934652000	-2.384647000	0.074801000
H	3.683655000	1.706623000	-1.165067000
C	-1.014427000	1.070981000	0.833342000
H	-0.535876000	0.641484000	1.709330000
C	-2.194157000	0.392115000	0.371891000
C	-3.052060000	0.892391000	-0.638567000
C	-2.541495000	-0.860738000	0.942044000
C	-4.171485000	0.181317000	-1.048541000
H	-2.837887000	1.845247000	-1.106721000
C	-3.658641000	-1.564502000	0.527072000
H	-1.906825000	-1.268808000	1.722049000
C	-4.487169000	-1.050646000	-0.474514000
H	-4.807508000	0.592982000	-1.825174000

H	-3.892981000	-2.519088000	0.986157000
H	-5.363050000	-1.599838000	-0.799769000
C	-0.617176000	2.477289000	0.482533000
H	-1.051420000	2.815122000	-0.459799000
H	-0.932283000	3.190229000	1.257633000
H	0.469277000	2.568700000	0.400632000

S.3 Model showing monolayer distribution of V_2O_5 over TiO_2 (Fig. 7)

Ti	**-4.290973000**	**-2.607014000**	**1.902548000**
Ti	**-4.290229000**	**-2.629912000**	**-1.886583000**
Ti	**-0.509760000**	**-2.264029000**	**1.901217000**
Ti	**-0.509016000**	**-2.286927000**	**-1.887913000**
Ti	**3.258967000**	**-1.922175000**	**1.899891000**
Ti	**3.259711000**	**-1.945074000**	**-1.889239000**
O	**-6.208382000**	**-2.400663000**	**-1.888345000**
O	**-6.209126000**	**-2.377764000**	**1.900786000**
O	**-2.439655000**	**-2.058809000**	**-1.889671000**
O	**-2.440399000**	**-2.035911000**	**1.899460000**
O	**1.340814000**	**-1.692926000**	**1.898129000**
O	**1.341558000**	**-1.715824000**	**-1.891001000**
O	**5.110285000**	**-1.373971000**	**-1.892327000**
O	**5.109541000**	**-1.351072000**	**1.896803000**
O	**-4.254330000**	**-3.018314000**	**0.010406000**
O	**-0.473118000**	**-2.675329000**	**0.009076000**
O	**3.295610000**	**-2.333476000**	**0.007749000**

Ti	-6.385518000	-0.388858000	2.069216000
Ti	-6.384128000	-0.417928000	-2.056565000
Ti	-2.617027000	-0.060964000	2.068507000
Ti	-2.615653000	-0.091243000	-2.058124000
Ti	1.156902000	0.283252000	2.068859000
Ti	1.158033000	0.254966000	-2.058091000
Ti	4.924871000	0.621850000	2.066428000
Ti	4.926335000	0.593026000	-2.060292000
O	-4.465977000	-0.655293000	1.731607000
O	-4.465628000	-0.673143000	-1.719872000
O	-0.689976000	-0.348573000	-1.794777000
O	-0.690351000	-0.328475000	1.802648000
O	3.078875000	0.013876000	-1.721831000
O	3.078376000	0.031032000	1.730066000
O	-6.615373000	1.254460000	-1.378097000
O	-6.612266000	1.273525000	1.370480000
O	-2.694966000	1.595659000	-1.374331000
O	-2.699506000	1.617838000	1.369608000
O	0.905327000	1.925530000	-1.377887000
O	0.912656000	1.945212000	1.371149000
O	4.845817000	2.301582000	1.367543000
O	4.851170000	2.282687000	-1.379949000
V	-6.409762000	2.364658000	-0.013221000
V	-3.102542000	2.651145000	-0.013272000
V	1.118982000	3.034245000	-0.013069000

V	4.436535000	3.331605000	-0.015768000
O	-4.808635000	3.097726000	-0.022962000
O	2.725465000	3.752757000	-0.025694000
O	-7.428781000	3.588343000	-0.023604000
O	-2.319703000	4.037511000	-0.028552000
O	0.114260000	4.270561000	-0.020458000
O	5.201649000	4.728527000	-0.027709000

S.4. Catalyst model used for the calculation representing all type of the oxygen (Fig.8)

Ti	-1.826292000	0.492864000	1.625975000
Ti	-5.571059000	0.450078000	1.558378000
O	-1.750728000	-1.474818000	1.836692000
O	-5.499372000	-1.518026000	1.759318000
O	-3.522799000	0.679857000	1.627595000
Ti	-3.684732000	-1.865302000	1.970919000
Ti	-1.809120000	-0.033596000	-1.595799000
Ti	-5.554952000	-0.076917000	-1.680251000
O	-1.734292000	-2.002901000	-1.409319000
O	-5.482423000	-2.045255000	-1.478422000
O	-3.506178000	0.152067000	-1.604183000
Ti	-3.668060000	-2.392620000	-1.267629000
Ti	-5.574524000	-1.740241000	0.025976000
O	-5.563796000	0.191992000	-0.029106000
O	-1.776604000	0.139754000	0.016083000
Ti	-1.748059000	-1.740060000	0.206984000

V	-5.265573000	2.907070000	-0.397360000
V	-1.672239000	2.928181000	-0.384471000
O	-5.823408000	2.256489000	1.231741000
O	-5.793417000	1.839383000	-1.736278000
O	-5.985637000	4.307835000	-0.616267000
O	-0.881941000	4.297502000	-0.584351000
O	-1.172632000	2.172001000	1.208795000
O	-1.209338000	1.797526000	-1.686553000
O	-3.463756000	3.056821000	-0.390476000

S.5. The Transition State (TS) structures for first hydrogen atom abstraction (Fig.2)

Ti	1.241268000	-1.888197000	-1.589698000
Ti	1.853577000	1.805256000	-1.702523000
O	3.157367000	-2.253092000	-1.247195000
O	3.768153000	1.445132000	-1.350939000
O	1.330786000	-0.189451000	-1.728535000
Ti	3.868824000	-0.411773000	-1.366656000
Ti	0.888368000	-1.682995000	1.649227000
Ti	1.496985000	2.012950000	1.552327000
O	2.799730000	-2.045137000	2.015425000
O	3.411778000	1.651981000	1.903732000
O	0.976638000	0.017041000	1.520233000
Ti	3.512389000	-0.204641000	1.888604000
Ti	3.533480000	1.647032000	0.370668000
O	1.678635000	1.907781000	-0.107167000

O	1.144140000	-1.838611000	0.055598000
Ti	2.978793000	-2.143201000	0.390599000
V	-1.032657000	2.064027000	-0.477084000
V	-1.577603000	-1.487974000	-0.288495000
O	0.087148000	2.403478000	-1.884344000
O	-0.292127000	2.604921000	1.050893000
O	-2.378374000	2.888096000	-0.688860000
O	-3.108934000	-1.897195000	-0.439293000
O	-0.582001000	-2.268643000	-1.609914000
O	-0.943845000	-2.075012000	1.289061000
O	-1.384326000	0.280167000	-0.403785000
C	-6.042977000	-0.547577000	-1.036424000
H	-5.094090000	-1.713660000	-0.958012000
H	-5.082082000	-0.232742000	-0.613106000
C	-6.236590000	0.136844000	-2.414737000
H	-7.174017000	-0.184807000	-2.888546000
H	-6.269345000	1.229209000	-2.308887000
H	-5.404736000	-0.115940000	-3.085457000
C	-7.171500000	-0.231698000	-0.066844000
C	-7.123346000	0.924410000	0.746375000
C	-8.310792000	-1.063694000	0.024165000
C	-8.181257000	1.242636000	1.619016000
H	-6.249622000	1.572683000	0.697052000
C	-9.372384000	-0.751088000	0.895239000
H	-8.361844000	-1.963858000	-0.586799000

C	-9.312384000	0.405795000	1.696808000
H	-8.121393000	2.135583000	2.237965000
H	-10.238481000	-1.407619000	0.952111000
H	-10.129671000	0.648509000	2.372550000

S.6. The TS structure for methyl H removal by V-OH (Fig.3)

Ti	1.733716000	1.946449000	1.401873000
Ti	0.791855000	-1.649871000	1.858631000
O	3.644910000	1.477083000	1.180683000
O	2.700074000	-2.123925000	1.628683000
O	1.121713000	0.378269000	1.683461000
Ti	3.543949000	-0.471508000	1.502699000
Ti	1.452711000	1.560828000	-1.827618000
Ti	0.507081000	-2.037956000	-1.386771000
O	3.359374000	1.088363000	-2.072500000
O	2.415833000	-2.511309000	-1.616592000
O	0.839425000	-0.009061000	-1.555805000
Ti	3.259562000	-0.859188000	-1.743144000
Ti	2.470075000	-2.394611000	-0.084091000
O	0.651835000	-1.840686000	0.267951000
O	1.688144000	1.767508000	-0.236661000
Ti	3.500218000	1.276560000	-0.451857000
V	-1.873246000	-0.885254000	0.447683000
V	-0.945486000	2.526645000	-0.058285000
O	-1.048648000	-1.487031000	2.014174000

O	-1.420506000	-1.830867000	-0.957332000
O	-3.607215000	-0.941543000	0.733978000
O	-2.419724000	3.490283000	0.200189000
O	0.266205000	3.005646000	1.355424000
O	-0.139196000	2.631602000	-1.643207000
O	-1.452174000	0.801253000	0.208771000
C	-4.823775000	-0.337152000	0.213094000
H	-2.751608000	4.412660000	0.197245000
H	-4.563406000	0.197236000	-0.716724000
C	-5.281920000	0.709644000	1.248998000
H	-6.194454000	1.214584000	0.907886000
H	-5.492880000	0.217265000	2.205463000
H	-3.036181000	2.520136000	0.462629000
C	-5.807102000	-1.448594000	-0.142491000
C	-5.749476000	-2.704171000	0.495178000
C	-6.818409000	-1.206930000	-1.096550000
C	-6.695463000	-3.699975000	0.188378000
H	-4.952308000	-2.894970000	1.207368000
C	-7.765765000	-2.201084000	-1.403075000
H	-6.864424000	-0.246007000	-1.608279000
C	-7.708069000	-3.452531000	-0.758808000
H	-6.638698000	-4.667794000	0.682113000
H	-8.537253000	-2.004112000	-2.144168000
H	-8.436614000	-4.224259000	-0.997005000

S.7. TS structure for methyl H removal by O2 (Fig.4)

Ti	1.739225000	1.944865000	1.408801000
Ti	0.784730000	-1.650219000	1.848753000
O	3.649716000	1.470429000	1.192406000
O	2.692262000	-2.129301000	1.623572000
O	1.121431000	0.377536000	1.682369000
Ti	3.541648000	-0.479039000	1.506720000
Ti	1.468162000	1.572265000	-1.823067000
Ti	0.509945000	-2.025212000	-1.399048000
O	3.374194000	1.094833000	-2.063182000
O	2.418012000	-2.503595000	-1.624098000
O	0.849113000	0.003268000	-1.559285000
Ti	3.267253000	-0.853625000	-1.741519000
Ti	2.467333000	-2.392830000	-0.090990000
O	0.649604000	-1.834616000	0.256894000
O	1.698747000	1.772230000	-0.230543000
Ti	3.510032000	1.276496000	-0.441366000
V	-1.873128000	-0.872066000	0.431558000
V	-0.933132000	2.538828000	-0.058348000
O	-1.055788000	-1.482277000	1.998589000
O	-1.418463000	-1.813782000	-0.975452000
O	-3.608238000	-0.924071000	0.711683000
O	-2.405279000	3.506040000	0.198696000
O	0.275150000	3.008760000	1.361310000
O	-0.121068000	2.647253000	-1.640085000

O	-1.446046000	0.814018000	0.200456000
C	-4.688840000	-0.015763000	1.063681000
H	-3.225414000	3.298752000	0.694018000
H	-4.300675000	1.014681000	0.989943000
C	-5.099732000	-0.299993000	2.522844000
H	-5.915015000	0.367183000	2.829815000
H	-5.443950000	-1.336621000	2.616020000
H	-2.561896000	1.216053000	1.541108000
C	-5.850489000	-0.187277000	0.089087000
C	-6.042502000	-1.395649000	-0.610472000
C	-6.774050000	0.864867000	-0.088117000
C	-7.147433000	-1.551247000	-1.468120000
H	-5.313494000	-2.191752000	-0.492730000
C	-7.880028000	0.710081000	-0.944058000
H	-6.628343000	1.809775000	0.434640000
C	-8.071388000	-0.501639000	-1.636620000
H	-7.283370000	-2.486044000	-2.007883000
H	-8.581897000	1.530553000	-1.076032000
H	-8.923179000	-0.622422000	-2.302159000

S.8. TS structure for methyl H removal by O3 (Fig.5)

Ti	1.705431000	1.948506000	1.431565000
Ti	0.877742000	-1.683337000	1.823860000
O	3.634162000	1.546052000	1.231765000
O	2.803780000	-2.090447000	1.615194000

O	1.142179000	0.356961000	1.682084000
Ti	3.593739000	-0.409295000	1.524823000
Ti	1.483167000	1.600800000	-1.806795000
Ti	0.652018000	-2.033400000	-1.430498000
O	3.407808000	1.195443000	-2.030393000
O	2.578564000	-2.439793000	-1.639020000
O	0.918827000	0.007646000	-1.566092000
Ti	3.368395000	-0.758932000	-1.729964000
Ti	2.607196000	-2.343667000	-0.104399000
O	0.766685000	-1.855530000	0.228776000
O	1.689040000	1.792007000	-0.209815000
Ti	3.519352000	1.364611000	-0.405376000
V	-1.764022000	-0.957061000	0.328171000
V	-0.958251000	2.491794000	-0.073762000
O	-1.018319000	-1.567348000	1.976178000
O	-1.275762000	-1.870500000	-1.069704000
O	-3.407876000	-1.078018000	0.757700000
O	-2.457589000	3.406300000	0.190234000
O	0.223699000	2.972202000	1.376127000
O	-0.128447000	2.626713000	-1.646812000
O	-1.392123000	0.741888000	0.153142000
C	-4.684196000	0.090450000	1.472030000
H	-3.279352000	3.179673000	0.672235000
H	-4.336978000	1.141617000	1.366021000
C	-4.613061000	-0.353748000	2.906717000

H	-5.212819000	0.261780000	3.587946000
H	-4.928207000	-1.401208000	2.992694000
H	-2.217812000	-1.071542000	2.492604000
C	-5.982887000	-0.040283000	0.697855000
C	-6.312849000	-1.195603000	-0.043872000
C	-6.909239000	1.023461000	0.760188000
C	-7.548176000	-1.283981000	-0.710712000
H	-5.592896000	-2.006841000	-0.089329000
C	-8.146378000	0.933475000	0.096284000
H	-6.663937000	1.925523000	1.319778000
C	-8.470476000	-0.221051000	-0.643205000
H	-7.790055000	-2.177611000	-1.282248000
H	-8.848647000	1.762484000	0.148509000
H	-9.424631000	-0.288970000	-1.160818000

S.9. TS structure for methyl H removal by O1 (Radical adsorb on O2 site).(Fig.6(a))

Ti	0.754048000	-1.827724000	-1.679312000
Ti	1.671682000	1.802459000	-1.640167000
O	2.604101000	-2.359613000	-1.214103000
O	3.519976000	1.276371000	-1.165302000
O	0.991373000	-0.140081000	-1.761725000
Ti	3.469975000	-0.581665000	-1.228628000
Ti	0.184312000	-1.670493000	1.530317000
Ti	1.097141000	1.962527000	1.585618000
O	2.028079000	-2.199323000	2.020126000

O	2.945677000	1.435511000	2.061006000
O	0.420028000	0.018584000	1.458215000
Ti	2.895631000	-0.422256000	1.998166000
Ti	3.177855000	1.456756000	0.540740000
O	1.390081000	1.882078000	-0.058957000
O	0.541958000	-1.809381000	-0.044787000
Ti	2.316184000	-2.274346000	0.409756000
V	-1.241581000	2.386426000	-0.625835000
V	-2.218221000	-1.532104000	-0.602069000
O	-0.064086000	2.616630000	-1.928959000
O	-0.627886000	2.754281000	0.982295000
O	-2.531848000	3.276969000	-0.925487000
O	-3.677619000	-2.571609000	-0.751501000
O	-1.043288000	-2.168950000	-1.922659000
O	-1.578095000	-1.991467000	1.071239000
O	-2.065990000	0.621995000	-0.729874000
C	-3.462206000	0.467410000	-1.071548000
H	-3.628075000	-3.543093000	-0.702223000
H	-3.856651000	1.435157000	-0.953599000
C	-3.760935000	0.151219000	-2.558702000
H	-4.686073000	-0.418777000	-2.653927000
H	-3.312373000	1.953203000	-2.251882000
H	-2.959298000	-0.460301000	-2.989734000
C	-4.480446000	0.262132000	0.116543000
C	-4.257991000	0.948612000	1.326167000

C	-5.640728000	-0.527543000	-0.043431000
C	-5.197077000	0.844606000	2.368768000
H	-3.368861000	1.560112000	1.459306000
C	-6.588804000	-0.595264000	0.992920000
H	-5.766258000	-1.111593000	-0.945927000
C	-6.369814000	0.084928000	2.206373000
H	-5.013918000	1.376839000	3.299951000
H	-7.477967000	-1.209863000	0.866140000
H	-7.096999000	0.020677000	3.012108000

S.10. TS structure for methyl H removal by O3 (Radical adsorb on O2 site). (Fig.6(b))

Ti	0.533692263	-1.871977042	-1.747697131
Ti	1.455860263	1.757155958	-1.719141131
O	2.383993263	-2.405018042	-1.284801131
O	3.304428263	1.229940958	-1.246600131
O	0.772929263	-0.184832042	-1.834664131
Ti	3.252021263	-0.628180042	-1.305323131
Ti	-0.029591737	-1.706268042	1.462644869
Ti	0.887806263	1.925746958	1.507358869
O	1.814475263	-2.236183042	1.950144869
O	2.736616263	1.397604958	1.980423869
O	0.208058263	-0.017662042	1.385987869
Ti	2.684165263	-0.460246042	1.922186869
Ti	2.965856263	1.414879958	0.459661869
O	1.177440263	1.840952958	-0.137584131
O	0.324811263	-1.849412042	-0.112811131

Ti	2.099348263	-2.315463042	0.339403869
V	-1.439269737	2.325745958	-0.712649131
V	-2.414811737	-1.587838042	-0.655278131
O	-0.266611737	2.555283958	-2.010599131
O	-0.848116737	2.721058958	0.900263869
O	-2.729385737	3.198544958	-1.057660131
O	-3.833657737	-2.687294042	-0.818158131
O	-1.262646737	-2.202405042	-1.989939131
O	-1.779400737	-2.043567042	1.017334869
O	-2.217819737	0.544476958	-0.785434131
C	-3.516316959	0.307183180	-1.251906670
H	-3.743902737	-3.650146042	-0.775612131
H	-3.931302032	1.250396823	-1.368883747
C	-3.358976095	-0.351973442	-2.694858287
H	-4.184638184	-1.030215706	-2.902872634
H	-3.270526223	0.442048446	-3.441981892
H	-2.338968737	-1.281536042	-2.564467131
C	-4.771876024	0.185216481	-0.285899378
C	-4.847905569	1.059116813	0.815735740
C	-5.841462752	-0.700577155	-0.551205464
C	-5.984495887	1.047857068	1.643658673
H	-4.032830954	1.747550116	1.029600250
C	-6.987791966	-0.678063262	0.262733055
H	-5.751233420	-1.416879423	-1.352736975
C	-7.063400234	0.190223927	1.367581817

H	-6.027476616	1.726344698	2.492757864
H	-7.805534088	-1.365037440	0.054015218
H	-7.945110542	0.196411271	2.003781198

S.11. TS structure for methyl H removal by VOH group (Radical adsorb on O2 site). (Fig.6(c))

Ti	0.749796000	-1.830571000	-1.674202000
Ti	1.671964000	1.798562000	-1.645646000
O	2.600097000	-2.363612000	-1.211306000
O	3.520532000	1.271347000	-1.173105000
O	0.989033000	-0.143426000	-1.761169000
Ti	3.468125000	-0.586774000	-1.231828000
Ti	0.186512000	-1.664862000	1.536140000
Ti	1.103910000	1.967153000	1.580854000
O	2.030579000	-2.194777000	2.023640000
O	2.952720000	1.439011000	2.053919000
O	0.424162000	0.023744000	1.459483000
Ti	2.900269000	-0.418840000	1.995682000
Ti	3.181960000	1.456286000	0.533157000
O	1.393544000	1.882359000	-0.064089000
O	0.540915000	-1.808006000	-0.039316000
Ti	2.315452000	-2.274057000	0.412899000
V	-1.238596000	2.388577000	-0.627064000
V	-2.220002000	-1.528676000	-0.591895000
O	-0.063362000	2.614171000	-1.933032000
O	-0.621316000	2.759570000	0.978971000

O	-2.528350000	3.279983000	-0.926363000
O	-3.680965000	-2.566739000	-0.735965000
O	-1.048429000	-2.170168000	-1.913221000
O	-1.577180000	-1.984773000	1.081273000
O	-2.065374000	0.624918000	-0.725219000
C	-3.462442000	0.471228000	-1.063799000
H	-3.632518000	-3.538161000	-0.684428000
H	-3.855467000	1.439743000	-0.947430000
C	-3.764458000	0.151803000	-2.549598000
H	-4.221395000	-1.416055000	-1.756142000
H	-3.820841000	1.095986000	-3.103191000
H	-2.964415000	-0.461747000	-2.980705000
C	-4.478616000	0.270084000	0.126766000
C	-4.252959000	0.959218000	1.334287000
C	-5.640177000	-0.518544000	-0.029034000
C	-5.190138000	0.858896000	2.378963000
H	-3.362821000	1.569942000	1.464211000
C	-6.586313000	-0.582585000	1.009322000
H	-5.768183000	-1.104624000	-0.929865000
C	-6.364122000	0.100274000	2.220693000
H	-5.004510000	1.393157000	3.308494000
H	-7.476476000	-1.196392000	0.885764000
H	-7.089813000	0.038872000	3.027996000

S.12. TS structure for methyl H removal by O1(Radical adsorb on O3 site). (Fig.7(a))

Ti	-0.596617000	-0.134988000	2.545910000
Ti	-3.051148000	1.241835000	0.074295000
O	-1.497748000	-1.898464000	2.544690000
O	-3.949138000	-0.522362000	0.063215000
O	-1.642700000	0.681503000	1.472560000
Ti	-3.024348000	-1.486382000	1.357011000
Ti	1.202687000	-1.255869000	0.063288000
Ti	-1.242493000	0.117618000	-2.421553000
O	0.315478000	-3.025333000	0.043047000
O	-2.140267000	-1.647067000	-2.431918000
O	0.161829000	-0.442334000	-1.018066000
Ti	-1.215284000	-2.611175000	-1.138744000
Ti	-3.011397000	-1.038198000	-1.320374000
O	-2.164925000	0.691271000	-1.149539000
O	0.292171000	-0.792063000	1.322308000
Ti	-0.591129000	-2.462197000	1.285093000
V	-0.639574000	3.124174000	-0.931673000
V	1.681752000	1.931490000	1.401195000
O	-2.346584000	2.898072000	-0.179187000
O	-0.589620000	1.922576000	-2.477898000
O	-0.300489000	4.632275000	-1.316140000
O	2.821798000	3.091630000	2.037412000
O	0.774739000	1.143292000	2.799365000
O	2.522641000	0.157803000	0.656607000
O	0.462976000	2.587110000	0.516830000

C	3.361486000	0.579581000	-0.508171000
H	3.136315000	3.981629000	2.250518000
H	2.766836000	0.252362000	-1.379030000
C	3.270566000	2.058342000	-0.449020000
H	3.895446000	2.610965000	0.258921000
H	3.207536000	2.580640000	-1.405763000
H	1.424129000	2.916421000	-1.074535000
C	4.554785000	-0.353233000	-0.680032000
C	4.784080000	-0.974270000	-1.923391000
C	5.467330000	-0.619469000	0.375010000
C	5.884846000	-1.831191000	-2.115216000
H	4.113050000	-0.780359000	-2.763838000
C	6.557852000	-1.483720000	0.198101000
H	5.297998000	-0.143410000	1.339145000
C	6.775404000	-2.091704000	-1.058235000
H	6.040441000	-2.290431000	-3.088769000
H	7.239375000	-1.675970000	1.023507000
H	7.624474000	-2.753760000	-1.209744000

S.13. TS structure for methyl H removal by O2(Radical adsorb on O3 site). (Fig.7(b))

Ti	-0.598793000	-0.135437000	2.544314000
Ti	-3.050548000	1.246324000	0.072699000
O	-1.503473000	-1.897096000	2.543094000
O	-3.952088000	-0.516061000	0.061619000
O	-1.643231000	0.683158000	1.470964000
Ti	-3.029240000	-1.481941000	1.355415000

Ti	1.198250000	-1.259938000	0.061692000
Ti	-1.244160000	0.118468000	-2.423149000
O	0.307481000	-3.027613000	0.041451000
O	-2.145484000	-1.644406000	-2.433514000
O	0.159032000	-0.444310000	-1.019662000
Ti	-1.222444000	-2.610374000	-1.140340000
Ti	-3.015387000	-1.033784000	-1.321970000
O	-2.165435000	0.693977000	-1.151135000
O	0.288670000	-0.794300000	1.320712000
Ti	-0.597991000	-2.462653000	1.283497000
V	-0.635189000	3.123805000	-0.933269000
V	1.683731000	1.926450000	1.399599000
O	-2.342651000	2.901140000	-0.180783000
O	-0.587654000	1.922108000	-2.479494000
O	-0.293069000	4.631220000	-1.317736000
O	2.826110000	3.084292000	2.035816000
O	0.775133000	1.140079000	2.797769000
O	2.521048000	0.151073000	0.655011000
O	0.466278000	2.584522000	0.515234000
C	3.360740000	0.571162000	-0.509767000
H	3.142419000	3.973656000	2.248922000
H	2.765433000	0.245141000	-1.380626000
C	3.272797000	2.050103000	-0.450616000
H	3.898789000	2.601467000	0.257325000
H	3.210819000	2.572527000	-1.407359000

H	1.784702000	2.347947000	-0.310204000
C	4.552159000	-0.364053000	-0.681628000
C	4.780203000	-0.985550000	-1.924987000
C	5.464166000	-0.632125000	0.373414000
C	5.879242000	-1.844685000	-2.116812000
H	4.109565000	-0.790289000	-2.765434000
C	6.552946000	-1.498570000	0.196505000
H	5.295793000	-0.155726000	1.337549000
C	6.769273000	-2.106991000	-1.059831000
H	6.033912000	-2.304238000	-3.090365000
H	7.234080000	-1.692192000	1.021911000
H	7.617009000	-2.770755000	-1.211340000

S.14. TS structure for methyl H removal by O3(Radical adsorb on O3 site). (Fig.7(c))

Ti	-0.596617000	-0.134988000	2.545910000
Ti	-3.051148000	1.241835000	0.074295000
O	-1.497748000	-1.898464000	2.544690000
O	-3.949138000	-0.522362000	0.063215000
O	-1.642700000	0.681503000	1.472560000
Ti	-3.024348000	-1.486382000	1.357011000
Ti	1.202687000	-1.255869000	0.063288000
Ti	-1.242493000	0.117618000	-2.421553000
O	0.315478000	-3.025333000	0.043047000
O	-2.140267000	-1.647067000	-2.431918000
O	0.161829000	-0.442334000	-1.018066000

Ti	-1.215284000	-2.611175000	-1.138744000
Ti	-3.011397000	-1.038198000	-1.320374000
O	-2.164925000	0.691271000	-1.149539000
O	0.292171000	-0.792063000	1.322308000
Ti	-0.591129000	-2.462197000	1.285093000
V	-0.639574000	3.124174000	-0.931673000
V	1.681752000	1.931490000	1.401195000
O	-2.346584000	2.898072000	-0.179187000
O	-0.589620000	1.922576000	-2.477898000
O	-0.300489000	4.632275000	-1.316140000
O	2.821798000	3.091630000	2.037412000
O	0.774739000	1.143292000	2.799365000
O	2.522641000	0.157803000	0.656607000
O	0.462976000	2.587110000	0.516830000
C	3.361486000	0.579581000	-0.508171000
H	3.136315000	3.981629000	2.250518000
H	2.766836000	0.252362000	-1.379030000
C	3.270566000	2.058342000	-0.449020000
H	3.895446000	2.610965000	0.258921000
H	3.207536000	2.580640000	-1.405763000
H	0.663084000	2.254617000	-1.712876000
C	4.554785000	-0.353233000	-0.680032000
C	4.784080000	-0.974270000	-1.923391000
C	5.467330000	-0.619469000	0.375010000
C	5.884846000	-1.831191000	-2.115216000

H	**4.113050000**	**-0.780359000**	**-2.763838000**
C	**6.557852000**	**-1.483720000**	**0.198101000**
H	**5.297998000**	**-0.143410000**	**1.339145000**
C	**6.775404000**	**-2.091704000**	**-1.058235000**
H	**6.040441000**	**-2.290431000**	**-3.088769000**
H	**7.239375000**	**-1.675970000**	**1.023507000**
H	**7.624474000**	**-2.753760000**	**-1.209744000**