

Theoretical Insights into the Gas-Phase Oxidation of 3-Methyl-2-Butene-1-Thiol by the OH Radical: Thermochemical and Kinetic Analysis

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SUPPORTING INFORMATION

Tables S1-S12 present the optimized geometries of all the stationary points computed at the M06-2X level of theory; vibrational frequencies, rotational constants, and imaginary frequencies of various transition states obtained at the M06-2X level; calculated total electronic energies including zero-point energy corrections calculated at various levels of theory; T1 diagnostic values for all the stationary points; rate coefficients for all possible paths for the MBT-II + OH radical reaction; weight factors and mole fractions of MBT-III; lower vibrational modes for various stationary points treated as hindered rotors; rate coefficients for the MBT + OH radical reaction with the hindered rotor (HR) treatment; rate coefficients for the H-abstraction and addition paths following the introduction of the uncertainty of 1 kcal mol⁻¹ in the CCSD(T) barriers for the MBT + OH radical reaction; and MESMER input files. Figure S1 presents optimized geometries of the post-reactive complexes and products; Figures S2-S4 present the PES diagrams for the various abstraction and addition paths associated with the MBT-II + OH radical reaction.

Table S1: The M06-2X/aug-cc-pV(T+d)Z level optimized geometries of reactants, pre-reactive complexes, transition states, post-reactive complexes, and products involved in the MBT + \cdot OH reaction.

MBT-I

C	0.00525200	0.01894900	-0.02394800
H	1.09119800	0.04786600	-0.04039000
H	-0.30382000	-0.58208600	0.83403200
H	-0.36267700	1.03162200	0.15636700
C	-0.60055700	-0.53942000	-1.27920200
C	-2.09316000	-0.69539300	-1.22636100
H	-2.37968900	-1.36716500	-0.41384500
H	-2.57164900	0.26555900	-1.02348800
H	-2.49126500	-1.09017800	-2.15875000
C	0.08539100	-0.88809600	-2.36651900
H	-0.45949200	-1.31357700	-3.20295700
C	1.56167900	-0.79872900	-2.55545500
H	1.79854100	-0.41763800	-3.54822000
H	2.04178200	-0.14729600	-1.83248900
S	2.36865100	-2.44010400	-2.51528000
H	1.87431500	-2.80601500	-1.32829600

MBT-II

C	-0.00843700	0.00059400	0.00870500
H	1.07608600	0.05803100	0.07455700
H	-0.43628100	0.82330500	0.58626300
H	-0.30324100	0.15864400	-1.03100800
C	-0.52825500	-1.31583200	0.50705900
C	-2.02129000	-1.45964400	0.46279300
H	-2.49328700	-0.72909000	1.12404800
H	-2.38110600	-1.24902200	-0.54631700
H	-2.36333200	-2.45433700	0.73578500
C	0.29864800	-2.26512000	0.94031600
H	1.36641300	-2.08112400	0.89587100
C	-0.11029900	-3.60966700	1.45582700
H	0.63653400	-3.99117100	2.14682000
H	-1.06991000	-3.57414500	1.96363400
S	-0.22650600	-4.76049800	0.03578700
H	-0.42993700	-5.88052300	0.73985900

MBT-III

C	0.05358200	0.12803100	-0.04224200
H	1.13718900	0.15093300	0.03313000
H	-0.20523800	0.13967800	-1.10322600
H	-0.30826900	-0.82076200	0.36057700
C	-0.61232900	1.27891300	0.65142500

C	-2.10591400	1.31703900	0.51336600
H	-2.39088000	1.37610400	-0.53960800
H	-2.55058200	0.40106300	0.90912700
H	-2.53884900	2.16645700	1.03792700
C	0.04417600	2.22018700	1.32591000
H	-0.52838600	3.03309200	1.76126400
C	1.52351200	2.29464700	1.52884100
H	1.76031900	2.83071800	2.44412400
H	1.97633100	1.30827000	1.60297000
S	2.42038600	3.09262600	0.14420100
H	1.65215300	4.18510300	0.08161600

TS1-R1

C	-0.04866600	-0.18197700	0.00158900
H	1.03543200	-0.23732000	0.02370300
H	-0.43060300	-0.82234600	0.79979000
H	-0.35161500	0.83868700	0.24554900
C	-0.64563800	-0.59563300	-1.31298600
C	-2.14727300	-0.65450100	-1.31862200
H	-2.50835900	-1.35759400	-0.56428700
H	-2.56559400	0.32114800	-1.06151900
H	-2.53794400	-0.95399000	-2.28880600
C	0.05298400	-0.89394300	-2.41020200
H	-0.49276700	-1.20082500	-3.29706100
C	1.53786700	-0.87110800	-2.56831000
H	1.80866200	-0.32190900	-3.47059700
H	2.04962200	-0.40373000	-1.73370500
S	2.24783600	-2.53185500	-2.84509600
H	2.05781600	-2.98721500	-1.55069700
O	0.95334200	-3.37431700	-0.54729500
H	0.19827700	-2.88527500	-0.92279200

RC1

C	-0.44489600	1.32590500	1.64171200
H	0.61394700	1.52536600	1.49432000
H	-0.53637400	0.51662300	2.37076700
H	-0.90524800	2.21118600	2.08394800
C	-1.15713100	0.93845100	0.37938400
C	-2.64507500	0.79638500	0.51604900
H	-2.88744400	0.06274300	1.28952100
H	-3.09217400	1.74158500	0.83073600
H	-3.11081200	0.48629600	-0.41736600
C	-0.53668900	0.67970000	-0.77204500
H	-1.13266500	0.35600300	-1.61940800
C	0.94090600	0.75203600	-0.99822100

H	1.16009100	0.88078600	-2.05575500
H	1.40221500	1.58064800	-0.46806100
S	1.82327100	-0.78819900	-0.54536600
H	1.60254900	-0.70425700	0.77199100
O	-0.30053800	-2.12162600	1.00865200
H	-0.74496400	-1.52129500	0.38334800

PC1

C	-0.41759000	1.41473700	1.62460900
H	0.65217100	1.57702900	1.52190500
H	-0.57318500	0.66062800	2.39843200
H	-0.88702400	2.33750400	1.97270200
C	-1.07088700	0.95108300	0.35845300
C	-2.52897800	0.62549700	0.48568200
H	-2.66558600	-0.17262900	1.21893000
H	-3.08019600	1.49479200	0.85035000
H	-2.96050200	0.31108500	-0.46238600
C	-0.43119200	0.80820300	-0.80773400
H	-0.97481400	0.41711900	-1.66000600
C	1.02597500	1.09693400	-1.04103400
H	1.20902000	1.31485600	-2.08987500
H	1.39115200	1.91596600	-0.42862400
S	1.82159700	-0.45740800	-0.58711600
H	0.21132700	-2.23538400	1.73936600
O	-0.67312200	-1.97011100	1.47581500
H	-0.53953700	-1.46715000	0.66547000

(CH₃)₂C=CHCH₂S[•] (P1)

C	-0.41358200	1.40785500	1.62476500
H	0.65729500	1.55946600	1.52021100
H	-0.57015300	0.66825200	2.41250100
H	-0.87360300	2.33708200	1.96903800
C	-1.06950200	0.94268300	0.35939200
C	-2.52957300	0.62391000	0.48360000
H	-2.68386200	-0.16654700	1.22150800
H	-3.08170900	1.49743500	0.83755500
H	-2.95671600	0.30305400	-0.46406900
C	-0.43402700	0.81228400	-0.80724600
H	-0.97837300	0.42152800	-1.65882200
C	1.02271000	1.09869900	-1.04039100
H	1.20487700	1.31484500	-2.08998500
H	1.38541500	1.92294400	-0.43281800
S	1.83076400	-0.44809500	-0.58095100

TS2-R2

C	-0.03235000	0.25091000	-0.13412000
H	1.04864500	0.32839900	-0.19700700
H	-0.29226400	-0.18186800	0.83432200
H	-0.44443000	1.26249900	-0.14450100
C	-0.64750200	-0.55656500	-1.23768400
C	-2.13491200	-0.71988600	-1.12604100
H	-2.39577200	-1.20904700	-0.18472800
H	-2.62452500	0.25675900	-1.11873600
H	-2.54127000	-1.30579500	-1.94736000
C	0.02024000	-1.10202700	-2.25939400
H	-0.54046800	-1.65906000	-3.00249500
C	1.47461800	-1.03093200	-2.50690000
H	1.66761500	-0.36412000	-3.42448800
H	2.04849000	-0.57978400	-1.70459400
S	2.22596700	-2.60137200	-3.02133100
H	2.01231300	-3.25695000	-1.87501300
O	2.34124800	0.29900700	-4.58593200
H	3.16134900	-0.22188600	-4.57856900

RC2

C	-0.52541900	1.21117400	1.78281800
H	0.48558800	1.24974500	1.38453400
H	-0.48072400	0.73659000	2.76544200
H	-0.87047700	2.23446400	1.94792300
C	-1.49755500	0.47098700	0.91018300
C	-2.85677400	0.27828100	1.51746500
H	-2.78259700	-0.28620300	2.44966700
H	-3.30142800	1.24374000	1.76928000
H	-3.53039200	-0.24850300	0.84478400
C	-1.21906900	0.00069600	-0.30495500
H	-1.98602300	-0.55300200	-0.83606100
C	0.08645500	0.13190400	-1.01257600
H	-0.06248900	0.29419700	-2.07882600
H	0.68236000	0.95843800	-0.63443600
S	1.07728900	-1.41228800	-0.93750000
H	0.90181300	-1.62167500	0.37192600
O	2.88183600	1.03716700	0.24791200
H	2.80932000	0.15037300	-0.15953700

PC2

C	-0.61228500	1.46418600	1.80268500
H	0.07663100	2.05961000	1.19600300

H	-0.03352700	1.02884000	2.62092700
H	-1.34833900	2.14112900	2.23198200
C	-1.27521600	0.40246400	0.97911500
C	-2.74816200	0.51420000	0.76155200
H	-3.28230000	0.50827600	1.71595700
H	-2.99401700	1.46229200	0.27462600
H	-3.13242700	-0.29756200	0.14652200
C	-0.54980900	-0.63078100	0.42707300
H	-1.09153200	-1.36819200	-0.15835900
C	0.82481300	-0.79035600	0.54952200
H	0.19088500	1.11892200	-1.01128100
H	1.42066400	-0.08875300	1.11681800
S	1.77017500	-2.05966300	-0.15619500
H	0.76494700	-2.70541000	-0.75834700
O	0.51193900	1.93812500	-1.40413600
H	1.29907300	1.68693200	-1.89182900

(CH₃)₂C=CHC^{*}HS^{*}H (P2)

C	-0.61105900	1.46615100	1.79695100
H	0.15395200	1.99850100	1.22523200
H	-0.11293800	1.03539100	2.66989000
H	-1.33396400	2.19851400	2.15180700
C	-1.27372400	0.40756500	0.96903800
C	-2.75139700	0.50475200	0.77510500
H	-3.27369200	0.48476800	1.73630600
H	-3.02139200	1.45141400	0.29762300
H	-3.13403200	-0.30889300	0.16139200
C	-0.54515800	-0.61708100	0.40940700
H	-1.08523400	-1.35237300	-0.17996200
C	0.82475700	-0.78236300	0.54073500
H	1.42140000	-0.08742100	1.11482300
S	1.76819000	-2.05985200	-0.15397900
H	0.76390600	-2.69879300	-0.76449000

TS3-R2

C	1.04665100	0.23218300	-0.64363700
H	2.12042300	0.38892200	-0.70844000
H	0.84838000	-0.57139800	0.07082600
H	0.59805900	1.13591100	-0.22628300
C	0.41070600	-0.09476000	-1.96244400
C	-1.08615400	-0.18606200	-1.93804700
H	-1.41017600	-0.93533600	-1.21215800
H	-1.51957600	0.76556800	-1.62277100

H	-1.49314300	-0.44771500	-2.91247600
C	1.09426000	-0.30662700	-3.08640200
H	0.54590600	-0.54825400	-3.99084700
C	2.57698000	-0.25786700	-3.22723100
H	2.87964500	-0.08041900	-4.25682000
H	3.00961400	0.62046800	-2.63367200
S	3.45961400	-1.75572700	-2.72274600
H	2.79290500	-1.93910600	-1.57811600
O	4.01018500	1.49756500	-1.92705000
H	4.66291800	0.77886800	-1.87750300

PC3

C	-0.93783800	-0.22790900	1.68150200
H	-0.25213000	0.53122700	2.07107100
H	-0.43192200	-1.19012100	1.70858000
H	-1.78798300	-0.26791900	2.36369500
C	-1.41692800	0.12390700	0.30509300
C	-2.64788300	0.97515600	0.25958000
H	-3.48278500	0.47585300	0.75926300
H	-2.48215600	1.91303600	0.79836800
H	-2.94604700	1.21470600	-0.75928900
C	-0.83658100	-0.29815800	-0.87165800
H	-1.39626300	-0.06196200	-1.77253900
C	0.34839700	-0.98583500	-1.13222200
H	0.51152300	-1.34514300	-2.13828600
H	0.48645400	1.60145600	-0.11711400
S	1.68885200	-1.36077300	-0.09580100
H	1.51597200	-0.38605000	0.80485200
O	1.12134000	2.03748400	0.46370000
H	1.89088300	2.20556400	-0.08498300

TS4-R3

C	-0.02670200	0.05513800	0.02128700
H	1.05697000	0.12690600	-0.01229700
H	-0.30503500	-0.58074500	0.86407100
H	-0.43135300	1.04834300	0.22556100
C	-0.62770000	-0.49176900	-1.24551200
C	-2.12144100	-0.64924700	-1.22221400
H	-2.41715000	-1.30348600	-0.39932100
H	-2.59986600	0.31695000	-1.04829600
H	-2.49341900	-1.06682900	-2.15463200
C	0.07979400	-0.80893500	-2.31892600
H	-0.53561500	-1.22928500	-3.25261800

C	1.53914500	-0.79810200	-2.58275000
H	1.75898600	-0.27998000	-3.51581400
H	2.09741400	-0.30841100	-1.78808200
S	2.20940200	-2.47816500	-2.84426900
H	1.82598500	-2.97033100	-1.66138200
O	-0.96385800	-2.01435300	-4.23371000
H	-0.27321400	-2.69350600	-4.15148700

RC3

C	-0.33419500	0.64827200	2.10594700
H	0.75340600	0.64029900	2.08918900
H	-0.67606900	-0.30757200	2.50936900
H	-0.66316400	1.42392400	2.80031600
C	-0.95281200	0.85663900	0.75613300
C	-2.44862300	0.95593700	0.75972100
H	-2.88177300	0.07346300	1.23265700
H	-2.76707500	1.82763200	1.33613500
H	-2.84760700	1.03508100	-0.24899700
C	-0.25328400	0.93604200	-0.37918500
H	-0.79835000	1.03446500	-1.31173700
C	1.23593600	0.87338000	-0.49301300
H	1.57281800	1.38571800	-1.39167100
H	1.73951000	1.33486900	0.35155900
S	1.89921000	-0.82637600	-0.68614200
H	1.54437400	-1.25532200	0.53142000
O	-1.34135900	-1.64468500	-0.16346300
H	-0.50531300	-1.69061500	-0.66323000

PC4

C	-0.31854000	1.42232100	2.37642600
H	0.76294300	1.47953800	2.27762400
H	-0.55472800	0.80743900	3.24701600
H	-0.70250800	2.42463500	2.57531700
C	-0.98323800	0.84871500	1.14742900
C	-2.48089700	0.72346500	1.22420800
H	-2.76309000	0.08883600	2.06675100
H	-2.93316900	1.70290300	1.39255600
H	-2.89491500	0.29828300	0.31302500
C	-0.30893400	0.48574500	0.08242300
H	-1.26620300	-0.30663400	-2.13148400
C	1.08200400	0.42925700	-0.37454300
H	1.17720800	0.83041700	-1.38360400

H	1.73649500	1.00821200	0.28103200
S	1.72523200	-1.27840700	-0.51089000
H	1.34212900	-1.67326800	0.70773400
O	-0.77421400	-0.81224600	-2.78464000
H	-0.20994700	-1.38670000	-2.25510300

(CH₃)₂C=C·CH₂SH (P3)

C	-0.31730300	1.40347100	2.37470100
H	0.76479900	1.44831800	2.27347000
H	-0.55746000	0.78345400	3.24082700
H	-0.68775300	2.40864800	2.58561500
C	-0.99141100	0.84900100	1.14189800
C	-2.49042400	0.73961800	1.22092500
H	-2.77897700	0.09376600	2.05306100
H	-2.93216800	1.72101600	1.40675700
H	-2.90744500	0.33482200	0.30218600
C	-0.32735400	0.48408100	0.07102100
C	1.06396900	0.41895400	-0.38227300
H	1.16732400	0.81843500	-1.39104600
H	1.71981600	1.00557500	0.26606500
S	1.70715200	-1.28788900	-0.50481300
H	1.45322600	-1.62317900	0.76410900

TS5-R4

C	0.20798000	0.28619100	-0.31152000
H	0.67493500	-0.48297800	0.39524200
H	-0.44790000	0.88791400	0.31628200
H	1.02700200	0.89203400	-0.68907500
C	-0.52997000	-0.47843100	-1.35021300
C	-1.91007400	-0.92247700	-0.96354800
H	-1.87079100	-1.51520400	-0.04662100
H	-2.55058600	-0.06194800	-0.76028200
H	-2.37149600	-1.52383200	-1.74386300
C	0.01690200	-0.83255100	-2.51727600
H	-0.56306800	-1.45250700	-3.19211200
C	1.40844700	-0.52037600	-2.94977900
H	1.47528500	-0.46127000	-4.03413100
H	1.77194000	0.41932800	-2.54428400
S	2.57282800	-1.85882900	-2.49328600
H	2.22435100	-1.90862700	-1.20023900
O	1.61524600	-1.48319000	1.10590800
H	2.30884800	-0.85098200	1.35532800

PC5

C	-0.90500400	1.79619900	0.81021500
H	0.14877500	0.02925200	1.93461300
H	-1.47921700	2.24957000	1.60571900
H	0.02560100	2.27474700	0.54252400
C	-1.37717300	0.68626000	0.15770900
C	-2.68000600	0.06228900	0.60071400
H	-2.49224800	-0.89859100	1.08199800
H	-3.20577400	0.70186600	1.30621400
H	-3.33231800	-0.11889300	-0.25294700
C	-0.70142100	0.05589900	-0.89628900
H	-1.15294600	-0.82789100	-1.33032300
C	0.62128100	0.43764300	-1.43686200
H	0.59610700	0.49380800	-2.52540500
H	0.97466700	1.39296500	-1.06234800
S	1.87462200	-0.85830800	-1.09697400
H	1.66108600	-0.91853600	0.22551500
O	0.70084200	-0.70799200	2.22293900
H	1.08715200	-0.43546400	3.05786600

(CH₃)(CH₂)C=CHCH₂SH (P4)

C	-0.74101900	1.59888000	0.85657700
H	-1.21484900	2.02643100	1.72820700
H	0.23121100	1.98700400	0.58710000
C	-1.35577200	0.61067200	0.13910100
C	-2.70525900	0.09071400	0.57236500
H	-2.64321900	-0.96656300	0.83170700
H	-3.07760200	0.63328000	1.43845000
H	-3.43376500	0.18850400	-0.23256800
C	-0.77410600	0.02475900	-0.99463800
H	-1.28479600	-0.80641800	-1.46422900
C	0.55482400	0.39240500	-1.52893400
H	0.64171300	0.14204300	-2.58388700
H	0.77401600	1.45055300	-1.41338900
S	1.89977600	-0.57925900	-0.72996900
H	1.55610400	-0.26397800	0.52356900

TS6-R4

C	-0.02833600	-0.28508000	0.19355700
H	1.04617000	-0.42209100	0.26992900
H	-0.53668100	-0.82162600	0.99474900
H	-0.23197700	0.82304500	0.44642000
C	-0.61609300	-0.58563100	-1.13823900

C	-2.11294200	-0.70439700	-1.15081600
H	-2.43595700	-1.53580100	-0.52087600
H	-2.56415200	0.20035200	-0.73673700
H	-2.49745200	-0.86053300	-2.15637400
C	0.09936200	-0.71319700	-2.25989200
H	-0.42410500	-0.95470900	-3.17913900
C	1.58095900	-0.61002900	-2.38216300
H	1.85206200	-0.03093200	-3.26434400
H	2.04555500	-0.13498800	-1.52372500
S	2.36213900	-2.23692900	-2.67408900
H	1.87099200	-2.82506700	-1.57843800
O	-0.56344000	2.26452000	0.31138800
H	-0.46836100	2.27768000	-0.65508900

PC6

C	-0.56013700	-0.22434000	1.66874200
H	0.50588700	-0.07620900	1.77547700
H	-1.11787400	-0.45418500	2.56537200
H	-0.44853900	2.15393000	1.08520300
C	-1.18606200	-0.15325200	0.45403900
C	-2.67212500	-0.39952800	0.35304400
H	-3.11479700	-0.55693500	1.33410000
H	-3.17296200	0.44522900	-0.12007800
H	-2.87047200	-1.28094200	-0.25737500
C	-0.49910700	0.13168800	-0.73816700
H	-1.05618000	0.10827500	-1.66610000
C	0.95953600	0.35663400	-0.82969100
H	1.20950100	0.96297200	-1.69716600
H	1.36859700	0.85074600	0.04645300
S	1.85301300	-1.22679300	-1.11268400
H	1.36945600	-1.84637900	-0.03041100
O	0.06708200	2.93162700	0.84424700
H	-0.07543200	3.56535900	1.55010000

TS7-R5

C	-0.05029100	0.10514200	-0.01898000
H	1.03210500	0.00792800	-0.02390100
H	-0.44039800	-0.43782900	0.84462000
H	-0.30154100	1.15771900	0.12702900
C	-0.70227800	-0.42083600	-1.26444900
C	-2.18634000	-0.45905100	-1.21653400
H	-2.49951400	-1.24894300	-0.43572600
H	-2.62431800	0.46176100	-0.82885400

H	-2.64891300	-0.74101600	-2.15900400
C	-0.04756500	-0.88816300	-2.33103600
H	-0.62692200	-1.29342600	-3.15425200
C	1.43215600	-0.95995700	-2.49243300
H	1.71841500	-0.75750200	-3.52319600
H	1.96014600	-0.25403400	-1.85934700
S	2.07366300	-2.64483200	-2.17962200
H	1.59869900	-2.74174700	-0.93275300
O	-2.48343000	-2.46572700	0.42617900
H	-1.94990000	-2.99595700	-0.18821900

PC7

C	-0.19031700	1.59018800	1.31919700
H	0.35856600	0.74030000	1.72761500
H	-0.90086500	1.92350500	2.07193900
H	0.52231800	2.39601000	1.14105100
C	-0.90363800	1.20736200	0.04516200
C	-2.26424300	1.36022000	-0.04912800
H	-1.64312300	-0.81695500	1.08270300
H	-2.83993700	1.78160900	0.76244200
H	-2.79179300	1.08874300	-0.95368200
C	-0.17440100	0.66901100	-1.02116400
H	-0.71171400	0.36984000	-1.91288200
C	1.26917400	0.35894600	-0.97019300
H	1.75295700	0.53789200	-1.92899400
H	1.79304000	0.92975700	-0.20911600
S	1.54910500	-1.43623000	-0.66505100
H	0.75603300	-1.51919800	0.41304900
O	-1.20585200	-1.44275200	1.67226400
H	-1.70780400	-2.25774200	1.60386700

TS8-R5

C	-0.69192100	0.07811700	-0.09840500
H	0.31641500	0.43444300	-0.28808300
H	-0.78625700	-0.12143500	0.97105600
H	-1.39698800	0.87874200	-0.33194000
C	-1.05073900	-1.15351800	-0.87759400
C	-2.43032300	-1.65165600	-0.63784600
H	-2.65217300	-2.58826500	-1.14302400
H	-2.68073400	-1.71345300	0.42227700
H	-3.17850400	-0.86780100	-1.03397500
C	-0.24932000	-1.78030300	-1.74424900
H	-0.61902800	-2.68048200	-2.22477700

C	1.15155300	-1.41089700	-2.09145700
H	1.31290400	-1.48996400	-3.16613100
H	1.41036700	-0.40033100	-1.79328200
S	2.36687500	-2.57940200	-1.38326600
H	1.98777700	-2.41877900	-0.11113400
O	-3.80708900	0.24192000	-1.80325200
H	-3.26340600	0.11343400	-2.59737300

PC8

C	-0.58560500	1.10974500	1.54857700
H	0.47931000	1.12711300	1.78546600
H	-1.14135500	1.21921300	2.47684900
H	-0.79498500	1.97379300	0.91658200
C	-0.96509900	-0.17322600	0.84852500
C	-1.97207300	-0.95830900	1.35588800
H	-2.25593600	-1.88055700	0.86770900
H	-2.50209400	-0.68133700	2.25531400
H	-1.89925600	1.09739900	-1.14503300
C	-0.29564100	-0.54854300	-0.31963200
H	-0.55208700	-1.49641400	-0.77778000
C	0.81922200	0.21329700	-0.92300300
H	0.78509800	0.17671300	-2.01060300
H	0.82107900	1.25756900	-0.62600300
S	2.44897000	-0.53843100	-0.51151800
H	2.29374000	-0.49322800	0.81593000
O	-1.75471200	1.95714700	-1.55437000
H	-2.61944600	2.25923200	-1.83961100

TS9-R6

C	-0.00495700	-0.03018600	-0.00590400
H	1.07949800	0.02588500	-0.05090900
H	-0.27699800	-0.66362800	0.84143400
H	-0.39742200	0.96523200	0.21837000
C	-0.63242300	-0.56631500	-1.25708000
C	-2.11922100	-0.72725700	-1.20059600
H	-2.39980800	-1.41981200	-0.40333900
H	-2.59119600	0.23149100	-0.97546900
H	-2.51868300	-1.09072500	-2.14407800
C	0.05006100	-0.87671000	-2.37616000
H	-0.49824500	-1.31487200	-3.20072100
C	1.52550700	-0.79705400	-2.56481100
H	1.74870700	-0.49246100	-3.58516100
H	2.00050700	-0.08339400	-1.89800900

S	2.33031200	-2.42647500	-2.38443200
H	1.90856100	-2.65884000	-1.13665300
O	-0.54190200	1.19519500	-3.17534700
H	-0.11129100	1.69831700	-2.46769900

(CH₃)₂C(OH)=C^{*}HCH₂SH (P5)

C	-0.33987400	0.74788100	1.91680400
H	0.73826000	0.58154100	1.92349800
H	-0.75487200	0.30320300	2.82160300
H	-0.49879800	1.83221900	2.00796500
C	-1.00449700	0.18951900	0.70129800
C	-2.47330700	-0.05218800	0.75504200
H	-2.76637800	-0.51740200	1.69705400
H	-3.03136300	0.88982100	0.67352700
H	-2.80265400	-0.68883000	-0.06623200
C	-0.39407300	0.41446400	-0.64760700
H	-0.87981700	-0.24254400	-1.37019000
C	1.10856600	0.16851700	-0.71263100
H	1.44812500	0.35849200	-1.72902500
H	1.64514900	0.85268100	-0.05509400
S	1.58364100	-1.54360400	-0.35899700
H	1.01689200	-1.61787100	0.85040000
O	-0.67283500	1.74020000	-1.12435800
H	-0.32736500	2.37292600	-0.48766300

TS10-R7

C	0.04439100	-0.11488500	0.00910400
H	1.10878400	0.07672800	-0.08929000
H	-0.09812600	-0.92417400	0.72976500
H	-0.42945000	0.77822000	0.41425900
C	-0.60955500	-0.48546400	-1.28493000
C	-2.09758700	-0.64427200	-1.21635000
H	-2.35759300	-1.43323900	-0.50672000
H	-2.55134600	0.28034200	-0.85916000
H	-2.52425300	-0.89721400	-2.18532400
C	0.07123500	-0.83299600	-2.40384100
H	-0.49617100	-1.20178000	-3.25207400
C	1.54611900	-0.78097600	-2.57562200
H	1.80102000	-0.51447700	-3.59946500
H	2.01225500	-0.05281000	-1.92104900
S	2.31423700	-2.42328500	-2.33198700
H	1.88603100	-2.59290700	-1.07621600
O	-0.39049700	1.52534300	-2.17415400

H -0.95539500 1.44466500 -2.95633800

(CH₃)₂C*CH(OH)CH₂SH (P6)

C -0.40506800 0.51691100 1.73163900
H 0.65198500 0.77565800 1.66801200
H -0.50411300 -0.50285400 2.10260300
H -0.88014100 1.20103200 2.43459200
C -1.06652500 0.65618400 0.36260700
C -2.55733700 0.35562700 0.45363600
H -2.72379400 -0.67278700 0.77508800
H -3.02741200 1.03080100 1.16702400
H -3.03262500 0.48886700 -0.52005400
C -0.41610900 -0.22463400 -0.66262400
H -0.95331800 -1.08458900 -1.04014600
C 1.01429200 -0.08605800 -0.99034200
H 1.20100600 -0.17532200 -2.06057600
H 1.41070900 0.86908800 -0.65404000
S 2.03850400 -1.45286000 -0.28848100
H 1.71198300 -1.24443400 0.99028300
O -0.86745600 2.03331200 0.01089100
H -1.24111500 2.17611400 -0.86414300

TS11-R1

C -0.09651400 0.00756600 0.02092000
H 0.97610100 0.17878500 0.08518100
H -0.60826300 0.78279700 0.59553100
H -0.40725500 0.12957900 -1.01908200
C -0.47582600 -1.35343900 0.52451200
C -1.94212500 -1.66566800 0.46875300
H -2.50537100 -0.93013300 1.04770200
H -2.29325100 -1.58724800 -0.56291300
H -2.18592000 -2.66180200 0.83095100
C 0.44348200 -2.20744400 0.97001100
H 1.48543600 -1.90895500 0.94689800
C 0.15625500 -3.58000200 1.49525100
H 0.97398000 -3.93868700 2.11479100
H -0.76212300 -3.61947300 2.07506300
S -0.07321600 -4.77560600 0.12792600
H -0.81547800 -5.69987900 0.84312300
O -2.32136200 -5.38419200 1.12123600
H -2.75561600 -5.41125400 0.25591300

RC4

C	0.45762200	2.98090600	-0.70260700
H	1.53798700	3.07769400	-0.78827900
H	0.07583900	3.82695300	-0.12669200
H	0.01925200	3.05649400	-1.69990800
C	0.05746800	1.68789000	-0.05387500
C	-1.42010400	1.51132000	0.13800300
H	-1.78726500	2.22363300	0.88116100
H	-1.93701300	1.74199100	-0.79574500
H	-1.69776100	0.50204800	0.42880500
C	0.97956900	0.79933400	0.31431000
H	2.02160500	1.01951900	0.10816700
C	0.71859700	-0.50688700	0.99201900
H	1.50259800	-0.72914800	1.71283600
H	-0.25156800	-0.55200900	1.47615100
S	0.73333800	-1.83846400	-0.25133200
H	0.68902200	-2.87996300	0.58439300
O	-1.49650400	-1.91468600	-0.05744900
H	-1.72270400	-2.09628000	-0.97851400

PC11

C	0.48383100	3.03190300	-0.59242700
H	1.54993800	3.23558600	-0.51880500
H	-0.05895800	3.80461300	-0.04352200
H	0.18274700	3.11957900	-1.63882300
C	0.13317500	1.67282000	-0.06365000
C	-1.32326500	1.32710400	-0.12767800
H	-1.90241500	2.05435500	0.44644900
H	-1.67001000	1.40057300	-1.16099600
H	-1.55668600	0.32984100	0.23531400
C	1.08096400	0.86782900	0.42583300
H	2.11346200	1.19516000	0.38863500
C	0.86151300	-0.51317400	0.97196600
H	1.62638100	-0.76433800	1.70249500
H	-0.12422200	-0.65291100	1.40600200
S	1.06820000	-1.54900200	-0.49496200
H	-1.25810700	-2.10735500	-0.07548600
O	-2.01754900	-2.05887400	0.52129800
H	-2.66236300	-2.67902800	0.17610300

RC5

C	0.57819000	2.67993200	-1.08656300
H	1.58432800	2.58359200	-1.48899100

H	0.50651600	3.62711100	-0.54757300
H	-0.12669400	2.73686300	-1.91880100
C	0.22332000	1.53454200	-0.18263100
C	-1.16419000	1.60693200	0.38253400
H	-1.31004200	2.56646300	0.88335800
H	-1.89700400	1.55621300	-0.42566100
H	-1.39653400	0.81507500	1.08907900
C	1.10556000	0.56549100	0.05838100
H	2.07566800	0.62509300	-0.42500900
C	0.90297600	-0.64500100	0.90925500
H	1.73751600	-0.77989300	1.59417400
H	-0.02178700	-0.60687200	1.47650200
S	0.85598600	-2.10417000	-0.20407400
H	0.75986800	-3.04365800	0.74469600
O	-2.33018700	-1.11744000	-0.17752500
H	-1.45498500	-1.50628600	-0.38890900

TS12-R2

C	-0.16747800	0.20965500	0.01983600
H	0.91057000	0.27493000	0.15076900
H	-0.63937500	1.00455800	0.60144900
H	-0.40423200	0.40355800	-1.02862200
C	-0.70320900	-1.12773000	0.43615000
C	-2.18113200	-1.30169800	0.25539200
H	-2.71341700	-0.47331500	0.72701600
H	-2.42945500	-1.27403600	-0.80818200
H	-2.55522400	-2.23145600	0.67352300
C	0.10500500	-2.06852600	0.92475300
H	1.16219800	-1.84455900	1.01689500
C	-0.30031100	-3.43750800	1.35650500
H	0.45997900	-3.90296700	1.97684700
H	-1.24098900	-3.39853500	2.00269200
S	-0.64101700	-4.49662000	-0.07432600
H	-0.69401900	-5.65726000	0.59144300
O	-2.54302100	-3.82760500	2.67535700
H	-2.80251500	-4.37135000	1.91248400

PC12

C	0.48296100	2.84155000	-0.04195200
H	1.43825500	2.98061000	0.46041900
H	-0.30044100	3.29172300	0.57477100
H	0.49837000	3.40524000	-0.97921200
C	0.18391700	1.39904300	-0.29864200

C	-1.12422000	1.10143500	-0.96890600
H	-1.57772500	2.01939100	-1.33988800
H	-1.00293200	0.42261700	-1.81412400
H	-1.83236900	0.64315800	-0.27270600
C	1.08880200	0.42792600	0.07986400
H	2.01377300	0.78758300	0.51947300
C	1.01789200	-0.95627700	0.00175800
H	1.86024100	-1.53647100	0.34371300
H	-0.63143100	0.20898600	1.93348300
S	-0.33062600	-1.89704900	-0.58535500
H	0.19572600	-3.08811700	-0.28920800
O	-1.45164700	-0.19456400	2.23464400
H	-1.50178200	-1.01173000	1.72984800

RC6

C	-0.37110600	2.84671700	-0.35613400
H	0.68918900	3.03155500	-0.19833800
H	-0.94282500	3.58740700	0.20764000
H	-0.60013200	3.00817600	-1.41167500
C	-0.76163000	1.45891900	0.05827400
C	-2.21420900	1.13066600	-0.12473900
H	-2.83168100	1.79376200	0.48551100
H	-2.50220700	1.30142800	-1.16404300
H	-2.45585600	0.10013300	0.12230500
C	0.13870100	0.60642700	0.54444200
H	1.17394500	0.92497300	0.61503300
C	-0.14193500	-0.79634500	0.98756900
H	0.62237600	-1.12938900	1.68410200
H	-1.11802900	-0.89335800	1.45420400
S	-0.08559300	-1.89316000	-0.48414900
H	-0.05538400	-3.06307600	0.16612100
O	2.92621200	-0.64000700	0.04089200
H	2.26558700	-1.21883000	-0.39159600

TS13-R3

C	-0.00460100	0.02813700	-0.00552700
H	1.08198700	-0.00900200	-0.01772600
H	-0.32625100	0.86258800	0.62128300
H	-0.36274800	0.23250000	-1.01653900
C	-0.59516500	-1.25670700	0.49978800
C	-2.09872100	-1.30392700	0.52115000
H	-2.48682200	-0.51655500	1.17024700
H	-2.48370500	-1.10980600	-0.48172100

H	-2.49242800	-2.25848800	0.85911700
C	0.17419400	-2.25719200	0.89948300
H	1.35332600	-2.08786000	0.81784500
C	-0.14818200	-3.62229100	1.38529800
H	0.47907900	-3.87503900	2.23713000
H	-1.19311800	-3.71163000	1.67318700
S	0.22213700	-4.80974600	0.03946000
H	0.38586300	-5.89111400	0.80889400
O	2.63084500	-2.26073300	0.49187700
H	2.52273900	-3.09662200	0.00781500

PC13

C	-0.36724300	2.85332700	-0.39661400
H	0.71160400	2.94397100	-0.29558900
H	-0.84329900	3.63377800	0.20038500
H	-0.63944500	3.03257800	-1.43855000
C	-0.85193800	1.49864900	0.03990300
C	-2.34121700	1.27036700	-0.05965700
H	-2.87470600	2.00319100	0.54870700
H	-2.66682700	1.40624500	-1.09258200
H	-2.62795200	0.27067700	0.25935700
C	-0.03680800	0.56900600	0.47681000
H	2.52223600	0.36769600	0.23706200
C	-0.12413500	-0.81446700	0.96329700
H	0.70818100	-1.03798500	1.62799900
H	-1.06201600	-0.97733900	1.49814300
S	-0.03358300	-1.95182600	-0.47229900
H	0.15882200	-3.07637200	0.22703800
O	2.98766800	-0.47333800	0.20813900
H	2.41070600	-1.04144300	-0.31502800

RC7

C	0.42789400	2.62066600	0.39679900
H	1.51510400	2.62252600	0.36149100
H	0.09958200	3.30094000	1.18575000
H	0.04871600	3.01052900	-0.54926400
C	-0.12107300	1.24425400	0.62974100
C	-1.61675700	1.18736500	0.71958800
H	-1.95626800	1.73976200	1.59883300
H	-2.04763500	1.67239000	-0.15666100
H	-2.01408800	0.17800700	0.77425300
C	0.70084200	0.19803200	0.75382100
H	1.76835800	0.37749300	0.66985200

C	0.31631000	-1.22724600	0.97928000
H	0.81686100	-1.62666900	1.85959100
H	-0.75453900	-1.35226600	1.09356600
S	0.87458600	-2.20059500	-0.47352100
H	0.26273200	-3.34814900	-0.16130400
O	-0.16159500	0.64347900	-1.95319400
H	-0.04612400	-0.32099900	-1.86397700

TS14-R4

C	0.05333300	0.28389600	0.31587000
H	1.14113400	0.28694800	0.32146100
H	-0.30402200	1.01943800	1.03900800
H	-0.29232600	0.60750200	-0.66836500
C	-0.50141300	-1.07465900	0.62575900
C	-1.97983200	-1.18532500	0.56910100
H	-2.48583600	-0.26861200	0.86901400
H	-2.28364800	-1.31672100	-0.54737200
H	-2.40088600	-2.04158700	1.08765400
C	0.30047500	-2.11664800	0.86367400
H	1.37315200	-1.96324900	0.83587900
C	-0.15931900	-3.51986600	1.09759100
H	0.58038400	-4.08138300	1.66119300
H	-1.10837000	-3.55688400	1.62431400
S	-0.36946100	-4.32582300	-0.53875600
H	-0.88238100	-5.48226400	-0.10225900
O	-2.46085500	-1.86007000	-1.87165900
H	-2.00156300	-2.69856900	-1.67887100

PC14

C	0.99086500	2.75442500	0.51435800
H	1.76136400	2.84214200	1.28067900
H	0.35146000	3.63212300	0.57345300
H	1.48971000	2.75723100	-0.45453700
C	0.19535000	1.48317700	0.70507700
C	-1.13870800	1.56332200	1.01827600
H	-1.61882700	2.52581800	1.11931700
H	-1.67254100	0.45040600	-1.18754000
H	-1.75283800	0.68973600	1.17829100
C	0.89136200	0.27889600	0.56632800
H	1.95156200	0.33120600	0.34448000
C	0.32652100	-1.08629900	0.71874100
H	0.75950700	-1.58839900	1.58485600
H	-0.75515900	-1.07661400	0.80939700

S	0.78663100	-2.05988000	-0.76730200
H	0.28382000	-3.22896000	-0.35534100
O	-2.07615200	-0.38975000	-1.42514800
H	-1.33187900	-0.96956000	-1.62493800

RC8

C	0.73607800	2.34087500	-1.03216500
H	1.77715800	2.46015200	-0.73958800
H	0.17049000	3.20542700	-0.67668600
H	0.67611200	2.35102400	-2.12229800
C	0.14410500	1.07321100	-0.49002800
C	-1.29722700	0.84785300	-0.84432600
H	-1.91753800	1.65326600	-0.44086600
H	-1.41432500	0.87452900	-1.92942200
H	-1.68257900	-0.10383400	-0.48867600
C	0.86734700	0.23187400	0.25236600
H	1.91366000	0.46212900	0.42170800
C	0.37628400	-1.05834900	0.83623100
H	0.96562700	-1.32296300	1.71004400
H	-0.66966000	-0.99988000	1.12663100
S	0.58115200	-2.37065800	-0.42302700
H	0.24634300	-3.40307600	0.35955900
O	-1.50276800	1.65103900	2.09754900
H	-0.62200000	1.46978500	1.71613700

TS15-R4

C	0.03372200	0.06836200	-0.24112500
H	1.10561800	0.15135000	-0.07459500
H	-0.45908100	0.93558800	0.20503200
H	-0.15850600	0.11274600	-1.31472600
C	-0.52428500	-1.19685600	0.33968200
C	-1.99997800	-1.36442600	0.23775200
H	-2.49183400	-0.89076000	1.17260200
H	-2.42588800	-0.81423400	-0.59941200
H	-2.33214900	-2.39954000	0.22433800
C	0.25314800	-2.09478500	0.95072600
H	1.32440000	-1.92991200	0.97775500
C	-0.24319200	-3.35789000	1.58062300
H	0.41332100	-3.65953800	2.39232800
H	-1.25261000	-3.24175200	1.96806100
S	-0.23392800	-4.67552800	0.30774800
H	-0.55916500	-5.68975500	1.11782200
O	-2.61655500	-0.38121400	2.55342100

H	-1.66797700	-0.47241200	2.74229500
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PC15

C	0.84128500	2.33321000	-1.20641500
H	1.70579200	2.06317900	-1.81327700
H	1.19536700	2.97227700	-0.39740800
H	0.15749500	2.90897100	-1.82621500
C	0.17373500	1.09430400	-0.65969400
C	-1.10930800	0.78442100	-1.02485000
H	-1.29690700	1.45920100	1.31623600
H	-1.65972300	1.42009800	-1.70363100
H	-1.59595300	-0.11924400	-0.68512600
C	0.91829700	0.28977700	0.21469600
H	1.94623300	0.56493400	0.41242300
C	0.41169800	-0.95247000	0.84915400
H	1.00417200	-1.19695200	1.72563000
H	-0.63046400	-0.85834800	1.14456600
S	0.57244700	-2.33660100	-0.35641100
H	0.25415200	-3.31953200	0.49403000
O	-1.48272800	1.28935100	2.24660400
H	-2.23869300	1.83866000	2.46303700

TS16-R5

C	-0.04305900	0.09096400	0.09311100
H	1.03017900	0.21320400	0.21464100
H	-0.58607300	0.93627700	0.51726800
H	-0.26043800	0.17816500	-1.04108600
C	-0.55558100	-1.22196500	0.56100600
C	-2.05024300	-1.35706000	0.55878400
H	-2.49105100	-0.69821600	1.31012500
H	-2.43833900	-1.03837800	-0.41071500
H	-2.38650700	-2.37424700	0.74082100
C	0.28861400	-2.20047300	0.89761200
H	1.35430200	-2.01411800	0.82144700
C	-0.10658500	-3.57595300	1.33108100
H	0.66416400	-4.01196800	1.96044300
H	-1.04744300	-3.57557800	1.87388700
S	-0.27912400	-4.60412700	-0.17505500
H	-0.41585000	-5.78792700	0.43435700
O	-0.57062200	-0.18630200	-2.43350700
H	-0.31017800	-1.11787600	-2.34084500

PC16

C	0.49856900	2.59126600	0.58369800
H	1.56204700	2.76011800	0.68431400
H	-0.12862900	3.44399500	0.36810700
H	0.14797900	1.41040600	-1.82345500
C	-0.03335200	1.33443300	0.73861200
C	-1.51977000	1.12085200	0.59603800
H	-1.96036500	0.81580200	1.54640900
H	-2.01000600	2.03492300	0.27036900
H	-1.73334600	0.34638200	-0.14138000
C	0.79944300	0.24803700	1.01566900
H	1.86503200	0.42236100	1.10025700
C	0.32792300	-1.15404200	1.11431000
H	0.91017500	-1.72025700	1.83662800
H	-0.72546200	-1.20698200	1.37403500
S	0.54839000	-1.94912800	-0.53746300
H	-0.16261200	-3.05701300	-0.29560700
O	-0.27421800	0.85509200	-2.48542600
H	-0.18481400	-0.03923500	-2.13851800

TS17-R5

C	-0.01083500	0.01806800	-0.11461200
H	1.07487900	0.06804600	-0.13567300
H	-0.37524300	0.88025600	0.56151700
H	-0.43165800	0.27502100	-1.08750100
C	-0.54153700	-1.26026200	0.42441500
C	-2.03270700	-1.40631700	0.35534500
H	-2.51046600	-0.58713200	0.89713200
H	-2.36009400	-1.33335700	-0.68350200
H	-2.38800700	-2.35426900	0.74970600
C	0.28346300	-2.17494000	0.94119700
H	1.35072500	-1.98491300	0.90788300
C	-0.12827600	-3.49111700	1.52008400
H	0.60775400	-3.83029700	2.24395200
H	-1.09843900	-3.43386900	2.00537900
S	-0.20977600	-4.71422500	0.15922800
H	-0.41389000	-5.79624500	0.92019600
O	-0.84031300	1.67010900	1.72964800
H	-0.44761100	1.08087500	2.39396700

PC17

C	0.54543800	1.80194000	-1.68323200
H	1.61732900	1.92358500	-1.75948600

H	0.14429200	1.94228900	1.50430600
H	-0.07668500	2.40669600	-2.32650600
C	-0.00126100	0.89654900	-0.80484100
C	-1.49888400	0.73909000	-0.71154200
H	-1.86074800	1.07100500	0.26300100
H	-1.99638900	1.32554800	-1.48037000
H	-1.78372400	-0.30658500	-0.83276200
C	0.82317300	0.12340200	0.01521200
H	1.89656800	0.21665800	-0.09796400
C	0.31942400	-0.88080500	0.98447000
H	1.00650300	-0.99260900	1.81871200
H	-0.66123400	-0.60800300	1.36526400
S	0.19072400	-2.50488900	0.12188500
H	-0.21224700	-3.21513800	1.18255200
O	-0.37057000	1.92363800	2.31804100
H	-0.35982600	2.82229600	2.65369700

RC9

C	0.43109200	2.42876800	-0.84673000
H	1.51230000	2.49522200	-0.73821400
H	-0.03029800	3.24896400	-0.29239400
H	0.17777200	2.57238500	-1.89915100
C	-0.10253000	1.11797700	-0.35409800
C	-1.58876000	0.96376300	-0.45050100
H	-2.07496200	1.69355500	0.19927500
H	-1.91244000	1.16883100	-1.47273900
H	-1.93199600	-0.03110600	-0.18150900
C	0.71771900	0.17244100	0.12494900
H	1.78691800	0.35792400	0.10167000
C	0.29438100	-1.16171200	0.64871300
H	1.01047000	-1.51665000	1.38470100
H	-0.68518900	-1.11214100	1.11324500
S	0.25766600	-2.34092000	-0.75154700
H	0.04309400	-3.44781300	-0.03087600
O	-0.08795600	1.45055500	2.19690000
H	0.81127400	1.81395900	2.20516400

TS18-R6

C	-0.03517900	-0.00276500	0.02562100
H	1.04381400	0.06189300	0.14209100
H	-0.49158900	0.81356100	0.59022700
H	-0.29171700	0.15424200	-1.02463100
C	-0.56394100	-1.31934900	0.50126200

C	-2.05132600	-1.48233400	0.42464400
H	-2.55022500	-0.73644900	1.04964700
H	-2.38623100	-1.29915300	-0.59851100
H	-2.39014000	-2.47335500	0.71417500
C	0.26739700	-2.26528900	0.97806000
H	1.33299400	-2.08348000	0.92388800
C	-0.14116900	-3.62390200	1.44958600
H	0.60842500	-4.01292300	2.13132400
H	-1.09881100	-3.60045300	1.96222700
S	-0.25679300	-4.72056400	-0.01107300
H	-0.41198800	-5.86930200	0.65744500
O	0.33944800	-1.24972600	3.01961500
H	-0.60784200	-1.05468900	3.08317100

TS19-R7

C	-0.03515500	0.01851700	0.03039100
H	1.03744900	0.12131500	0.18570900
H	-0.54679300	0.84806900	0.51823900
H	-0.23886700	0.09026000	-1.04036100
C	-0.55565200	-1.28140700	0.56157200
C	-2.02948300	-1.48670700	0.41140400
H	-2.56108700	-0.63200500	0.82740400
H	-2.27491700	-1.55455400	-0.65089500
H	-2.38181400	-2.39107400	0.89821500
C	0.29594100	-2.25243300	0.97383100
H	1.36031100	-2.04647700	0.94275700
C	-0.11137300	-3.60274100	1.45682800
H	0.65406000	-4.01532800	2.10770200
H	-1.04933600	-3.55300400	2.00112700
S	-0.29801000	-4.69837000	-0.00060500
H	-0.53339100	-5.82753400	0.67734200
O	-0.63388800	-0.88747300	2.72248200
H	0.26074200	-0.55539500	2.88629100

Table S2: Calculated positive frequencies (cm⁻¹) for reactants, complexes, transition states (TSs) and products at the M06-2X/aug-cc-pV(T+d)Z level of theory.

Species	Frequencies					
MBT-I	40	116	137	199	238	317
	348	403	474	519	705	771
	840	888	967	1007	1015	1046

	1106	1137	1180	1262	1270	1375
	1414	1422	1474	1478	1493	1496
	1505	1765	2730	3047	3054	3097
	3098	3101	3147	3151	3165	3173
MBT-II	50	112	129	199	244	316
	341	393	471	539	716	788
	856	922	953	969	1010	1040
	1107	1132	1163	1259	1265	1373
	1415	1423	1472	1482	1491	1496
	1514	1763	2717	3049	3054	3100
	3103	3106	3147	3152	3165	3177
MBT-III	48	106	124	180	206	310
	348	397	468	547	696	771
	839	879	965	979	1009	1057
	1106	1140	1187	1262	1277	1374
	1416	1422	1471	1478	1490	1496
	1508	1765	2729	3048	3055	3099
	3102	3104	3144	3146	3164	3168
TS1-R1	-841	42	66	101	125	149
	199	240	292	313	348	409
	478	514	678	723	778	834
	889	967	979	1017	1044	1107
	1137	1178	1253	1265	1379	1415
	1424	1467	1471	1489	1493	1500
	1755	1817	3048	3055	3089	3099
	3103	3148	3155	3166	3179	3704
RC1	36	68	73	122	135	157
	217	255	302	337	370	401
	447	475	546	684	764	829
	883	968	994	1011	1047	1108
	1143	1186	1257	1281	1371	1416
	1421	1472	1477	1493	1498	1502
	1754	2719	3046	3054	3099	3107
	3108	3145	3150	3157	3169	3722
PC1	34	49	87	111	125	140
	154	208	210	306	308	317
	393	480	534	738	790	869
	927	971	1008	1022	1108	1123
	1142	1223	1254	1365	1413	1419
	1469	1478	1490	1494	1512	1619
	1719	3051	3057	3103	3107	3111
	3149	3155	3165	3184	3833	3934

(CH ₃) ₂ C=CHCH ₂ S* (P1)	76	106	137	195	306	314
	390	469	535	739	790	868
	926	968	1006	1022	1104	1122
	1142	1223	1255	1366	1413	1420
	1470	1478	1489	1493	1510	1734
	3049	3055	3100	3100	3104	3149
	3150	3166	3186			
Water (H ₂ O)	1619	3868	3971			
TS2-R2	-639	37	66	91	118	131
	148	194	213	293	326	411
	473	494	622	730	794	846
	877	967	985	1017	1048	1070
	1104	1156	1206	1271	1319	1389
	1415	1423	1473	1486	1494	1497
	1638	1781	2724	3049	3056	3099
	3103	3150	3152	3171	3178	3770
RC2	31	60	76	119	139	144
	194	212	321	350	367	403
	421	476	526	694	770	843
	889	969	1003	1013	1044	1108
	1135	1186	1263	1278	1376	1415
	1425	1473	1477	1491	1497	1508
	1761	2723	3049	3054	3096	3100
	3103	3140	3147	3161	3171	3636
PC2	23	63	86	105	122	147
	159	174	189	249	302	309
	376	415	432	489	710	826
	828	911	985	986	1001	1055
	1076	1181	1233	1322	1401	1413
	1428	1472	1477	1490	1498	1519
	1615	2730	3033	3038	3078	3088
	3138	3141	3152	3214	3826	3940
(CH ₃) ₂ C=CHC*HSH (P2)	86	132	167	183	240	296
	301	415	416	488	708	826
	827	909	983	986	998	1052
	1072	1183	1234	1320	1399	1413
	1430	1473	1477	1487	1498	1519
	2732	3029	3035	3071	3081	3135
	3138	3153	3216			
TS3-R2	-713	54	83	118	126	158
	205	227	303	334	364	401

	458	528	643	708	784	839
	886	970	996	1004	1019	1071
	1107	1139	1234	1293	1355	1371
	1415	1424	1474	1487	1494	1500
	1703	1751	2730	3048	3051	3099
	3102	3131	3148	3166	3168	3759
PC3	55	80	106	131	160	174
	185	196	229	284	314	382
	399	439	480	643	671	721
	832	902	973	994	1004	1047
	1079	1188	1241	1350	1395	1412
	1428	1468	1479	1488	1505	1530
	1614	2724	3032	3039	3076	3100
	3139	3147	3153	3210	3807	3931
TS4-R3	-1051	62	85	113	120	144
	201	243	286	336	359	386
	422	512	571	719	767	846
	919	954	971	999	1028	1073
	1104	1158	1211	1255	1270	1403
	1416	1433	1462	1475	1488	1495
	1498	1765	2731	3051	3057	3090
	3104	3108	3140	3159	3164	3751
RC3	36	70	124	135	149	167
	212	246	314	353	399	441
	472	497	542	677	761	830
	884	970	994	1008	1049	1105
	1135	1190	1261	1280	1371	1416
	1417	1472	1475	1491	1495	1503
	1742	2718	3053	3056	3107	3107
	3113	3148	3154	3157	3175	3695
PC4	22	45	81	114	130	157
	197	201	217	259	294	329
	386	435	485	501	695	759
	828	960	962	992	1003	1097
	1160	1181	1227	1274	1395	1410
	1450	1473	1485	1492	1495	1632
	1792	2727	3051	3052	3055	3106
	3110	3115	3154	3154	3817	3908
(CH ₃) ₂ C=C*CH ₂ SH (P3)	22	107	158	165	202	236
	326	384	482	499	701	760
	825	961	962	1000	1007	1097
	1162	1180	1227	1268	1394	1408

	1454	1475	1484	1493	1495	1792
	2731	3046	3049	3053	3102	3106
	3109	3150	3156			
TS5-R4	-673	29	62	70	85	127
	200	243	304	326	351	404
	470	530	670	701	780	850
	891	986	989	1015	1048	1089
	1134	1175	1256	1269	1297	1346
	1380	1416	1470	1485	1497	1503
	1652	1834	2699	3050	3099	3103
	3107	3149	3151	3170	3178	3777
PC5	14	49	78	94	123	134
	149	218	282	321	369	400
	433	495	510	611	697	765
	778	837	892	962	1008	1050
	1064	1139	1195	1246	1286	1338
	1409	1452	1489	1496	1502	1560
	1610	2693	3066	3087	3128	3153
	3154	3178	3185	3266	3790	3935
(CH ₃)([•] CH ₂)C=CHCH ₂ SH (P4)	71	84	107	173	305	319
	429	485	525	604	655	738
	787	853	884	954	1005	1054
	1065	1129	1199	1253	1279	1335
	1411	1453	1489	1498	1506	1566
	2723	3067	3104	3127	3153	3153
	3175	3192	3264			
TS6-R4	-840	26	41	77	127	170
	206	275	308	335	355	400
	457	519	691	724	778	848
	891	927	986	1007	1047	1079
	1136	1181	1263	1270	1330	1358
	1402	1416	1465	1483	1496	1501
	1573	1762	2731	3050	3094	3099
	3103	3150	3152	3172	3179	3774
PC6	41	58	78	90	102	125
	147	194	271	299	330	332
	427	492	525	621	662	746
	786	857	883	954	1005	1054
	1065	1130	1205	1251	1284	1344
	1410	1453	1489	1497	1506	1565
	1614	2730	3067	3113	3127	3152
	3163	3173	3194	3261	3820	3943

TS7-R5	-817	16	48	53	89	129
	153	175	282	321	369	403
	467	526	699	735	777	838
	873	943	981	1008	1048	1069
	1136	1183	1258	1269	1345	1370
	1385	1424	1466	1481	1488	1506
	1600	1768	2723	3056	3085	3105
	3107	3152	3163	3166	3173	3774
PC7	56	72	98	119	121	152
	196	249	286	303	332	388
	437	497	522	613	679	778
	789	846	872	964	1006	1041
	1064	1129	1212	1245	1279	1391
	1422	1434	1488	1492	1503	1540
	1619	2694	3065	3099	3125	3153
	3156	3163	3185	3260	3806	3936
TS8-R5	-785	31	42	73	108	145
	164	207	292	315	355	411
	472	516	707	723	779	842
	877	941	989	1011	1047	1070
	1138	1182	1259	1268	1345	1375
	1393	1424	1463	1481	1487	1503
	1577	1763	2728	3058	3083	3098
	3107	3154	3164	3168	3176	3780
PC8	42	56	80	90	122	149
	175	184	197	290	303	331
	436	495	522	593	671	765
	783	843	860	956	1002	1026
	1064	1127	1212	1245	1272	1389
	1421	1434	1486	1493	1506	1536
	1607	2721	3062	3105	3121	3153
	3164	3167	3186	3264	3826	3944
TS9-R6	-163	26	47	92	115	130
	159	187	257	320	345	400
	470	525	608	706	771	839
	894	966	1001	1006	1048	1097
	1140	1184	1262	1270	1373	1415
	1419	1469	1476	1488	1493	1501
	1689	2724	3047	3051	3094	3102
	3109	3152	3157	3164	3196	3797
(CH ₃) ₂ C(OH)=C*HCH ₂ SH (P5)	48	95	111	129	169	224
	242	300	348	362	401	491

	547	706	783	839	934	965
	984	999	1042	1059	1103	1165
	1204	1265	1301	1321	1387	1404
	1410	1424	1468	1479	1480	1494
	1501	2730	2983	3004	3079	3084
	3086	3095	3126	3130	3143	3859
TS10-R7	155	32	101	119	127	169
	212	241	266	322	353	402
	420	527	666	694	766	828
	875	966	997	1002	1049	1084
	1139	1181	1262	1270	1370	1411
	1421	1468	1477	1488	1496	1503
	1667	2723	3054	3060	3111	3116
	3126	3148	3163	3172	3182	3806
(CH ₃) ₂ C [*] C(OH)HCH ₂ SH (P6)	68	100	225	234	252	291
	307	339	341	364	408	443
	542	562	667	733	821	914
	943	978	993	1025	1122	1128
	1180	1230	1239	1256	1347	1393
	1408	1417	1475	1483	1490	1503
	1512	2741	3056	3062	3084	3127
	3138	3144	3145	3148	3197	3851

Table S3: Calculated rotational constants (GHz) for reactants, complexes, transition states (TS), and products at the M06-2X/aug-cc-pV(T+d)Z level of theory.

Species	A	B	C
MBT-I	5.88	1.30	1.21
MBT-II	5.62	1.41	1.31
MBT-III	5.64	1.39	1.28
TS1-R1	2.96	1.16	1.02
RC1	2.61	1.29	1.08
PC1	2.26	1.39	1.07
(CH ₃) ₂ C=CHCH ₂ S [*] (P1)	5.48	1.53	1.42
TS2-R2	2.70	0.94	0.83
RC2	2.55	1.11	0.85
PC2	2.35	1.05	0.87
(CH ₃) ₂ C=CHC [*] HS [*] H (P2)	7.58	2.00	1.05
TS3-R2	2.50	1.20	0.98
PC3	2.44	1.28	1.09
TS4-R3	2.46	1.25	0.91
RC3	2.86	1.25	1.10

PC4	2.30	1.11	0.82
(CH ₃) ₂ C=C*CH ₂ SH (P3)	6.06	1.26	1.17
TS5-R4	2.14	1.35	0.96
PC5	2.40	1.21	0.98
(CH ₃)(*CH ₂)C=CHCH ₂ SH (P4)	5.99	1.42	1.34
TS6-R4	3.21	0.88	0.78
PC6	2.10	1.21	0.92
TS7-R5	2.72	0.98	0.86
PC7	2.34	1.30	1.03
TS8-R5	4.62	0.74	0.72
PC8	2.21	1.16	0.92
TS9-R6	2.81	1.14	0.98
(CH ₃) ₂ C(OH)=C*HCH ₂ SH (P5)	2.77	1.38	1.17
TS10-R7	3.29	1.10	1.02
(CH ₃) ₂ C*C(OH)HCH ₂ SH (P6)	4.01	1.10	1.07

Table S4: Imaginary frequencies of all transition states associated with the MBT + OH radical reactions obtained at the M06-2X/aug-cc-pV(T+d)Z level of theory.

Transition State	M06-2X/aug-cc-pV(T+d)Z
TS1-R1	841
TS2-R2	639
TS3-R2	713
TS4-R3	1051
TS5-R4	673
TS6-R4	840
TS7-R5	817
TS8-R5	785
TS9-R6	163
TS10-R7	155
TS11-R1	984
TS12-R2	725
TS13-R3	1047
TS14-R4	956
TS15-R4	902
TS16-R5	863
TS17-R5	796
TS18-R6	181
TS19-R7	178

Table S5: Calculated total electronic energies for reactants, pre- and post-reactive complexes, transition states (TSs), and products associated with the MBT + OH radical reaction at the M06-2X/aug-cc-pV(T+d)Z and CCSD(T)/aug-cc-pV(T+d)Z levels of theory. Zero-point energy (ZPE) corrections and thermal corrections to Gibbs free energies and enthalpies are given at the M06-2X level.

Species	M06-2X	ZPE (M06-2X)	CCSD(T)	Thermal correction to Gibbs free energy	Thermal correction to Enthalpy
MBT-I	-594.702270	0.137080	-593.927085	0.103855	0.146276
MBT-II	-594.701320	0.137089	-593.926091	0.104040	0.146275
MBT-III	-594.701082	0.136872	-593.925720	0.103562	0.146181
OH radical	-75.733809	0.008585	-75.6455842	-0.008335	0.011890
RC1	-670.445875	0.147995	-669.579797	0.110191	0.159997
TS1-R1	-670.441477	0.145986	-669.577436	0.109154	0.157224
PC1	-670.498912	0.151398	-669.632237	0.112510	0.163960
P1	-594.060617	0.127872	-593.282751	0.094890	0.136516
H ₂ O	-76.430105	0.021547	-76.3422883	0.003259	0.025327
TS2-R2	-670.434069	0.143644	-669.570271	0.105742	0.155321
RC2	-670.445298	0.147709	-669.580429	0.109327	0.159835
PC2	-670.500961	0.146806	-669.633810	0.107065	0.159946
P2	-594.063440	0.123269	-593.284119	0.090090	0.132417
TS3-R2	-670.436723	0.144502	-669.572452	0.108153	0.155632
PC3	-670.498261	0.147935	-669.630751	0.110478	0.160353
RC3	-670.448271	0.148455	-669.582192	0.111362	0.160177
TS4-R3	-670.433468	0.143309	-669.568693	0.106869	0.154576
PC4	-670.460199	0.147780	-669.591978	0.108207	0.160664
P3	-594.021073	0.123545	-593.242281	0.088805	0.132992
TS5-R4	-670.434763	0.144447	-669.571311	0.106482	0.155877
PC5	-670.491452	0.147379	-669.626683	0.107586	0.159996
P4	-594.078016	0.123406	-593.276655	0.089872	0.132438
TS6-R4	-670.434038	0.144468	-669.570020	0.106600	0.155717
PC6	-670.490733	0.147257	-669.625272	0.108055	0.160063

TS7-R5	-670.434527	0.143949	-669.570471	0.104636	0.155646
PC7	-670.493284	0.147792	-669.627798	0.110197	0.160092
TS8-R5	-670.434052	0.144187	-669.570065	0.105989	0.155691
PC8	-670.490974	0.146893	-669.625670	0.107826	0.159746
TS9-R6	-670.444330	0.147582	-669.580382	0.159194	0.109447
P5	-670.492009	0.151508	-669.623774	0.115529	0.162397
TS10-R7	-670.445083	0.148162	-669.581621	0.111621	0.159347
P6	-670.494168	0.151334	-669.626876	0.116897	0.161712
RC4	-670.449790	0.149687	-669.584639	0.112517	0.161173
TS11-R1	-670.438930	0.146942	-669.574654	0.109690	0.158298
PC11	-670.499908	0.151581	-669.634277	0.112553	0.164005
RC5	-670.445426	0.147996	-669.580454	0.109555	0.159899
TS12-R2	-670.435566	0.144256	-669.571315	0.107508	0.155565
PC12	-670.499584	0.147517	-669.631861	0.109598	0.160188
RC6	-670.444928	0.147834	-669.579897	0.109705	0.159873
TS13-R3	-670.431765	0.142960	-669.567104	0.105862	0.154480
PC13	-670.459507	0.147690	-669.591450	0.108118	0.160648
RC7	-670.446339	0.148102	-669.580890	0.110417	0.160073
TS14-R4	-670.436308	0.144808	-669.572394	0.108804	0.155545
PC14	-670.490442	0.147537	-669.624900	0.109225	0.159947
TS15-R4	-670.433095	0.144144	-669.568933	0.105580	0.155548
PC15	-670.488725	0.146839	-669.623559	0.107234	0.159822
TS16-R5	-670.433491	0.144195	-669.569318	0.106540	0.155527
PC16	-670.491190	0.147574	-669.625554	0.109791	0.159904
RC8	-670.443000	0.147273	-669.578166	0.159769	0.107762
TS17-R5	-670.432888	0.144203	-669.568874	0.106293	0.155627
PC17	-670.489732	0.147097	-669.624550	0.108392	0.159781
RC9	-670.444616	0.147816	-669.579814	0.109497	0.160092
TS18-R6	-670.443307	0.147402	-669.579377	0.109691	0.159128
TS19-R7	-670.443747	0.1482810	-669.580402	0.112255	0.159410

Table S6: T1 diagnostic values for all the stationary points involved in the MBT + OH radical reaction calculated at the CCSD(T)/aug-cc-pV(T+d)Z level on M06-2X optimized geometries.

Species	T1 values	Species	T1 value
MBT-I	0.010	TS7-R5	0.019
[•] OH	0.010	PC7	0.020
RC1	0.013	TS8-R5	0.019
TS1-R1	0.018	PC8	0.020
PC1	0.016	RC4	0.013
P1	0.017	TS9-R6	0.022
H ₂ O	0.010	P5	0.012
RC2	0.011	TS10-R6	0.022
TS2-R2	0.019	P6	0.013
PC2	0.020	MBT-II	0.010
P2	0.020	MBT-III	0.010
TS3-R2	0.019		
PC3	0.020		
RC3	0.011		
TS4-R3	0.021		
PC4	0.021		
P3	0.022		
TS5-R4	0.021		
PC5	0.020		
P4	0.022		
TS6-R4	0.019		
PC6	0.020		

Table S7: Rate coefficients for the various possible abstraction and addition channels associated with the MBT-II + OH radical reaction in the temperature range between 200 – 320 K and 1 atm pressure.

T (K)	TS11-R1	TS12-R2^a	TS13-R3	TS14-R4	TS15-R4^a	TS16-R5
200	5.02×10^{-12}	2.01×10^{-12}	6.29×10^{-13}	2.28×10^{-12}	7.32×10^{-13}	8.87×10^{-13}
220	4.53×10^{-12}	1.68×10^{-12}	4.45×10^{-13}	1.87×10^{-12}	7.17×10^{-13}	7.00×10^{-13}
240	4.10×10^{-12}	1.44×10^{-12}	3.39×10^{-13}	1.56×10^{-12}	7.16×10^{-13}	5.91×10^{-13}
250	3.91×10^{-12}	1.35×10^{-12}	3.03×10^{-13}	1.44×10^{-12}	7.20×10^{-13}	5.56×10^{-13}
260	3.73×10^{-12}	1.27×10^{-12}	2.76×10^{-13}	1.33×10^{-12}	7.27×10^{-13}	5.28×10^{-13}
280	3.42×10^{-12}	1.15×10^{-12}	2.38×10^{-13}	1.14×10^{-12}	7.46×10^{-13}	4.93×10^{-13}
298	3.19×10^{-12}	1.06×10^{-12}	2.17×10^{-13}	1.01×10^{-12}	7.70×10^{-13}	4.76×10^{-13}
300	3.16×10^{-12}	1.06×10^{-12}	2.16×10^{-13}	1.00×10^{-12}	7.73×10^{-13}	4.75×10^{-13}
320	2.95×10^{-12}	9.86×10^{-13}	2.04×10^{-13}	8.87×10^{-13}	8.07×10^{-13}	4.69×10^{-13}

TS17-R5^a	TS18-R6	TS19-R7	$k_{\text{MBT-II}}^{\text{b}}$	X_2^{c}	k_2^{d}
1.36×10^{-12}	9.14×10^{-12}	8.15×10^{-12}	3.43×10^{-11}	0.11598	3.98×10^{-12}
1.37×10^{-12}	9.14×10^{-12}	7.89×10^{-12}	3.21×10^{-11}	0.13155	4.22×10^{-12}
1.41×10^{-12}	9.13×10^{-12}	7.60×10^{-12}	3.05×10^{-11}	0.14553	4.43×10^{-12}
1.44×10^{-12}	9.11×10^{-12}	7.44×10^{-12}	2.98×10^{-11}	0.15196	4.52×10^{-12}
1.47×10^{-12}	9.09×10^{-12}	7.27×10^{-12}	2.92×10^{-11}	0.15803	4.61×10^{-12}
1.54×10^{-12}	9.04×10^{-12}	6.94×10^{-12}	2.81×10^{-11}	0.16921	4.76×10^{-12}
1.61×10^{-12}	8.98×10^{-12}	6.63×10^{-12}	2.74×10^{-11}	0.17826	4.88×10^{-12}
1.62×10^{-12}	8.98×10^{-12}	6.59×10^{-12}	2.73×10^{-11}	0.17921	4.90×10^{-12}
1.71×10^{-12}	8.90×10^{-12}	6.25×10^{-12}	2.67×10^{-11}	0.18819	5.02×10^{-12}

^aThe degeneracy of TS12-R2, TS15-R4, and TS17-R5 is 2 and thus the contributions of the rate coefficients for these paths was multiplied by a factor of 2; ^b $k_{\text{MBT-II}}$ refers to the total rate coefficient for the MBT-II + OH radical reaction obtained by adding the corresponding site-specific reaction rate coefficients at each temperature; ^cthe mole fraction of MBT-II was calculated using eqn. 3; ^dthe total rate coefficient (k_2) was calculated by multiplying $k_{\text{MBT-II}}$ by X_2 at the present studied temperatures.

Table S8: Boltzmann weight factors and mole fractions of the MBT-III conformer, and calculated total rate coefficients for the MBT-III + OH radical reaction.

T (K)	Γ_1	Γ_2	Γ_3	$\Gamma_1 + \Gamma_2 + \Gamma_3$	X_3	k_3^a
200	1.0	0.15532	0.18388	1.33920	0.13730	4.71×10^{-12}
220	1.0	0.18397	0.21448	1.39845	0.15337	4.92×10^{-12}
240	1.0	0.21185	0.24384	1.45569	0.16751	5.10×10^{-12}
250	1.0	0.22542	0.25800	1.48342	0.17392	5.18×10^{-12}
260	1.0	0.23871	0.27180	1.51051	0.17994	5.25×10^{-12}
280	1.0	0.26443	0.29831	1.56273	0.19089	5.37×10^{-12}
298	1.0	0.28655	0.32092	1.60747	0.19964	5.47×10^{-12}
300	1.0	0.28895	0.32336	1.61231	0.20056	5.48×10^{-12}
320	1.0	0.31226	0.34700	1.65926	0.20913	5.58×10^{-12}

^aThe mole fraction of MBT-III was calculated using eqn. 4; ^bThe total rate coefficient (k_3) was calculated by multiplying $k_{\text{MBT-III}}$ by X_3 at the present studied temperatures.

Table S9: Lower vibrational modes (in cm^{-1}) for various stationary points treated as hindered rotors at the M06-2X/aug-cc-pV(T+d)Z level of theory.

Species	M06-2X/aug-cc-pV(T+d)Z
MBT-I	40.3, 116.0, 137.2
TS1-R1	66.1, 101.2
TS2-R2	37.2, 91.5
TS3-R2	54.1
TS4-R3	61.6
TS5-R4	69.7, 200.1
TS6-R4	25.7
TS7-R5	48.4
TS8-R5	41.7
TS9-R6	26.2, 47.2, 91.8
TS10-R7	32.1, 101.1, 119.0

Table S10: Rate coefficients for the various possible abstraction and addition channels associated with the MBT + OH radical reaction with the hindered rotor (HR) treatment in the temperature range between 200 – 320 K and 1 atm pressure.

T (K)	TS1-R1	TS2-R2	TS3-R2	TS4-R3	TS5-R4^a	TS6-R4	TS7-R5
200	4.26×10^{-11}	8.65×10^{-13}	8.79×10^{-13}	2.15×10^{-13}	7.03×10^{-13}	5.80×10^{-12}	2.39×10^{-12}
220	3.76×10^{-11}	7.48×10^{-13}	7.55×10^{-13}	1.60×10^{-13}	6.82×10^{-13}	3.31×10^{-12}	2.32×10^{-12}
240	3.33×10^{-11}	6.84×10^{-13}	6.66×10^{-13}	1.28×10^{-13}	6.84×10^{-13}	2.17×10^{-12}	2.30×10^{-12}
250	3.14×10^{-11}	6.66×10^{-13}	6.31×10^{-13}	1.17×10^{-13}	6.91×10^{-13}	1.83×10^{-12}	2.30×10^{-12}
260	2.97×10^{-11}	6.53×10^{-13}	6.00×10^{-13}	1.09×10^{-13}	7.02×10^{-13}	1.57×10^{-12}	2.31×10^{-12}
280	2.66×10^{-11}	6.42×10^{-13}	5.52×10^{-13}	9.76×10^{-14}	7.31×10^{-13}	1.23×10^{-12}	2.35×10^{-12}
298	2.42×10^{-11}	6.44×10^{-13}	5.19×10^{-13}	9.20×10^{-14}	7.65×10^{-13}	1.04×10^{-12}	2.40×10^{-12}
300	2.39×10^{-11}	6.44×10^{-13}	5.16×10^{-13}	9.16×10^{-14}	7.69×10^{-13}	1.02×10^{-12}	2.40×10^{-12}
320	2.17×10^{-11}	6.56×10^{-13}	4.88×10^{-13}	8.91×10^{-14}	8.15×10^{-13}	8.87×10^{-13}	2.48×10^{-12}

TS8-R5^a	TS9-R6	TS10-R7	k_{global}^b
6.04×10^{-13}	1.90×10^{-11}	3.37×10^{-10}	4.03×10^{-10}
5.17×10^{-13}	1.94×10^{-11}	2.75×10^{-10}	3.33×10^{-10}
4.76×10^{-13}	1.97×10^{-11}	2.25×10^{-10}	2.77×10^{-10}
4.66×10^{-13}	1.99×10^{-11}	2.04×10^{-10}	2.54×10^{-10}
4.61×10^{-13}	2.00×10^{-11}	1.85×10^{-10}	2.33×10^{-10}
4.62×10^{-13}	2.03×10^{-11}	1.52×10^{-10}	1.97×10^{-10}
4.71×10^{-13}	2.06×10^{-11}	1.28×10^{-10}	1.71×10^{-10}
4.73×10^{-13}	2.06×10^{-11}	1.26×10^{-10}	1.69×10^{-10}
4.92×10^{-13}	2.08×10^{-11}	1.05×10^{-10}	1.46×10^{-10}

^aThe degeneracy of TS5-R4 and TS8-R5 is 2 and thus the contribution of the rate coefficients for TS5-R4 and TS8-R5 were multiplied by a factor of 2. ^bThe global rate coefficients (k_{global}) for the MBT + OH radical reaction were obtained by adding the rate coefficients for all the individual reaction paths at the corresponding temperatures.

Table S11. The rate coefficients for the various H-abstraction and addition paths with the introduction of an uncertainty of 1 kcal mol⁻¹ in the CCSD(T) barriers for the MBT + OH radical reaction, calculated in the temperature range between 200 – 320 K and 1 atm pressure.

T (K)	TS1-R1	TS2-R2	TS3-R2	TS4-R3	TS5-R4^a	TS6-R4	TS7-R5
200	3.06×10^{-11}	3.91×10^{-13}	3.45×10^{-13}	1.55×10^{-13}	2.10×10^{-13}	3.13×10^{-12}	5.02×10^{-13}
220	2.58×10^{-11}	2.81×10^{-13}	2.63×10^{-13}	1.03×10^{-13}	1.70×10^{-13}	1.46×10^{-12}	4.60×10^{-13}
240	2.20×10^{-11}	2.23×10^{-13}	2.14×10^{-13}	7.24×10^{-14}	1.54×10^{-13}	7.92×10^{-13}	4.60×10^{-13}
250	2.04×10^{-11}	2.06×10^{-13}	1.97×10^{-13}	6.24×10^{-14}	1.52×10^{-13}	6.17×10^{-13}	4.70×10^{-13}
260	1.90×10^{-11}	1.94×10^{-13}	1.83×10^{-13}	5.46×10^{-14}	1.53×10^{-13}	4.98×10^{-13}	4.86×10^{-13}
280	1.65×10^{-11}	1.81×10^{-13}	1.65×10^{-13}	4.40×10^{-14}	1.62×10^{-13}	3.56×10^{-13}	5.30×10^{-13}
298	1.47×10^{-11}	1.79×10^{-13}	1.54×10^{-13}	3.82×10^{-14}	1.75×10^{-13}	2.88×10^{-13}	5.81×10^{-13}
300	1.46×10^{-11}	1.79×10^{-13}	1.53×10^{-13}	3.78×10^{-14}	1.77×10^{-13}	2.82×10^{-13}	5.88×10^{-13}
320	1.29×10^{-11}	1.84×10^{-13}	1.47×10^{-13}	3.43×10^{-14}	1.98×10^{-13}	2.42×10^{-13}	6.56×10^{-13}

TS8-R5^a	TS9-R6	TS10-R7	k_{global}^b
2.59×10^{-13}	1.76×10^{-11}	1.27×10^{-10}	1.81×10^{-10}
1.77×10^{-13}	1.76×10^{-11}	9.82×10^{-11}	1.45×10^{-10}
1.37×10^{-13}	1.76×10^{-11}	7.68×10^{-11}	1.19×10^{-10}
1.25×10^{-13}	1.76×10^{-11}	6.83×10^{-11}	1.08×10^{-10}
1.18×10^{-13}	1.76×10^{-11}	6.10×10^{-11}	9.95×10^{-11}
1.13×10^{-13}	1.76×10^{-11}	4.92×10^{-11}	8.52×10^{-11}
1.15×10^{-13}	1.76×10^{-11}	4.11×10^{-11}	7.53×10^{-11}
1.16×10^{-13}	1.76×10^{-11}	4.03×10^{-11}	7.43×10^{-11}
1.24×10^{-13}	1.76×10^{-11}	3.36×10^{-11}	6.61×10^{-11}

^aThe degeneracy of TS5-R4 and TS8-R5 is 2 and thus the contribution of the rate coefficients for TS5-R4 and TS8-R5 were multiplied by a factor of 2. ^bThe global rate coefficients (k_{global}) for the MBT + OH radical reaction were obtained by adding the rate coefficients for all the individual reaction paths at the corresponding temperatures.

Table S12: MESMER input files for the various possible abstraction and addition channels associated with the MBT-I + OH radical reaction.

Mesmer script for TS1

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS1</me:title>
<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">102.05032</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
      </property>
    </propertyList>
    <me:DOSCMETHOD name="ClassicalRotors"/>
  </molecule>
  <molecule id="OH">
```

```

<propertyList>
  <property dictRef="me:ZPE">
    <scalar units="kcal/mol">0.0</scalar>
  </property>
  <property dictRef="me:rotConsts">
    <array units="cm-1">18.83025</array>
  </property>
  <property dictRef="me:vibFreqs">
    <array units="cm-1">3768.5403</array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">17.00274</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
</propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="RC1">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-3.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.08699 0.04316 0.03617</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.8244 67.5886 72.8471 122.4920 134.5751 156.6399
217.2786 255.0761 301.6535 336.9823 370.1718 400.8085 447.0932 474.5829 545.6857
684.2300 763.5315 829.0335 883.0211 968.2325 993.8452 1011.0493 1047.0903 1107.8475
1133.4125 1185.6253 1257.4277 1280.8523 1371.0997 1415.5526 1420.7184 1472.0298
1476.8668 1492.6928 1497.9832 1501.8395 1753.7393 2718.8594 3045.7800 3053.9183
3098.5793 3106.6719 3108.3600 3145.2134 3149.7155 3156.6792 3169.2441
3722.1643</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">

```

```

    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">119.05306</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:epsilon">
    <scalar>306.5</scalar>
  </property>
  <property dictRef="me:sigma">
    <scalar>4.42</scalar>
  </property>
</propertyList>
<me:DOSMethod name="ClassicalRotors"/>
<me:energyTransferModel xsi:type="me:ExponentialDown">
  <me:deltaEDown units="cm-1">200</me:deltaEDown>
</me:energyTransferModel>
</molecule>
<molecule id="TS1">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-2.8</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09892 0.03862 0.03410</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">42.0949 66.0832 101.1661 125.1211 149.2984 199.2532
239.7764 291.9091 312.9310 347.7784 408.6016 478.4386 513.6131 677.7916 721.6769
777.7024 834.2156 888.6888 966.8135 978.5449 1016.6894 1044.4787 1106.7130 1137.1491
1177.7503 1253.4574 1264.7619 1379.1132 1415.3825 1424.0299 1466.7154 1471.2219
1489.3623 1493.3814 1500.3525 1755.1678 1816.9381 3048.0655 3055.1320 3089.2471
3098.7352 3102.5719 3148.0541 3155.4809 3166.3512 3179.0713 3703.6759</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:imFreqs">

```

```

      <array units="cm-1">841.2870</array>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="PC1">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-33.8</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07527 0.04649 0.03575</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">33.9848 49.4617 86.8056 111.0586 125.1645 140.1312 154.2511
207.9138 209.6167 306.3430 308.4153 316.7423 393.0498 479.7644 533.7893 737.6537
789.7403 868.5491 927.1859 970.7603 1007.5822 1022.0066 1108.0001 1122.6240 1141.5243
1223.4369 1254.2351 1365.2863 1413.6310 1418.5516 1469.0884 1477.9441 1489.9130
1493.5207 1511.5155 1619.1846 1719.2404 3051.1728 3056.9746 3103.1631 3107.0268
3111.4326 3148.5694 3154.7557 3164.7785 3183.9198 3833.0212 3933.5262</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="P1">

```

```

<propertyList>
  <property dictRef="me:ZPE">
    <scalar units="kcal/mol">-30.5</scalar>
  </property>
  <property dictRef="me:rotConsts">
    <array units="cm-1">0.18295 0.05091 0.04745</array>
  </property>
  <property dictRef="me:vibFreqs">
    <array units="cm-1">76.1362 105.5411 138.7874 194.5983 305.8958 314.2413
390.0590 469.3094 534.9709 738.9309 790.0075 868.4685 925.6677 968.1145 1006.4569
1021.9085 1104.4419 1121.6659 1142.2676 1223.4815 1254.8085 1366.3424 1413.7055
1420.3833 1469.9065 1478.1165 1489.0891 1492.5590 1510.3855 1733.5672 3049.1930
3054.7838 3099.5313 3100.3730 3104.2002 3148.9958 3150.1356 3165.8914
3186.1982</array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">101.04250</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
</propertyList>
<me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
  </propertyList>

```

```

    </property>
    <property dictRef="me:MW">
      <scalar units="amu">18.01056</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC1" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>
      <molecule ref="RC1" me:type="modelled" />

```

```

</reactant>
<product>
  <molecule ref="PC1" me:type="modelled" />
</product>
<me:MCRCMethod name="SimpleRRKM"/>
<me:transitionState>
  <molecule ref="TS1" me:type="transitionState" />
</me:transitionState>
<me:tunneling name="Eckart"/>
<me:MCRCMethod name="SimpleRRKM"/>
</reaction>
<reaction id="R2">
  <reactant>
    <molecule ref="PC1" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="P1" me:type="sink" />
  </product>
  <product>
    <molecule ref="H2O" me:type="sink" />
  </product>
  <me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
  </me:MCRCMethod>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>

```

```

    <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkFE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS2

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS2</me:title>
<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">

```

```

    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">102.05032</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>1</scalar>
  </property>
</propertyList>
<me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="RC2">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-3.6</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.08517 0.03711 0.02850</array>
    </property>
    <property dictRef="me:vibFreqs">

```

```

      <array units="cm-1">30.9451 59.5534 76.3263 119.2061 138.7491 143.7835
194.2656 211.8785 321.4811 350.3024 366.8120 403.1757 420.7014 476.0277 526.3855
694.4637 769.5880 842.5191 888.7272 969.1120 1002.7876 1012.6180 1043.9410 1107.5784
1135.2397 1185.8401 1263.2303 1278.1043 1376.2153 1415.4743 1424.7868 1473.0708
1477.4287 1491.0373 1496.6969 1508.3204 1760.6348 2722.9847 3048.8728 3054.3520
3096.4679 3099.9312 3102.7838 3139.8262 3146.6642 3160.5663 3170.6882
3636.4704</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS2">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09008 0.03140 0.02766</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">37.2233 66.0951 91.4529 117.5456 130.7354 148.0437 194.1105
213.3783 292.8273 325.8488 411.4233 473.0285 493.9977 621.6636 729.7601 794.2550
845.6756 876.7480 965.9339 984.8741 1016.7366 1048.1924 1070.1797 1104.4464 1156.0603
1205.8746 1270.6841 1319.2335 1389.3366 1414.8371 1422.8234 1472.7195 1485.7538

```

```

1493.8369 1496.8494 1637.8881 1780.5584 2724.2276 3048.6126 3056.4088 3099.2003
3103.0540 3150.0282 3152.2242 3170.5693 3177.6220 3770.0306</array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:imFreqs">
    <array units="cm-1">639.3869</array>
  </property>
</propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="PC2">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-37.7</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07832 0.03496 0.02899</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">23.0995 63.3937 85.5867 104.7036 121.7524 146.7136
159.0430 173.7303 188.6086 248.7931 301.7819 308.8988 375.9968 415.0212 431.8803
489.4436 709.6454 826.2063 827.8796 911.0493 984.8586 986.0326 1001.2220 1054.7847
1076.1949 1181.1402 1232.6067 1321.5332 1400.5774 1412.8669 1428.4705 1471.5487
1476.8718 1489.6631 1497.7943 1519.2144 1615.2924 2729.6385 3032.6506 3037.5521
3077.5323 3087.8488 3137.7997 3141.0299 3152.3600 3214.1938 3826.3140
3939.6610</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>

```

```

    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="P2">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-34.3</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.25302 0.04002 0.03500</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">85.9610 131.5048 167.2374 183.4367 239.9712 296.4347
301.4346 414.9136 416.4955 487.9792 707.6603 826.1410 827.4161 908.9132 982.6487
986.0236 997.9192 1051.9220 1071.8936 1183.2122 1233.6460 1320.0262 1399.3124
1413.0270 1429.8451 1472.6476 1477.2247 1487.1721 1498.3179 1518.7724 2731.6411
3029.0204 3035.3446 3070.8564 3080.9120 3135.1767 3137.6291 3153.3105
3215.6986</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">101.04250</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>

```

```

    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">18.01056</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
  </reaction>
</reactionList>

```

```

</reactant>
<product>
  <molecule ref="RC2" me:type="modelled" />
</product>
<me:excessReactantConc>1.00E11</me:excessReactantConc>
<me:MCRCMethod name="MesmerILT"/>
<me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
<me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
<me:TInfinity>298.0</me:TInfinity>
<me:nInfinity>0.1</me:nInfinity>
</reaction>
<reaction id="R1">
  <reactant>
    <molecule ref="RC2" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="PC2" me:type="modelled" />
  </product>
  <me:MCRCMethod name="SimpleRRKM"/>
  <me:transitionState>
    <molecule ref="TS2" me:type="transitionState" />
  </me:transitionState>
  <me:tunneling name="Eckart"/>
  <me:MCRCMethod name="SimpleRRKM"/>
</reaction>
<reaction id="R2">
  <reactant>
    <molecule ref="PC2" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="P2" me:type="sink" />
  </product>
  <product>
    <molecule ref="H2O" me:type="sink" />
  </product>
  <me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
  </me:MCRCMethod>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
  </me:PTs>
</me:conditions>

```

```

    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkFE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS3

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
  <me:title>321MBT_OH_TS3</me:title>
  <moleculeList>
    <molecule id="321MBT">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kcal/mol">0.0</scalar>
        </property>

```

```

    <property dictRef="me:rotConsts">
      <array units="cm-1">0.19625 0.04349 0.04035</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">102.05032</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="RC2">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-3.6</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.08517 0.03711 0.02850</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">30.9451 59.5534 76.3263 119.2061 138.7491 143.7835
194.2656 211.8785 321.4811 350.3024 366.8120 403.1757 420.7014 476.0277 526.3855
694.4637 769.5880 842.5191 888.7272 969.1120 1002.7876 1012.6180 1043.9410 1107.5784
1135.2397 1185.8401 1263.2303 1278.1043 1376.2153 1415.4743 1424.7868 1473.0708
1477.4287 1491.0373 1496.6969 1508.3204 1760.6348 2722.9847 3048.8728 3054.3520
3096.4679 3099.9312 3102.7838 3139.8262 3146.6642 3160.5663 3170.6882
3636.4704</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>

```

```

</molecule>
<molecule id="TS3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-0.6</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.08346 0.04007 0.03267</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">54.0947 83.2553 118.3007 125.6138 157.5346 205.2766
227.4529 303.4782 333.6271 364.4011 400.6841 458.4511 527.7319 642.7992 708.3367
783.7738 839.0881 885.7854 969.6718 995.9431 1003.8838 1018.1515 1070.8042 1106.9919
1139.3129 1233.9186 1293.3450 1354.9366 1370.8811 1415.2991 1423.8579 1474.3771
1487.3076 1493.8521 1500.9895 1702.6804 1750.9828 2730.1104 3047.7597 3051.3324
3098.7995 3101.7639 3131.2167 3148.1992 3166.3075 3167.6935 3758.9747</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:imFreqs">
      <array units="cm-1">712.6057</array>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="PC3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-35.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.08132 0.04265 0.03667</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">55.4689 80.4249 105.5655 130.8053 160.0274 174.2451
185.2565 195.6544 228.5039 284.2631 313.6031 382.4919 399.0561 439.3943 479.5350
642.7475 670.8147 721.2254 831.9396 901.8402 973.3853 994.3111 1004.1593 1046.6868
1079.3530 1187.7562 1240.6789 1349.8699 1394.5517 1411.7850 1428.1242 1467.6537
1478.5038 1487.5133 1504.8049 1530.1162 1614.4298 2724.2542 3031.7968 3039.4596

```

```

3076.0297 3100.5408 3139.1144 3147.3579 3152.9604 3209.9383 3807.1956
3930.5755</array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">119.05306</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:epsilon">
    <scalar>306.5</scalar>
  </property>
  <property dictRef="me:sigma">
    <scalar>4.42</scalar>
  </property>
</propertyList>
<me:DOSCMMethod name="ClassicalRotors"/>
<me:energyTransferModel xsi:type="me:ExponentialDown">
  <me:deltaEDown units="cm-1">200</me:deltaEDown>
</me:energyTransferModel>
</molecule>
<molecule id="P2">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-34.3</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.25302 0.04002 0.03500</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">85.9610 131.5048 167.2374 183.4367 239.9712 296.4347
301.4346 414.9136 416.4955 487.9792 707.6603 826.1410 827.4161 908.9132 982.6487
986.0236 997.9192 1051.9220 1071.8936 1183.2122 1233.6460 1320.0262 1399.3124
1413.0270 1429.8451 1472.6476 1477.2247 1487.1721 1498.3179 1518.7724 2731.6411
3029.0204 3035.3446 3070.8564 3080.9120 3135.1767 3137.6291 3153.3105
3215.6986</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">101.04250</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">18.01056</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC2" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>
      <molecule ref="RC2" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="PC3" me:type="modelled" />
    </product>
    <me:MCRCMethod name="SimpleRRKM"/>
    <me:transitionState>
      <molecule ref="TS3" me:type="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
  <reaction id="R2">
    <reactant>
      <molecule ref="PC3" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="P2" me:type="sink" />
    </product>
  </reaction>

```

```

<product>
  <molecule ref="H2O" me:type="sink" />
</product>
<me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
  <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
  <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
</me:MCRCMethod>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkfE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS4

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS4</me:title>
<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">102.05032</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
      </property>
    </propertyList>
    <me:DOSCMMethod name="ClassicalRotors"/>
  </molecule>
  <molecule id="OH">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">

```

```

    <array units="cm-1">18.83025</array>
  </property>
  <property dictRef="me:vibFreqs">
    <array units="cm-1">3768.5403</array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">17.00274</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
</propertyList>
<me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="RC4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685
1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">1.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.08196 0.04176 0.03030</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">61.6182 85.2881 112.7779 119.7991 143.5582 200.9902
242.8835 285.9543 336.4634 359.2971 385.9420 421.8287 512.0487 570.9763 718.7670
767.4449 846.1386 918.9615 954.0719 970.6884 999.0001 1028.0538 1073.0507 1104.4189
1158.2480 1210.8840 1254.7939 1270.1725 1403.1304 1416.2523 1432.7579 1461.8221
1474.9686 1487.9694 1495.4168 1497.7200 1765.5753 2730.8391 3051.0688 3056.5845
3090.4073 3103.6427 3107.7840 3140.3700 3159.4925 3164.3095 3751.1729</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:imFreqs">
      <array units="cm-1">1050.6351</array>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>

```

```

<molecule id="PC4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-10.8</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07681 0.03713 0.02754</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">22.4349 44.8066 80.9505 113.8549 130.3917 157.3695
197.2901 201.0511 216.9150 258.5526 294.1073 329.1240 385.6252 435.1540 484.9063
500.8854 694.9506 758.5933 827.7770 960.0182 962.2941 992.0986 1002.7179 1096.8418
1160.4741 1180.6012 1227.1721 1274.1628 1394.9922 1410.1872 1450.1471 1473.8863
1484.5462 1492.4252 1494.9803 1632.2453 1792.1724 2726.7728 3051.4333 3052.2792
3055.7834 3106.6732 3109.8471 3115.1144 3153.7505 3154.2609 3817.1806
3908.1584</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="P3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-7.8</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:rotConsts">
      <array units="cm-1">0.20236 0.04214 0.03913</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">22.1968 106.7002 157.5756 165.4530 202.2801 236.2518
325.7176 383.5624 481.9971 499.3667 701.2744 759.9462 824.6916 960.9838 961.6871
1000.1917 1007.2531 1096.8221 1161.5167 1180.3116 1226.8022 1268.1354 1393.5657
1408.3855 1454.0446 1474.7789 1484.2937 1493.1533 1494.9373 1792.2713 2730.7672
3046.1017 3048.9892 3052.9036 3102.3538 3106.1425 3109.7860 3150.4080
3156.3167</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">101.04250</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">18.01056</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
</molecule>
<me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC4" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>
      <molecule ref="RC4" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="PC4" me:type="modelled" />
    </product>
  </reaction>
</reactionList>

```

```

    <me:MCRCMethod name="SimpleRRKM"/>
    <me:transitionState>
      <molecule ref="TS4" me:type="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
<reaction id="R2">
  <reactant>
    <molecule ref="PC4" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="P3" me:type="sink" />
  </product>
  <product>
    <molecule ref="H2O" me:type="sink" />
  </product>
  <me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
  </me:MCRCMethod>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>

```

```

<me:calcMethod>simpleCalc</me:calcMethod>
<me:testMicroRates/>
<me:testRateConstants/>
<me:printGrainDOS/>
<me:printGrainkFE/>
<me:testDOS/>
<me:printSpeciesProfile/>
<me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS5

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS5</me:title>
<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:MW">

```

```

    <scalar units="amu">102.05032</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>1</scalar>
  </property>
</propertyList>
<me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="RC4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685

```

```

1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">119.05306</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:epsilon">
    <scalar>306.5</scalar>
  </property>
  <property dictRef="me:sigma">
    <scalar>4.42</scalar>
  </property>
</propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
<me:energyTransferModel xsi:type="me:ExponentialDown">
  <me:deltaEDown units="cm-1">200</me:deltaEDown>
</me:energyTransferModel>
</molecule>
<molecule id="TS5">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.1</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07149 0.04513 0.03212</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">28.6170 61.8380 69.6561 85.1467 126.6149 200.0631 242.5912
303.8256 326.4587 350.9916 404.3258 469.5836 530.3024 659.9723 700.6092 780.0433
850.4146 890.7515 986.1829 989.3063 1015.0759 1048.4634 1088.7973 1133.7156 1174.5231
1256.0586 1268.8694 1297.1101 1346.3755 1380.1763 1415.8177 1469.7101 1484.6887
1496.6332 1503.1557 1651.9180 1834.2824 2698.7971 3049.9313 3098.7108 3102.8794
3106.6524 3148.8284 3151.1037 3169.9836 3178.3116 3777.1637</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">

```

```

    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:imFreqs">
    <array units="cm-1">672.5616</array>
  </property>
</propertyList>
<me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="PC5">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-32.8</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07994 0.04041 0.03260</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">13.5305 48.7653 77.6952 93.8775 123.0928 133.6944 149.4398
217.7222 282.1693 320.9817 368.6389 400.4006 432.9467 495.0649 510.1087 610.6688
696.8584 764.8488 778.0469 837.3752 891.8374 962.2114 1007.8148 1049.8337 1064.1513
1139.0611 1195.3793 1245.8069 1285.6929 1337.5492 1409.7436 1451.9716 1489.2094
1495.9265 1502.3226 1559.7554 1610.1095 2693.3733 3065.8029 3087.2562 3127.9529
3152.5663 3154.9492 3178.3625 3185.4555 3266.4262 3790.4952 3934.8556</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">

```

```

    <scalar>4.42</scalar>
  </property>
</propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
<me:energyTransferModel xsi:type="me:ExponentialDown">
  <me:deltaEDown units="cm-1">200</me:deltaEDown>
</me:energyTransferModel>
</molecule>
<molecule id="P4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-29.5</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.19971 0.04750 0.04455</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">70.8637 84.4487 106.9806 173.0253 304.6887 318.7750
428.7644 484.8145 525.1031 603.7048 654.6832 737.5220 787.4276 852.8379 883.6111
953.9823 1004.5478 1053.8957 1064.6069 1128.7833 1198.6969 1253.3244 1278.7220
1334.8805 1410.6218 1452.6993 1489.3660 1497.6437 1505.8495 1566.0557 2722.9610
3067.1244 3104.7070 3126.7407 3152.6138 3153.1238 3175.3520 3191.6923
3263.6723</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">101.04250</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>

```

```

    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">18.01056</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC4" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
  </reaction>
</reactionList>

```

```

    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>
      <molecule ref="RC4" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="PC5" me:type="modelled" />
    </product>
    <me:MCRCMethod name="SimpleRRKM"/>
    <me:transitionState>
      <molecule ref="TS5" me:type="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
  <reaction id="R2">
    <reactant>
      <molecule ref="PC5" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="P4" me:type="sink" />
    </product>
    <product>
      <molecule ref="H2O" me:type="sink" />
    </product>
    <me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
      <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
      <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
    </me:MCRCMethod>
  </reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
  </me:PTs>
</me:conditions>

```

```

    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkFE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS6

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
  <me:title>321MBT_OH_TS6</me:title>
  <moleculeList>
    <molecule id="321MBT">
      <propertyList>
        <property dictRef="me:ZPE">
          <scalar units="kcal/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
          <array units="cm-1">0.19625 0.04349 0.04035</array>
        </property>
        <property dictRef="me:vibFreqs">
          <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843

```

1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>

```
</property>
<property dictRef="me:frequenciesScaleFactor">
  <scalar>1.0</scalar>
</property>
<property dictRef="me:symmetryNumber">
  <scalar>1</scalar>
</property>
<property dictRef="me:MW">
  <scalar units="amu">102.05032</scalar>
</property>
<property dictRef="me:spinMultiplicity">
  <scalar>1</scalar>
</property>
</propertyList>
<me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
```

```

<molecule id="RC3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685
1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS6">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.9</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:rotConsts">
      <array units="cm-1">0.10717 0.02936 0.02603</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">25.7405 40.8974 76.8288 127.0523 170.2731 205.7722
275.2253 307.8860 334.8656 355.1619 399.6303 456.7797 518.8199 691.4698 724.3039
778.4553 847.7091 890.6651 927.3391 986.1267 1007.0235 1046.8732 1079.2518 1135.7936
1180.9345 1262.8779 1270.3855 1330.2329 1357.9731 1401.9276 1415.6109 1464.9566
1483.2003 1496.2669 1500.7625 1573.1114 1762.2473 2730.7254 3050.3192 3094.3751
3098.6697 3103.3654 3149.9910 3151.8375 3171.8320 3178.6494 3774.1384</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:imFreqs">
      <array units="cm-1">840.4725</array>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="PC6">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-32.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07002 0.04041 0.03059</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">40.9478 57.6632 77.5579 89.6561 102.4130 125.3057 147.1574
193.6143 270.9335 299.2407 330.0015 332.3976 427.5682 492.3255 524.6881 621.4944
662.2332 745.8907 785.5782 857.2700 882.5822 954.4076 1005.3014 1053.6974 1064.7058
1130.3767 1205.4824 1251.9821 1284.1326 1344.2845 1409.5232 1453.0177 1488.9770
1497.3274 1506.2104 1565.3358 1614.6441 2729.6381 3066.6144 3113.6135 3126.8483
3152.2594 3162.6530 3172.8092 3193.8730 3261.1397 3820.2561 3942.5234</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">

```

```

    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">119.05306</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:epsilon">
    <scalar>306.5</scalar>
  </property>
  <property dictRef="me:sigma">
    <scalar>4.42</scalar>
  </property>
</propertyList>
<me:DOSMethod name="ClassicalRotors"/>
<me:energyTransferModel xsi:type="me:ExponentialDown">
  <me:deltaEDown units="cm-1">200</me:deltaEDown>
</me:energyTransferModel>
</molecule>
<molecule id="P4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-29.5</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.19971 0.04750 0.04455</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">70.8637 84.4487 106.9806 173.0253 304.6887 318.7750
428.7644 484.8145 525.1031 603.7048 654.6832 737.5220 787.4276 852.8379 883.6111
953.9823 1004.5478 1053.8957 1064.6069 1128.7833 1198.6969 1253.3244 1278.7220
1334.8805 1410.6218 1452.6993 1489.3660 1497.6437 1505.8495 1566.0557 2722.9610
3067.1244 3104.7070 3126.7407 3152.6138 3153.1238 3175.3520 3191.6923
3263.6723</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">101.04250</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">

```

```

        <scalar>2</scalar>
    </property>
</propertyList>
<me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
    <propertyList>
        <property dictRef="me:ZPE">
            <scalar units="kcal/mol">0.0</scalar>
        </property>
        <property dictRef="me:rotConsts">
            <array units="cm-1">27.82574 14.37796 9.47967</array>
        </property>
        <property dictRef="me:vibFreqs">
            <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
        </property>
        <property dictRef="me:frequenciesScaleFactor">
            <scalar>1.0</scalar>
        </property>
        <property dictRef="me:symmetryNumber">
            <scalar>1</scalar>
        </property>
        <property dictRef="me:MW">
            <scalar units="amu">18.01056</scalar>
        </property>
        <property dictRef="me:spinMultiplicity">
            <scalar>1</scalar>
        </property>
    </propertyList>
    <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
    <propertyList>
        <property dictRef="me:MW">
            <scalar units="amu">28</scalar>
        </property>
        <property dictRef="me:epsilon">
            <scalar>48</scalar>
        </property>
        <property dictRef="me:sigma">
            <scalar>3.9</scalar>
        </property>
    </propertyList>
    <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>

```

```

<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC3" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>
      <molecule ref="RC3" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="PC6" me:type="modelled" />
    </product>
    <me:MCRCMethod name="SimpleRRKM"/>
    <me:transitionState>
      <molecule ref="TS6" me:type="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
  <reaction id="R2">
    <reactant>
      <molecule ref="PC6" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="P4" me:type="sink" />
    </product>
    <product>
      <molecule ref="H2O" me:type="sink" />
    </product>
    <me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
      <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
      <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
    </me:MCRCMethod>
  </reaction>
</reactionList>

```

```

</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkFE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS7

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS7</me:title>

```

```

<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">102.05032</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
      </property>
    </propertyList>
    <me:DOSCMETHOD name="ClassicalRotors"/>
  </molecule>
  <molecule id="OH">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">18.83025</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">3768.5403</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
    </propertyList>
  </molecule>
</moleculeList>

```

```

    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="RC3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685
1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
  </propertyList>

```

```

    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS7">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.3</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09072 0.03277 0.02879</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">16.0204 48.4106 52.9496 88.5500 128.5910 153.4464 175.4564
281.7447 321.4985 369.4382 402.9132 466.6106 526.1255 699.4136 735.1559 776.7005
838.4552 873.3316 942.9405 981.2934 1008.0600 1048.1974 1068.8525 1136.4200 1182.5012
1257.8003 1268.6326 1344.8670 1369.7109 1384.8211 1423.5340 1466.2438 1480.8049
1488.3898 1506.4530 1600.5106 1768.0477 2722.5350 3056.2131 3085.0381 3104.5783
3107.4167 3152.4447 3162.7849 3165.6032 3173.4238 3773.5649</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:imFreqs">
      <array units="cm-1">816.9770</array>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="PC7">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-33.3</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07804 0.04345 0.03443</array>
    </property>
  </propertyList>

```

```

    <property dictRef="me:vibFreqs">
      <array units="cm-1">55.8438 71.9342 97.6493 118.5241 120.5299 152.0781
196.2032 249.2345 285.5973 302.6743 331.5793 387.7059 436.5461 497.3363 522.3877
613.0238 679.1093 778.3144 789.0915 846.2190 871.6731 963.5673 1006.2403 1040.9771
1064.4964 1128.7595 1211.6587 1245.3430 1279.1541 1390.5166 1421.9198 1433.7368
1487.8844 1492.2097 1502.5765 1539.6187 1618.7390 2694.4757 3064.6384 3099.2954
3124.7513 3152.8415 3156.1097 3163.3306 3185.0587 3260.1016 3805.8521
3935.9889</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="P4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-29.5</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.19971 0.04750 0.04455</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">70.8637 84.4487 106.9806 173.0253 304.6887 318.7750
428.7644 484.8145 525.1031 603.7048 654.6832 737.5220 787.4276 852.8379 883.6111
953.9823 1004.5478 1053.8957 1064.6069 1128.7833 1198.6969 1253.3244 1278.7220
1334.8805 1410.6218 1452.6993 1489.3660 1497.6437 1505.8495 1566.0557 2722.9610

```

3067.1244 3104.7070 3126.7407 3152.6138 3153.1238 3175.3520 3191.6923
3263.6723</array>

```
</property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">101.04250</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
</propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">18.01056</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
```

```

    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC3" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>
      <molecule ref="RC3" me:type="modelled" />
    </reactant>
    <product>
      <molecule ref="PC7" me:type="modelled" />
    </product>
    <me:MCRCMethod name="SimpleRRKM"/>
    <me:transitionState>
      <molecule ref="TS7" me:type="transitionState" />
    </me:transitionState>
    <me:tunneling name="Eckart"/>
    <me:MCRCMethod name="SimpleRRKM"/>
  </reaction>
  <reaction id="R2">

```

```

<reactant>
  <molecule ref="PC7" me:type="modelled" />
</reactant>
<product>
  <molecule ref="P5" me:type="sink" />
</product>
<product>
  <molecule ref="H2O" me:type="sink" />
</product>
<me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
  <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
  <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
</me:MCRCMethod>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkFE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>

```

```
</me:control>
</me:mesmer>
```

Mesmer script for TS8

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS8</me:title>
<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">102.05032</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
      </property>
    </propertyList>
    <me:DOSCMMethod name="ClassicalRotors"/>
  </molecule>
```

```

<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="RC3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685
1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS8">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.7</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.15399 0.02466 0.02419</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">30.6757 41.6766 73.4407 107.8500 145.1592 164.0789
207.2901 292.2301 315.1860 354.6026 410.6572 472.0270 515.7597 707.0783 723.1794
779.1989 842.3616 876.5669 940.9674 989.4162 1010.9132 1047.0812 1070.4799 1137.9524
1181.9020 1259.3732 1267.9818 1344.6340 1375.1342 1393.1437 1423.7420 1462.7199
1480.7076 1486.7340 1502.7156 1576.9646 1763.4371 2728.3617 3057.5925 3083.4232
3098.2185 3106.9773 3153.9214 3163.7114 3167.7461 3176.1543 3779.7212</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:imFreqs">
      <array units="cm-1">784.9387</array>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="PC8">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-32.5</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.07363 0.03875 0.03066</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">41.5274 56.2853 79.6581 90.3410 122.3193 149.3645 174.8784
184.2657 197.0733 290.4644 303.1590 331.4885 435.7107 494.6252 522.4119 593.0760
671.0966 764.5478 782.9395 843.2608 860.1001 955.7228 1001.6914 1026.2241 1064.4523
1127.4246 1211.5839 1244.5059 1272.1483 1389.2253 1421.2783 1434.2002 1486.2066
1493.1029 1506.1397 1536.0069 1607.8255 2720.8493 3062.1756 3105.0893 3121.0503
3152.6976 3163.9878 3166.7584 3185.6494 3263.6129 3826.1344 3944.4559</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>

```

```

<molecule id="P4">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-29.4</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.19971 0.04750 0.04455</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">70.8637 84.4487 106.9806 173.0253 304.6887 318.7750
428.7644 484.8145 525.1031 603.7048 654.6832 737.5220 787.4276 852.8379 883.6111
953.9823 1004.5478 1053.8957 1064.6069 1128.7833 1198.6969 1253.3244 1278.7220
1334.8805 1410.6218 1452.6993 1489.3660 1497.6437 1505.8495 1566.0557 2722.9610
3067.1244 3104.7070 3126.7407 3152.6138 3153.1238 3175.3520 3191.6923
3263.6723</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">101.04250</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="H2O">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">27.82574 14.37796 9.47967</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">1618.8285 3867.7498 3971.3807</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">

```

```

    <scalar>1</scalar>
  </property>
  <property dictRef="me:MW">
    <scalar units="amu">18.01056</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>1</scalar>
  </property>
</propertyList>
<me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC3" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>
  <reaction id="R1">
    <reactant>

```

```

    <molecule ref="RC3" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="PC8" me:type="modelled" />
  </product>
  <me:MCRCMethod name="SimpleRRKM"/>
  <me:transitionState>
    <molecule ref="TS8" me:type="transitionState" />
  </me:transitionState>
  <me:tunneling name="Eckart"/>
  <me:MCRCMethod name="SimpleRRKM"/>
</reaction>
<reaction id="R2">
  <reactant>
    <molecule ref="PC8" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="P4" me:type="sink" />
  </product>
  <product>
    <molecule ref="H2O" me:type="sink" />
  </product>
  <me:MCRCMethod name="MesmerILT" xsi:type="MesmerILT" >
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol" reverse="true">0.01</me:activationEnergy>
  </me:MCRCMethod>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>

```

```

    <me:grainSize units="cm-1">20</me:grainSize>
    <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
    <me:eigenvalues>1</me:eigenvalues>
    <me:calcMethod>simpleCalc</me:calcMethod>
    <me:testMicroRates/>
    <me:testRateConstants/>
    <me:printGrainDOS/>
    <me:printGrainkFE/>
    <me:testDOS/>
    <me:printSpeciesProfile/>
    <me:printGrainedSpeciesProfile/>
</me:control>
</me:mesmer>

```

Mesmer script for TS9

```

<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type="text/xsl" href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type="text/xsl" href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS9</me:title>
<moleculeList>
    <molecule id="321MBT">
        <propertyList>
            <property dictRef="me:ZPE">
                <scalar units="kcal/mol">0.0</scalar>
            </property>
            <property dictRef="me:rotConsts">
                <array units="cm-1">0.19625 0.04349 0.04035</array>
            </property>
            <property dictRef="me:vibFreqs">
                <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
            </property>
            <property dictRef="me:frequenciesScaleFactor">
                <scalar>1.0</scalar>
            </property>

```

```

    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">102.05032</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>1</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMethod name="ClassicalRotors"/>
</molecule>
<molecule id="RC3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
  </propertyList>

```

```

    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685
1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS9">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-3.6</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09389 0.03807 0.03293</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">26.2264 47.2168 91.8250 114.8459 129.7682 159.1357
186.7684 257.4149 320.4654 345.2027 400.1665 470.0443 524.5307 607.6665 706.4594
771.2090 838.5007 893.8448 965.7258 1000.7088 1006.0154 1048.3292 1096.6255 1139.7318
1183.8080 1261.9979 1269.6890 1372.8911 1415.1093 1418.7983 1468.8109 1475.5142

```

```

1487.5908 1492.8336 1500.7525 1688.5043 2724.3976 3047.1545 3051.1969 3094.4425
3102.9133 3109.2972 3152.5627 3157.1357 3164.3036 3195.9171 3796.9432 </array>
  </property>
  <property dictRef="me:frequenciesScaleFactor">
    <scalar>1.0</scalar>
  </property>
  <property dictRef="me:symmetryNumber">
    <scalar>1</scalar>
  </property>
  <property dictRef="me:spinMultiplicity">
    <scalar>2</scalar>
  </property>
  <property dictRef="me:imFreqs">
    <array units="cm-1">163.3461</array>
  </property>
</propertyList>
<me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="P5">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-28.4</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09246 0.04614 0.03902</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">48.2695 95.0670 110.7283 128.7449 168.5714 224.3486
241.9731 299.7620 348.4495 362.2111 400.6299 490.8469 546.5858 706.2912 783.0783
839.4414 934.2286 964.5744 983.5206 998.8696 1041.8782 1059.4890 1103.4461 1164.5261
1204.4894 1264.9071 1301.1823 1320.8069 1387.4638 1403.5968 1409.9486 1423.9114
1468.3775 1479.3799 1480.2073 1494.6184 1500.5191 2729.9402 2983.2072 3003.6207
3078.5631 3084.4952 3086.4299 3095.4275 3126.1039 3129.9591 3142.9208
3858.7365</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
  </propertyList>

```

```

    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="N2">
  <propertyList>
    <property dictRef="me:MW">
      <scalar units="amu">28</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>48</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>3.9</scalar>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
</moleculeList>
<reactionList>
  <reaction id="R0">
    <reactant>
      <molecule ref="OH" me:type="deficientReactant" />
    </reactant>
    <reactant>
      <molecule ref="321MBT" me:type="excessReactant" />
    </reactant>
    <product>
      <molecule ref="RC3" me:type="modelled" />
    </product>
    <me:excessReactantConc>1.00E11</me:excessReactantConc>
    <me:MCRCMethod name="MesmerILT"/>
    <me:preExponential units="cm3molecule-1s-1">1.00E-11</me:preExponential>
    <me:activationEnergy units="kcal/mol">0.01</me:activationEnergy>
    <me:TInfinity>298.0</me:TInfinity>
    <me:nInfinity>0.1</me:nInfinity>
  </reaction>

```

```

<reaction id="R1">
  <reactant>
    <molecule ref="RC3" me:type="modelled" />
  </reactant>
  <product>
    <molecule ref="P5" me:type="modelled" />
  </product>
  <me:MCRCMethod name="SimpleRRKM"/>
  <me:transitionState>
    <molecule ref="TS9" me:type="transitionState" />
  </me:transitionState>
  <me:tunneling name="Eckart"/>
  <me:MCRCMethod name="SimpleRRKM"/>
</reaction>
</reactionList>
<me:conditions>
  <me:bathGas>N2</me:bathGas>
  <me:PTs>
    <me:PTpair me:units="Torr" me:P="760" me:T="200" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="220" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="240" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="250" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="260" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="280" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="298" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="300" me:precision="qd" />
    <me:PTpair me:units="Torr" me:P="760" me:T="320" me:precision="qd" />
  </me:PTs>
  <me:InitialPopulation>
    <molecule ref="OH" me:population="1.0"/>
  </me:InitialPopulation>
</me:conditions>
<me:modelParameters>
  <me:grainSize units="cm-1">20</me:grainSize>
  <me:energyAboveTheTopHill>25</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
  <me:eigenvalues>1</me:eigenvalues>
  <me:calcMethod>simpleCalc</me:calcMethod>
  <me:testMicroRates/>
  <me:testRateConstants/>
  <me:printGrainDOS/>
  <me:printGrainkFE/>
  <me:testDOS/>
  <me:printSpeciesProfile/>
  <me:printGrainedSpeciesProfile/>

```

```
</me:control>
</me:mesmer>
```

Mesmer script for TS10

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns:cml="http://www.xml-
cml.org/schema">
<me:title>321MBT_OH_TS10</me:title>
<moleculeList>
  <molecule id="321MBT">
    <propertyList>
      <property dictRef="me:ZPE">
        <scalar units="kcal/mol">0.0</scalar>
      </property>
      <property dictRef="me:rotConsts">
        <array units="cm-1">0.19625 0.04349 0.04035</array>
      </property>
      <property dictRef="me:vibFreqs">
        <array units="cm-1">40.2728 115.9719 137.1856 199.4724 238.1814 316.9590
347.5624 402.8403 474.4488 519.2721 704.7871 770.9793 839.5900 887.5999 966.7843
1007.2573 1014.6785 1046.3552 1106.3000 1137.0336 1180.0570 1262.0525 1270.0480
1375.0776 1414.1651 1421.7355 1473.8347 1477.9148 1492.9447 1495.8890 1504.7109
1764.7289 2730.2078 3047.3869 3054.1175 3097.3687 3097.8866 3100.6151 3147.0004
3151.3191 3164.8649 3173.6496</array>
      </property>
      <property dictRef="me:frequenciesScaleFactor">
        <scalar>1.0</scalar>
      </property>
      <property dictRef="me:symmetryNumber">
        <scalar>1</scalar>
      </property>
      <property dictRef="me:MW">
        <scalar units="amu">102.05032</scalar>
      </property>
      <property dictRef="me:spinMultiplicity">
        <scalar>1</scalar>
      </property>
    </propertyList>
    <me:DOSCMMethod name="ClassicalRotors"/>
  </molecule>
```

```

<molecule id="OH">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">0.0</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">18.83025</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">3768.5403</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">17.00274</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
</molecule>
<molecule id="RC3">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.2</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.09554 0.04198 0.03662</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">35.7787 70.3183 124.2449 134.5829 149.0950 166.9956
212.3151 246.2130 313.5306 352.5367 398.8715 441.4619 471.5616 497.1640 542.3588
677.0556 761.2820 829.7183 883.5424 969.8058 993.5754 1007.5748 1048.6448 1105.4685
1135.4445 1189.7518 1261.3261 1280.1405 1370.7399 1416.1810 1417.3408 1472.0102
1475.0698 1490.8198 1494.6929 1503.2930 1741.5790 2717.6292 3052.9388 3056.2290
3106.6369 3107.3552 3112.5705 3148.3617 3154.0865 3156.7024 3174.6065
3694.8463</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:MW">
      <scalar units="amu">119.05306</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
    <property dictRef="me:epsilon">
      <scalar>306.5</scalar>
    </property>
    <property dictRef="me:sigma">
      <scalar>4.42</scalar>
    </property>
  </propertyList>
  <me:DOSCMETHOD name="ClassicalRotors"/>
  <me:energyTransferModel xsi:type="me:ExponentialDown">
    <me:deltaEDown units="cm-1">200</me:deltaEDown>
  </me:energyTransferModel>
</molecule>
<molecule id="TS10">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-4.1</scalar>
    </property>
    <property dictRef="me:rotConsts">
      <array units="cm-1">0.10980 0.03675 0.03400</array>
    </property>
    <property dictRef="me:vibFreqs">
      <array units="cm-1">32.0942 101.0686 118.9414 127.0030 168.5388 212.3980
241.4481 266.0674 322.3978 352.7545 402.1087 420.2565 527.0139 666.1398 694.4273
766.3680 828.3863 875.4150 966.2979 997.2202 1001.8028 1049.4057 1084.3023 1138.8260
1180.6026 1261.7491 1269.5908 1369.6422 1411.2670 1421.4273 1467.7326 1476.7156
1487.8799 1496.2318 1502.7733 1667.1187 2722.8291 3054.1110 3060.1918 3111.1732
3116.5225 3125.7223 3147.5319 3162.9815 3172.3329 3182.4874 3806.3731</array>
    </property>
    <property dictRef="me:frequenciesScaleFactor">
      <scalar>1.0</scalar>
    </property>
    <property dictRef="me:symmetryNumber">
      <scalar>1</scalar>
    </property>
    <property dictRef="me:spinMultiplicity">
      <scalar>2</scalar>
    </property>
  </propertyList>

```

```

    <property dictRef="me:imFreqs">
      <array units="cm-1">154.6911</array>
    </property>
  </propertyList>
  <me:DOSCMMethod name="ClassicalRotors"/>
</molecule>
<molecule id="P6">
  <propertyList>
    <property dictRef="me:ZPE">
      <scalar units="kcal/mol">-30.5</scalar>
    </property>
    <property dictRef="me:rotConsts">
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1179.7350 1229.6198 1238.8820 1256.4236 1347.3065 1393.1077 1408.1080 1416.8142
1475.1413 1483.5874 1490.3369 1502.9972 1511.8245 2741.3841 3056.2361 3062.4746
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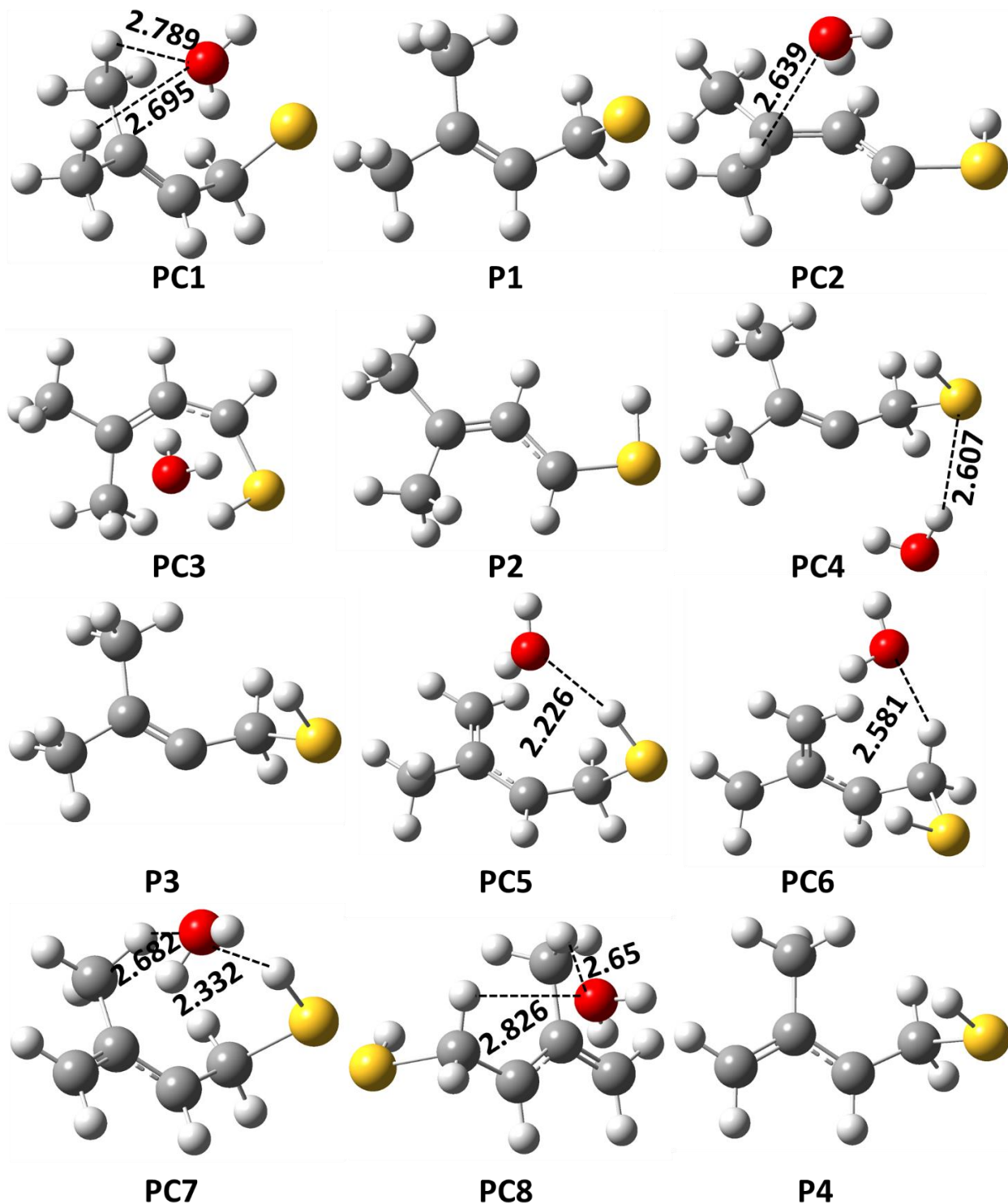


Figure S1. Optimized geometries of post-reactive complexes and products for the H-abstraction and addition paths associated with the MBT + $\cdot\text{OH}$ reaction obtained at the M06-2X/aug-cc-pV(T+d)Z level of theory. The black, yellow, red, and white colors denote C, S, O, and H-atoms, respectively.

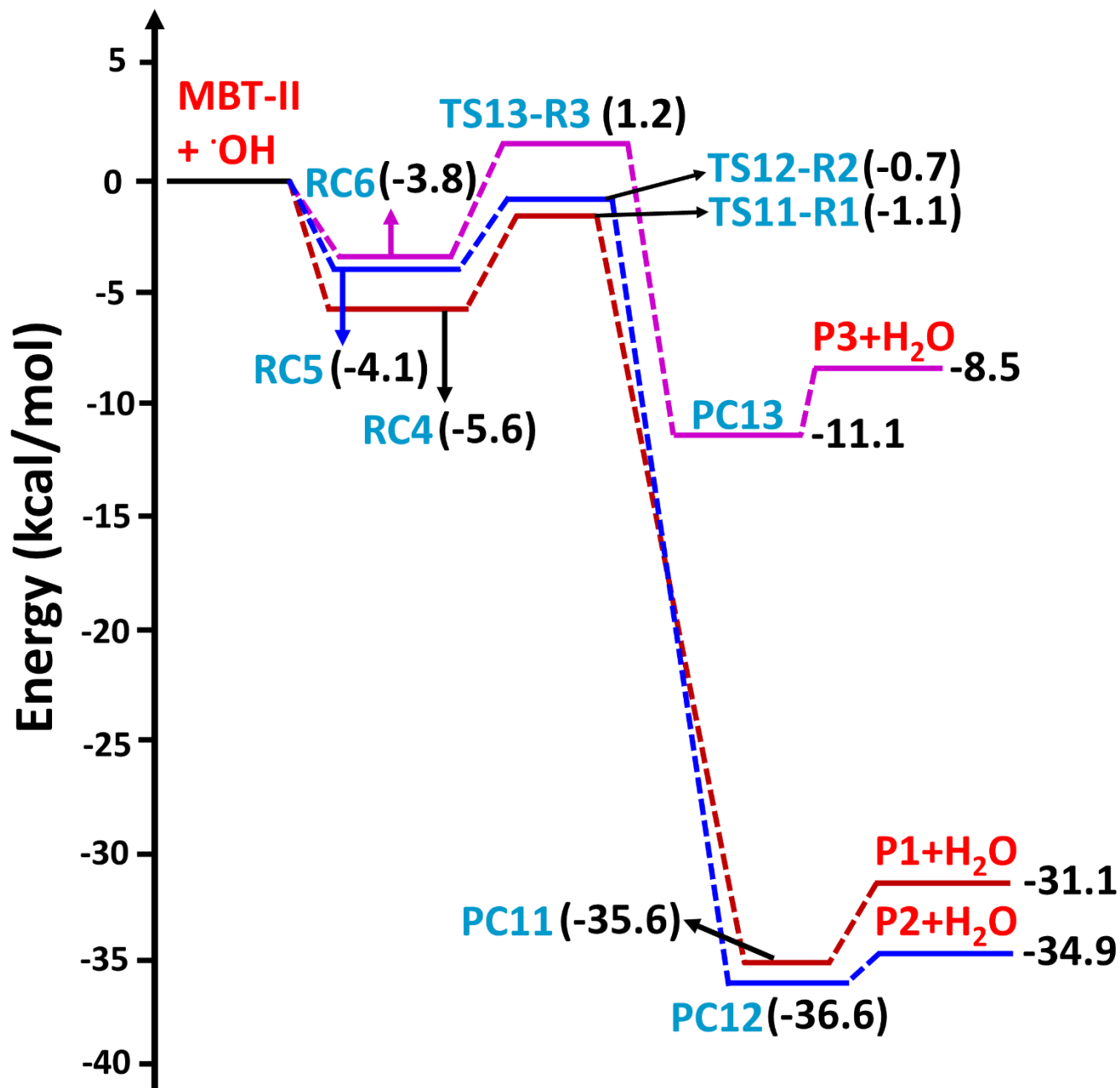


Figure S2. The potential energy surface profiles for H-abstraction from the -SH, -CH₂, and -CH sites in the reaction of MBT-II + OH radical computed at the CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory. The RCs, TSs, PCs, and Ps refer to pre-reactive complexes, transition states, product complexes and products, respectively.

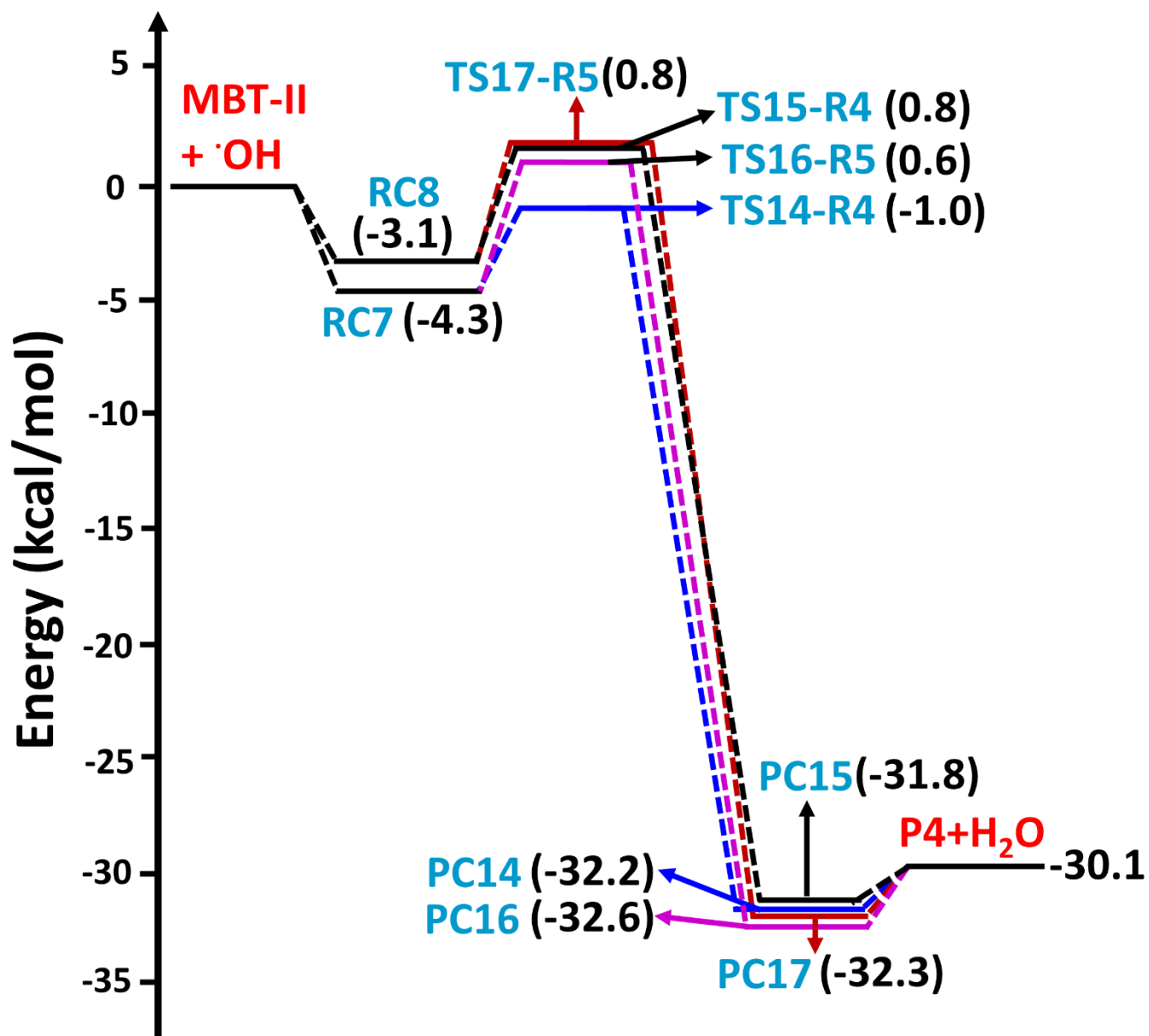


Figure S3. The potential energy surface profiles for H-abstraction from the two methyl groups involved in the reaction of MBT-II + OH radical computed at the CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory. The RCs, TSs, PCs, and Ps refer to pre-reactive complexes, transition states, product complexes and products, respectively.

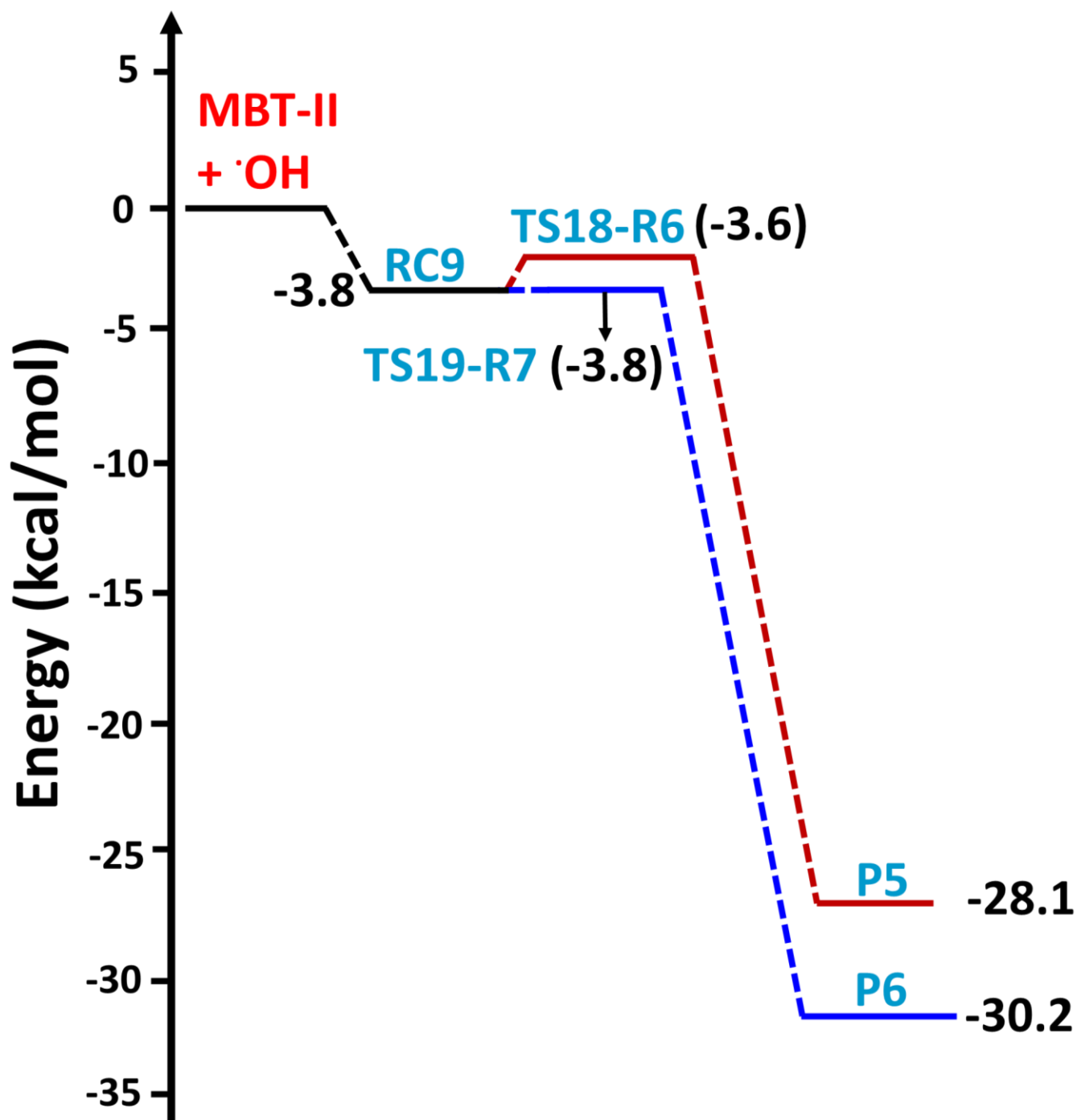


Figure S4. The potential energy surface profiles for the two possible OH addition paths involved in the reaction of MBT-II + OH radical computed at the CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory. The RCs, TSs and Ps refer to pre-reactive complexes, transition states, and products, respectively.

Master equation simulations:^{1,2}

In essence, the energy associated with the intermediate complexes along the potential energy surfaces (PESs) is partitioned into discrete units, which serve as the foundational components for constructing the chemical master equation model.^{1,2} The specific formulation of the energy-grained master equation employed in this study is presented in eqn. 1^{1,2}

$$\frac{d}{dt} \mathbf{p} = \mathbf{M} \mathbf{p} \quad (1)$$

In eqn. 1, 'p' represents a vector that encompasses the population distributions, while 'M' is a matrix responsible for determining how these energy grains within the populations evolve through collision-induced energy transfer processes. These energy transfer events are characterized using an exponential decay model.^{1,2}

We employed a single exponential down model with an average transfer energy of $\Delta E_d = 200 \text{ cm}^{-1}$ to simulate the collision energy transfer processes between the RCs and PCs, and the bath gas (N_2) in the various possible H-abstraction and addition paths involving MBT-I + OH radical and MBT-II + OH radical reactions. This choice of ΔE_d was based on prior studies in the literature that investigated analogous reactions with OH radicals.^{2,3}

In addition to this, Lennard-Jones' (L-J) potentials were essential for computing collision frequencies. Therefore, we adopted the L-J parameters for the RCs and PCs involved in the PES profiles associated with the MBT-I + OH radical and MBT-II + OH radical reactions. The RCs and PC's L-J parameters used were $\sigma = 4.42 \text{ \AA}$ and $\varepsilon = 306.5 \text{ K}$. These L-J parameters were derived based on the nearest-sized alkane.⁴ For the bath gas, N_2 was used in the calculations, and its L-J parameters were $\sigma = 3.9 \text{ \AA}$ and $\varepsilon = 48 \text{ K}$ as per Glowacki et al.⁵

The zero-point-corrected energies for all stationary points located on the PESs as shown in Figures 3, 4 and 5 for the MBT-I + OH radical reaction, and Figures S1, S2 and S3 for MBT-II + OH radical reaction respectively, along with the rotational constants and vibrational frequencies, were obtained from the current calculations. These data were utilized as input parameters for the Mesmer rate calculations. The interaction between MBT-I and OH radical, and MBT-II and OH radical respectively, to form the corresponding intermediate complexes is barrierless. Therefore, for these barrierless reactions, we employed the Inverse Laplace Transform (ILT) method.⁵ The Arrhenius pre-exponential factor utilized in the ILT approach for the MBT-I + OH radical and MBT-II + OH radical barrierless reactions was $1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, as shown in Figures 3, 4 and 5. We set an activation energy value of 0 kcal mol^{-1} and a modified Arrhenius parameter of 0.1 for all the barrierless reaction pathways used in the rate coefficient calculations. To consider the effects of tunneling corrections on reaction rates, we applied the Eckart tunneling correction method.⁶

References:

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