

## Supplementary information (SI)

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# The Hydroxyl Radical Scavenging of Indole-3-carbinol: A Mechanistic and Kinetic Study

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### List of supporting information:

#### Table of Contents

Table S1: Cartesian coordinates and molecular enthalpies of TSs of in water and pentyl ethanoate.....S2

**Table S1: Cartesian coordinates and molecular enthalpies of TSs in water and pentyl ethanoate.**

Water				Pentyl ethanoate			
<b>Name: TS-O11-H-OH-HAT</b>							
Cartesian Coordinates							
C	2.69524400	0.04216100	0.28121600	C	2.58922000	0.63924400	0.37978500
C	2.70530600	-1.32947900	-0.01084000	C	3.02400300	-0.67607600	0.33779500
C	1.54448100	-2.00672100	-0.40386200	C	2.15683600	-1.72513700	-0.03400800
C	0.32622600	-1.34317500	-0.51675600	C	0.83524700	-1.47888800	-0.36889000
C	0.28856100	0.03265700	-0.22909800	C	0.36762300	-0.15391900	-0.33895300
C	1.48288000	0.68437100	0.16260700	C	1.25479900	0.88302900	0.03637800
H	3.59252200	0.56560800	0.58420800	H	3.25386700	1.44542500	0.66621200
H	3.63664800	-1.87497900	0.07053900	H	4.05078300	-0.90449600	0.59729600
H	1.59698800	-3.06574800	-0.61992200	H	2.53395300	-2.74044400	-0.05152000
H	-0.56979700	-1.86681700	-0.81535400	H	0.17000000	-2.28942900	-0.64076400
C	-0.11646600	2.24122900	0.16674400	C	-0.73728200	1.81219100	-0.40078800
H	-0.56790000	3.21446600	0.28691300	H	-1.45347700	2.61403900	-0.49852800
N	1.17038200	2.03444500	0.38987200	N	0.55263900	2.06544400	-0.01403600
H	1.83003600	2.74224200	0.69035800	H	0.92467700	2.97590200	0.20202000
C	-0.74308900	1.01664300	-0.23099700	C	-0.90442600	0.46570200	-0.61638700
H	-2.69347800	-1.06075100	0.43551200	H	-2.84246000	-0.90962400	0.76090700
C	-2.19081100	0.90946700	-0.55130800	C	-2.16233500	-0.20881300	-1.05345100
H	-2.71801500	1.38077200	0.30383400	H	-2.97171800	0.51976200	-1.15349300
H	-2.36605400	1.61658100	-1.38577900	H	-2.02069400	-0.69154300	-2.02840500
O	-2.65222200	-0.36326600	-0.83086400	O	-2.54373000	-1.28262600	-0.20821300
O	-2.72223800	-1.50363700	1.38953500	O	-2.73383500	-0.21505900	1.81040300
H	-2.89193800	-2.44017500	1.24497800	H	-1.83500300	0.15978400	1.77812400
Frequency and Energy							
Zero-point correction= 0.173623 (Hartree/Particle)				Zero-point correction= 0.170691 (Hartree/Particle)			
Thermal correction to Energy= 0.184379				Thermal correction to Energy= 0.181492			
Thermal correction to Enthalpy= 0.185323				Thermal correction to Enthalpy= 0.182436			
Thermal correction to Gibbs Free Energy= 0.135319				Thermal correction to Gibbs Free Energy= 0.133037			
Sum of electronic and zero-point Energies= -553.930108				Sum of electronic and zero-point Energies= -553.897646			
Sum of electronic and thermal Energies= -553.919352				Sum of electronic and thermal Energies= -553.886844			
Sum of electronic and thermal Enthalpies= -553.918407				Sum of electronic and thermal Enthalpies= -553.885900			
Sum of electronic and thermal Free Energies= -553.968411				Sum of electronic and thermal Free Energies= -553.935299			
<b>Name: TS-N1-H-OH-HAT</b>							
Cartesian Coordinates							
C	-2.26089700	0.25385000	-0.23086300	C	-2.24390800	0.17420400	-0.17449200
C	-2.80516100	-1.00796700	0.00789800	C	-2.74068900	-1.11363100	0.02362200

C	-1.98411200	-2.12856200	0.20015600	C	-1.87833000	-2.21053000	0.16390400
C	-0.59377500	-2.01636300	0.17582400	C	-0.49303600	-2.04917200	0.13120000
C	-0.03839700	-0.75899400	-0.05226100	C	0.01720600	-0.76618900	-0.06075100
C	-0.87914200	0.35663000	-0.28048000	C	-0.86809000	0.32186100	-0.24799500
H	-2.87942100	1.12991000	-0.34500200	H	-2.87512500	1.04658500	-0.22492800
H	-3.87774100	-1.12261300	0.05130800	H	-3.80752600	-1.26840900	0.07936400
H	-2.43795500	-3.09167200	0.37879200	H	-2.29600800	-3.19545200	0.31151800
H	0.03503500	-2.88042000	0.33290000	H	0.16445000	-2.89713600	0.25242000
C	1.25368900	1.09211500	-0.35593200	C	1.22524400	1.15194100	-0.31033800
H	2.06218600	1.78782800	-0.46890500	H	2.01096300	1.87362400	-0.42321500
N	-0.06848200	1.47708000	-0.53845000	N	-0.10538300	1.47998400	-0.47472200
H	-0.52193400	2.51851500	-0.34184600	H	-0.65643000	2.50093500	-0.31616700
C	1.32478500	-0.25505800	-0.10123500	C	1.35608600	-0.20450000	-0.09765500
H	3.65535100	0.31886800	1.02449800	H	3.64236400	0.39025300	1.11673700
C	2.58444600	-1.03937800	0.03226500	C	2.65874500	-0.92408600	-0.01206100
H	2.50920900	-1.72199600	0.88318000	H	2.61320300	-1.68816100	0.77107700
H	2.75856000	-1.63537900	-0.86446600	H	2.88187400	-1.42249900	-0.95622100
O	3.73308800	-0.14485600	0.15064200	O	3.74833700	0.02354700	0.20000900
O	-1.20701300	3.16314800	0.52442500	O	-1.49768700	3.08838700	0.40943000
H	-0.64113300	3.23342500	1.34592000	H	-1.14464500	3.12550400	1.34435900
Frequency and Energy							
Zero-point correction= 0.175957 (Hartree/Particle)				Zero-point correction= 0.171113 (Hartree/Particle)			
Thermal correction to Energy= 0.187477				Thermal correction to Energy= 0.182574			
Thermal correction to Enthalpy= 0.188421				Thermal correction to Enthalpy= 0.183518			
Thermal correction to Gibbs Free Energy= 0.136005				Thermal correction to Gibbs Free Energy= 0.132626			
Sum of electronic and zero-point Energies= -553.908110				Sum of electronic and zero-point Energies= -553.895816			
Sum of electronic and thermal Energies= -553.896591				Sum of electronic and thermal Energies= -553.884354			
Sum of electronic and thermal Enthalpies= -553.895646				Sum of electronic and thermal Enthalpies= -553.883410			
Sum of electronic and thermal Free Energies= -553.948062				Sum of electronic and thermal Free Energies= -553.934303			
<b>Name: TS-C5-H-OH-HAT</b>							
Cartesian Coordinates							
C	-2.65138000	-0.23356900	0.15520700	C	-2.53518300	-0.68530800	0.13667900
C	-2.70940300	1.14988300	0.09666700	C	-2.82088700	0.66386100	0.27013400
C	-1.54120000	1.92980400	-0.06420100	C	-1.79941600	1.63919400	0.22357800
C	-0.32077500	1.30147700	-0.18764500	C	-0.48929400	1.24222000	0.06737400
C	-0.20139900	-0.09069500	-0.13670500	C	-0.14173500	-0.10443900	-0.07238600
C	-1.39474100	-0.83856400	0.03914300	C	-1.19554100	-1.05394500	-0.03362800
H	-3.54565300	-0.82936700	0.29072100	H	-3.32192200	-1.42982700	0.15999000
H	-3.66639300	1.64932800	0.18452700	H	-3.84743000	0.98219600	0.40535400
H	-1.61155700	3.01004200	-0.08979600	H	-2.04938700	2.68906500	0.31617600

H	0.65731300	1.97356400	-0.31259900	H	0.37137600	2.08419000	0.03221800
C	0.31486200	-2.27838800	-0.07870800	C	0.72991700	-2.15894100	-0.33355400
H	0.78854500	-3.24799700	-0.08437900	H	1.35742200	-3.02639500	-0.47376700
N	-1.04352400	-2.16640600	0.06738500	N	-0.62823100	-2.29428000	-0.19814800
H	-1.68282000	-2.93816000	0.17657500	H	-1.12871800	-3.16803900	-0.21992200
C	0.88203300	-1.03618200	-0.21491200	C	1.08373600	-0.83436700	-0.26383200
H	2.68701400	-0.33832200	1.47653500	H	2.75805400	-0.62391200	1.61766000
C	2.33079500	-0.74836700	-0.42276700	C	2.47310800	-0.28466400	-0.28551200
H	2.88531800	-1.68580000	-0.49423400	H	3.15333300	-1.02995500	-0.70935500
H	2.49376300	-0.17692400	-1.33688600	H	2.52774000	0.61762200	-0.89311200
O	2.89205400	0.07032200	0.62577400	O	2.92259100	0.11115000	1.01661200
O	1.82909000	2.56141500	-0.08552000	O	1.08934600	3.05037800	-0.48536500
H	2.27723400	1.76219600	0.27932500	H	0.65342000	3.13112500	-1.35130900
Frequency and Energy							
Zero-point correction= 0.171542 (Hartree/Particle)				Zero-point correction= 0.171019 (Hartree/Particle)			
Thermal correction to Energy= 0.182059				Thermal correction to Energy= 0.182339			
Thermal correction to Enthalpy= 0.183003				Thermal correction to Enthalpy= 0.183283			
Thermal correction to Gibbs Free Energy= 0.135045				Thermal correction to Gibbs Free Energy= 0.133126			
Sum of electronic and zero-point Energies= -553.901623				Sum of electronic and zero-point Energies= -553.890353			
Sum of electronic and thermal Energies= -553.891106				Sum of electronic and thermal Energies= -553.879033			
Sum of electronic and thermal Enthalpies= -553.890162				Sum of electronic and thermal Enthalpies= -553.878089			
Sum of electronic and thermal Free Energies= -553.938121				Sum of electronic and thermal Free Energies= -553.928246			
<b>Name: TS-C6-H-OH-HAT</b>							
Cartesian Coordinates							
C	1.18936800	-1.98458800	-0.22165500	C	-1.17796400	1.99545000	-0.21323100
C	2.26418500	-1.10724900	-0.25528600	C	-2.25444500	1.12110700	-0.25012100
C	2.03702000	0.27168800	-0.12173500	C	-2.03092900	-0.25889600	-0.12725600
C	0.79364300	0.83504100	0.07217900	C	-0.78907900	-0.82649400	0.05949600
C	-0.30575300	-0.04287500	0.10600800	C	0.31265700	0.04766900	0.09912800
C	-0.08577100	-1.43535000	-0.04238100	C	0.09616700	1.44174700	-0.03742500
H	1.33200700	-3.05305900	-0.32852100	H	-1.32101800	3.06452100	-0.31556100
H	3.27058400	-1.48289100	-0.39009500	H	-3.26035800	1.49915500	-0.38334400
H	2.97062600	0.98975400	-0.18579600	H	-2.97937500	-0.98203500	-0.19987700
H	0.66383200	1.90474200	0.18720000	H	-0.66050700	-1.89811600	0.15529700
C	-2.28376400	-1.10754900	0.22909900	C	2.29609900	1.10310200	0.21859800
H	-3.31942200	-1.39766200	0.32009600	H	3.33389200	1.38749700	0.30637000
N	-1.30949000	-2.05428600	0.03838900	N	1.32305900	2.05462500	0.04264700
H	-1.46810100	-3.04767600	-0.02548400	H	1.48683300	3.04597700	-0.02411200
C	-1.72282300	0.14414200	0.28034300	C	1.73043500	-0.14608000	0.26516900
H	-2.80223100	1.75890500	-1.44547800	H	2.52626100	-1.79815200	-1.48452200

C	-2.44433400	1.43764000	0.45827500	C	2.44712600	-1.44483800	0.43769800
H	-3.48157500	1.24525300	0.74118000	H	3.50485500	-1.25352000	0.64403400
H	-1.97839300	2.04013300	1.23804400	H	2.03739900	-2.00897200	1.27679100
O	-2.40363400	2.26062400	-0.72376900	O	2.30542000	-2.30737000	-0.69640100
O	4.05764300	1.72330400	0.15975400	O	-4.02551300	-1.69805200	0.18013700
H	4.09639200	1.48568500	1.10316900	H	-3.94905000	-1.59194500	1.14416300
Frequency and Energy							
Zero-point correction= 0.170440 (Hartree/Particle)				Zero-point correction= 0.170777 (Hartree/Particle)			
Thermal correction to Energy= 0.181821				Thermal correction to Energy= 0.182195			
Thermal correction to Enthalpy= 0.182765				Thermal correction to Enthalpy= 0.183139			
Thermal correction to Gibbs Free Energy= 0.131711				Thermal correction to Gibbs Free Energy= 0.132304			
Sum of electronic and zero-point Energies= -553.898650				Sum of electronic and zero-point Energies= -553.892313			
Sum of electronic and thermal Energies= -553.887269				Sum of electronic and thermal Energies= -553.880895			
Sum of electronic and thermal Enthalpies= -553.886325				Sum of electronic and thermal Enthalpies= -553.879950			
Sum of electronic and thermal Free Energies= -553.937379				Sum of electronic and thermal Free Energies= -553.930786			
<b>Name: TS-C7-H-OH-HAT</b>							
Cartesian Coordinates							
C	-1.68629200	1.01271400	-0.18608800	C	-1.69328800	1.00099200	-0.20615300
C	-2.27295600	-0.23382500	-0.12004000	C	-2.26781200	-0.25137500	-0.15193900
C	-1.57053600	-1.42993400	0.09353800	C	-1.55450100	-1.44095700	0.05846300
C	-0.18926700	-1.39055400	0.22660000	C	-0.17461300	-1.38888500	0.19584500
C	0.46569700	-0.14928000	0.15483400	C	0.46799600	-0.14103300	0.13657700
C	-0.29179800	1.03106100	-0.05085100	C	-0.29932900	1.03270700	-0.06665800
H	-2.25999200	1.91831700	-0.33869400	H	-2.27952400	1.89939200	-0.35641000
H	-3.44298500	-0.29990500	-0.26511500	H	-3.45108800	-0.32528300	-0.30361400
H	-2.10280200	-2.37116200	0.14583100	H	-2.07729300	-2.38832700	0.09893000
H	0.37348000	-2.30370400	0.38194700	H	0.39998500	-2.29641300	0.33908100
C	1.86163500	1.61652600	0.10111600	C	1.85012100	1.63630700	0.09646400
H	2.69946400	2.29694100	0.11332600	H	2.68283300	2.32328000	0.11652200
N	0.58486500	2.08723800	-0.07634700	N	0.56951900	2.09601300	-0.08521800
H	0.33175200	3.05442900	-0.20410100	H	0.31092500	3.06086100	-0.21185100
C	1.84579000	0.25283100	0.25142600	C	1.84443400	0.27229600	0.24240800
H	3.38780600	-0.94794100	-1.45117500	H	3.19625300	-1.05453600	-1.44239100
C	3.02881400	-0.63417300	0.45230500	C	3.03260300	-0.60744100	0.45575000
H	3.91702100	-0.02792100	0.64369900	H	3.92584200	0.01107500	0.58934600
H	2.87592600	-1.30259800	1.29971600	H	2.90880900	-1.22001500	1.35022300
O	3.26086100	-1.50371000	-0.67252500	O	3.22555200	-1.54275800	-0.61186100
O	-4.78642900	-0.33946900	-0.10238000	O	-4.74296000	-0.33928200	-0.02490200
H	-4.81570100	-0.33388700	0.87119300	H	-4.69778000	-0.30147900	0.94624700
Frequency and Energy							

Zero-point correction=	0.170200 (Hartree/Particle)	Zero-point correction=	0.170744 (Hartree/Particle)
Thermal correction to Energy=	0.181597	Thermal correction to Energy=	0.182087
Thermal correction to Enthalpy=	0.182541	Thermal correction to Enthalpy=	0.183031
Thermal correction to Gibbs Free Energy=	0.131328	Thermal correction to Gibbs Free Energy=	0.132439
Sum of electronic and zero-point Energies=	-553.898675	Sum of electronic and zero-point Energies=	-553.892014
Sum of electronic and thermal Energies=	-553.887278	Sum of electronic and thermal Energies=	-553.880671
Sum of electronic and thermal Enthalpies=	-553.886334	Sum of electronic and thermal Enthalpies=	-553.879727
Sum of electronic and thermal Free Energies=	-553.937547	Sum of electronic and thermal Free Energies=	-553.930319
<b>Name: TS-C8-H-OH-HAT</b>			
Cartesian Coordinates			
C	1.95169800	0.21449000	-0.14637700
C	2.04474500	1.58786500	-0.08100400
C	0.87296000	2.36000300	0.09141700
C	-0.37108500	1.75979400	0.21131200
C	-0.46495400	0.35845600	0.15991600
C	0.71424300	-0.41021400	-0.01485500
H	2.92199500	-0.44964400	-0.32716200
H	3.00742800	2.07596400	-0.16884600
H	0.95872500	3.43898500	0.13104400
H	-1.26160800	2.36301100	0.34550600
C	-1.00213300	-1.82998900	0.13947900
H	-1.48319400	-2.79561200	0.16668900
N	0.35782900	-1.73403700	-0.02325300
H	0.99323100	-2.51070000	-0.12024000
C	-1.55440900	-0.57991100	0.25822600
H	-3.44060500	-0.22388000	-1.47829500
C	-3.00223900	-0.26474500	0.43386700
H	-3.55082400	-1.17944400	0.66941700
H	-3.15104900	0.44682900	1.24593900
O	-3.57560900	0.36619500	-0.72680600
O	3.98541200	-1.24127000	-0.19626800
H	4.08972000	-1.20115200	0.77143000
C	1.94963300	0.22616900	-0.17247800
C	2.02570000	1.59953400	-0.08817500
C	0.84582200	2.35474200	0.09866900
C	-0.38960800	1.73813300	0.21727800
C	-0.46678500	0.33714900	0.15008700
C	0.71997700	-0.41495100	-0.04129200
H	2.93559300	-0.43232800	-0.36674200
H	2.98211800	2.10066800	-0.17487800
H	0.91749600	3.43450900	0.14858900
H	-1.28825300	2.32701900	0.35803500
C	-0.98169800	-1.85590400	0.10431000
H	-1.45307600	-2.82687400	0.11904200
N	0.37657400	-1.74211800	-0.06250700
H	1.01495500	-2.51145600	-0.18525400
C	-1.54618300	-0.61361700	0.24376800
H	-3.30581700	-0.01515700	-1.47936400
C	-2.99725000	-0.31074700	0.42983400
H	-3.54863500	-1.24521200	0.57401600
H	-3.15637300	0.31462100	1.30937100
O	-3.55053000	0.43292000	-0.66187500
O	3.95339500	-1.21798400	-0.12985400
H	4.08540700	-1.03350000	0.81656500
Frequency and Energy			
Zero-point correction=	0.170542 (Hartree/Particle)	Zero-point correction=	0.170963 (Hartree/Particle)
Thermal correction to Energy=	0.181856	Thermal correction to Energy=	0.182241
Thermal correction to Enthalpy=	0.182800	Thermal correction to Enthalpy=	0.183185
Thermal correction to Gibbs Free Energy=	0.132110	Thermal correction to Gibbs Free Energy=	0.132869
Sum of electronic and zero-point Energies=	-553.897211	Sum of electronic and zero-point Energies=	-553.891415
Sum of electronic and thermal Energies=	-553.885897	Sum of electronic and thermal Energies=	-553.880137
Sum of electronic and thermal Enthalpies=	-553.884953	Sum of electronic and thermal Enthalpies=	-553.879193

Sum of electronic and thermal Free Energies= -553.935643				Sum of electronic and thermal Free Energies= -553.929509			
<b>Name: TS-C10-H-OH-HAT</b>							
Cartesian Coordinates							
C	-2.72348600	0.29041600	0.14393100	C	-2.79057700	0.16805000	0.16791200
C	-2.88235800	-1.06743700	-0.08883000	C	-2.87874200	-1.20914000	0.03855300
C	-1.77263200	-1.90656500	-0.32403200	C	-1.72789700	-2.00499800	-0.13612200
C	-0.48153000	-1.40079200	-0.33414200	C	-0.46436000	-1.43819300	-0.18924500
C	-0.28976100	-0.02691300	-0.10128100	C	-0.34560900	-0.04377100	-0.06571500
C	-1.41866800	0.79384600	0.13566500	C	-1.51285100	0.73405900	0.11632800
H	-3.57207600	0.93820800	0.32714600	H	-3.67342900	0.78060100	0.30626900
H	-3.87853100	-1.49276500	-0.08973000	H	-3.85148300	-1.68455700	0.07461300
H	-1.93630900	-2.96246600	-0.50161900	H	-1.83755300	-3.07886600	-0.22848100
H	0.36526200	-2.05247900	-0.52232800	H	0.41565600	-2.05543200	-0.32314200
C	0.40058700	2.09252300	0.24726400	C	0.23872400	2.13125100	0.11082900
H	0.95149100	3.01037600	0.38357100	H	0.74372200	3.08339300	0.16810600
N	-0.96395800	2.07597500	0.34410000	N	-1.12041700	2.05020900	0.22278500
H	-1.54278500	2.87781900	0.54004100	H	-1.73731600	2.83548100	0.35451400
C	0.86865100	0.83010200	-0.02919300	C	0.76873700	0.87400400	-0.07020800
H	2.04326900	-0.73362700	-1.72821400	H	1.89559400	-0.16048800	-2.00379600
C	2.29474600	0.45066300	-0.18391800	C	2.20203600	0.54860100	-0.20590200
H	2.95314300	1.28928800	0.03705000	H	2.82269600	1.44722900	-0.25649100
H	2.55120400	-0.35525800	0.57883600	H	2.56662400	-0.01754800	0.72923900
O	2.65715200	-0.03507100	-1.46870600	O	2.49623700	-0.34516700	-1.27178400
O	2.72553500	-1.65299100	1.50701300	O	3.28030400	-1.20576100	1.33976500
H	1.77825500	-1.88148600	1.46731800	H	3.34932000	-1.65303100	0.47725200
Frequency and Energy							
Zero-point correction= 0.173215 (Hartree/Particle)				Zero-point correction= 0.172481 (Hartree/Particle)			
Thermal correction to Energy= 0.184042				Thermal correction to Energy= 0.183438			
Thermal correction to Enthalpy= 0.184986				Thermal correction to Enthalpy= 0.184382			
Thermal correction to Gibbs Free Energy= 0.135677				Thermal correction to Gibbs Free Energy= 0.134460			
Sum of electronic and zero-point Energies= -553.905968				Sum of electronic and zero-point Energies= -553.899958			
Sum of electronic and thermal Energies= -553.895142				Sum of electronic and thermal Energies= -553.889001			
Sum of electronic and thermal Enthalpies= -553.894198				Sum of electronic and thermal Enthalpies= -553.888057			
Sum of electronic and thermal Free Energies= -553.943506				Sum of electronic and thermal Free Energies= -553.937979			
<b>Name: TS-C2-OH-RAF</b>							
Cartesian Coordinates							
C	2.39773500	-0.80872300	-0.38162200	C	2.39501700	-0.85187200	-0.34397300
C	3.03329500	0.35115600	0.05080100	C	3.05030900	0.28994900	0.09688900
C	2.30511200	1.48329300	0.46476100	C	2.34132100	1.44350600	0.49031500

C	0.91739100	1.48221200	0.45855100	C	0.95667400	1.47882500	0.45216500
C	0.25441100	0.32318800	0.02775300	C	0.26772000	0.33572300	0.01295700
C	1.00663900	-0.79882500	-0.38700500	C	1.00041000	-0.81008900	-0.38155100
H	2.95806900	-1.67904000	-0.69892500	H	2.94247600	-1.73647400	-0.64552600
H	4.11569600	0.38357500	0.06917700	H	4.13286900	0.29515300	0.13855100
H	2.84043600	2.36539200	0.79301400	H	2.89204800	2.31401100	0.82503600
H	0.35601500	2.35222500	0.77750200	H	0.41310600	2.36798300	0.74805000
C	-1.15106300	-1.35845700	-0.56764200	C	-1.17542500	-1.30312600	-0.59002800
H	-2.00333400	-1.95664100	-0.84524500	H	-2.03308800	-1.87609200	-0.90107000
N	0.10937700	-1.79149100	-0.76588500	N	0.09071500	-1.77354000	-0.77160500
H	0.36119800	-2.72080300	-1.06817600	H	0.31899200	-2.71804700	-1.03723700
C	-1.13143200	-0.03485100	-0.08850800	C	-1.12410900	0.01626800	-0.13723100
H	-2.55887500	1.49918400	-1.70400900	H	-2.30286400	1.75897400	-1.62733800
C	-2.31821500	0.84283300	0.13199400	C	-2.29636200	0.90064400	0.13425000
H	-3.22927300	0.24377000	0.11205700	H	-3.21960200	0.32560700	0.02936100
H	-2.24194900	1.33746600	1.09925200	H	-2.25330600	1.28733500	1.15294500
O	-2.38574200	1.89558800	-0.84107000	O	-2.31119000	2.05619400	-0.71056100
O	-1.67512200	-1.49366100	1.66678000	O	-1.81180900	-1.71486500	1.50672500
H	-0.75994500	-1.39107200	1.96637500	H	-1.03497200	-1.33326700	1.94639600
Frequency and Energy							
Zero-point correction= 0.177135 (Hartree/Particle)				Zero-point correction= 0.176765 (Hartree/Particle)			
Thermal correction to Energy= 0.187907				Thermal correction to Energy= 0.187673			
Thermal correction to Enthalpy= 0.188851				Thermal correction to Enthalpy= 0.188618			
Thermal correction to Gibbs Free Energy= 0.140064				Thermal correction to Gibbs Free Energy= 0.139412			
Sum of electronic and zero-point Energies= -553.915957				Sum of electronic and zero-point Energies= -553.905809			
Sum of electronic and thermal Energies= -553.905185				Sum of electronic and thermal Energies= -553.894901			
Sum of electronic and thermal Enthalpies= -553.904241				Sum of electronic and thermal Enthalpies= -553.893957			
Sum of electronic and thermal Free Energies= -553.953029				Sum of electronic and thermal Free Energies= -553.943162			
<b>Name: TS-C3-OH-RAF</b>							
Cartesian Coordinates							
C	-2.39759600	0.80864800	-0.38186700	C	2.42285300	-0.78923100	-0.36407400
C	-3.03325800	-0.35112600	0.05068700	C	3.02398800	0.40998200	-0.00302500
C	-2.30517900	-1.48322600	0.46493900	C	2.25923700	1.53367100	0.36340500
C	-0.91746400	-1.48221400	0.45888600	C	0.87206800	1.48068200	0.38360500
C	-0.25436500	-0.32330200	0.02793800	C	0.24309500	0.28107000	0.02872900
C	-1.00649900	0.79867900	-0.38711100	C	1.02905800	-0.82926800	-0.34625200
H	-2.95785300	1.67893400	-0.69939000	H	3.01086500	-1.65302900	-0.64929100
H	-4.11566300	-0.38349300	0.06893400	H	4.10485900	0.48232200	-0.00626300
H	-2.84058400	-2.36524200	0.79328400	H	2.76521400	2.45253900	0.63292800
H	-0.35617100	-2.35220100	0.77804800	H	0.28704000	2.34810900	0.66501700



C	1.15126300	1.35818500	-0.56756900	C	-1.11850400	-1.45276000	-0.49766900
H	2.00355500	1.95613700	-0.84559900	H	-1.94839100	-2.11684100	-0.68127900
N	-0.10915400	1.79122100	-0.76609500	N	0.16173000	-1.86397500	-0.66410900
H	-0.36089100	2.72044300	-1.06872800	H	0.43864200	-2.79689400	-0.92662200
C	1.13147600	0.03456000	-0.08838800	C	-1.14347400	-0.13697300	-0.02981900
H	2.55859400	-1.49999600	-1.70361000	H	-2.54894200	1.04840200	-1.88043600
C	2.31826400	-0.84309000	0.13225600	C	-2.34333000	0.75317200	0.04715000
H	3.22932100	-0.24401300	0.11203000	H	-3.24051300	0.14387700	0.17807700
H	2.24212200	-1.33743400	1.09966900	H	-2.25576400	1.41722800	0.90414100
O	2.38568000	-1.89612000	-0.84050000	O	-2.46607700	1.60384000	-1.09759800
O	1.67476600	1.49456100	1.66621600	O	-1.60278200	-0.94820500	1.94103300
H	0.75821900	1.39810100	1.96366500	H	-0.66420300	-1.02503500	2.17270700
Frequency and Energy							
Zero-point correction= 0.177174 (Hartree/Particle)				Zero-point correction= 0.177168 (Hartree/Particle)			
Thermal correction to Energy= 0.187914				Thermal correction to Energy= 0.187859			
Thermal correction to Enthalpy= 0.188858				Thermal correction to Enthalpy= 0.188804			
Thermal correction to Gibbs Free Energy= 0.140171				Thermal correction to Gibbs Free Energy= 0.140459			
Sum of electronic and zero-point Energies= -553.915919				Sum of electronic and zero-point Energies= -553.905388			
Sum of electronic and thermal Energies= -553.905179				Sum of electronic and thermal Energies= -553.894697			
Sum of electronic and thermal Enthalpies= -553.904234				Sum of electronic and thermal Enthalpies= -553.893753			
Sum of electronic and thermal Free Energies= -553.952921				Sum of electronic and thermal Free Energies= -553.942097			
<b>Name: TS-C5-OH-RAF</b>							
Cartesian Coordinates							
C	2.38487800	0.71621600	0.30044400	C	2.33117200	0.86505300	0.24775300
C	2.76711700	-0.61251500	-0.02507900	C	2.79401400	-0.40669800	-0.08663900
C	1.86643300	-1.53488800	-0.52420500	C	1.92765300	-1.39533500	-0.57231700
C	0.50791900	-1.19095500	-0.72209700	C	0.55349200	-1.15184500	-0.71547800
C	0.11308700	0.13290500	-0.40451500	C	0.06750800	0.13371500	-0.38118100
C	1.06601000	1.05315600	0.10219800	C	0.96482700	1.11497700	0.09912600
H	3.10458000	1.42058400	0.69689500	H	3.00718800	1.62684200	0.61686400
H	3.80172700	-0.89879800	0.11309700	H	3.84765800	-0.63132600	0.02282000
H	2.20145900	-2.53122400	-0.77991700	H	2.32156600	-2.36828300	-0.83756600
H	-0.15262000	-1.84546800	-1.26895600	H	-0.07905600	-1.87014400	-1.21991000
C	-0.91941500	2.06815900	0.07540300	C	-1.09558200	1.98868700	0.11022200
H	-1.62894100	2.86747800	0.22538200	H	-1.84537900	2.74587800	0.28232700
N	0.38255700	2.23391700	0.35979900	N	0.22437000	2.24105600	0.37334800
H	0.79763600	3.08534700	0.71403100	H	0.59056300	3.11085300	0.72581000
C	-1.14244200	0.76638000	-0.40421300	C	-1.24428400	0.70309300	-0.35812200
H	-1.92348100	-1.36844200	0.64854900	H	-2.00226000	-1.44605300	0.63651100
C	-2.44973900	0.08731800	-0.66538000	C	-2.50835200	-0.04314900	-0.64260200

H	-3.24785500	0.82542600	-0.74560900	H	-3.35031900	0.64630300	-0.70670300
H	-2.39222300	-0.46255400	-1.61037100	H	-2.42656400	-0.56638000	-1.60192600
O	-2.76496100	-0.79903300	0.40793100	O	-2.81856000	-0.97739800	0.39356700
O	-0.75300800	-2.19318100	1.01765600	O	-0.26335300	-2.27476900	1.05411200
H	-0.25750700	-1.70671800	1.68827200	H	0.27862900	-1.76872800	1.68232300
Frequency and Energy							
Zero-point correction= 0.175689 (Hartree/Particle)				Zero-point correction= 0.177361 (Hartree/Particle)			
Thermal correction to Energy= 0.185770				Thermal correction to Energy= 0.187831			
Thermal correction to Enthalpy= 0.186714				Thermal correction to Enthalpy= 0.188775			
Thermal correction to Gibbs Free Energy= 0.139564				Thermal correction to Gibbs Free Energy= 0.140775			
Sum of electronic and zero-point Energies= -553.912020				Sum of electronic and zero-point Energies= -553.905428			
Sum of electronic and thermal Energies= -553.901939				Sum of electronic and thermal Energies= -553.894958			
Sum of electronic and thermal Enthalpies= -553.900995				Sum of electronic and thermal Enthalpies= -553.894013			
Sum of electronic and thermal Free Energies= -553.948145				Sum of electronic and thermal Free Energies= -553.942014			
<b>Name: TS-C6-OH-RAF</b>							
Cartesian Coordinates							
C	1.88416600	1.42741200	0.04283100	C	1.83492900	1.47205600	0.01811200
C	2.63107500	0.34984500	-0.37633800	C	2.59975300	0.39767700	-0.36717700
C	2.01394000	-0.87940300	-0.74880100	C	2.00991700	-0.86848700	-0.68011600
C	0.61485000	-1.00120200	-0.77194600	C	0.60762800	-1.00583600	-0.71073900
C	-0.16087400	0.07899600	-0.34416300	C	-0.18534700	0.07204500	-0.30931800
C	0.48466700	1.27508600	0.06047200	C	0.43709000	1.29403100	0.05029300
H	2.34650900	2.35946900	0.34301300	H	2.28424300	2.42209700	0.28038100
H	3.71104600	0.42071100	-0.40535700	H	3.67802600	0.48670700	-0.40216600
H	2.62228900	-1.66549400	-1.17371300	H	2.62180700	-1.62158200	-1.15439000
H	0.15488100	-1.92808500	-1.09219800	H	0.16315800	-1.95088000	-0.99561500
C	-1.72432100	1.58005600	0.26058800	C	-1.77891300	1.56131100	0.25025100
H	-2.62298400	2.12993200	0.49389500	H	-2.68898300	2.10039400	0.46503600
N	-0.48652600	2.16327200	0.42059900	N	-0.55223600	2.17387900	0.38601900
H	-0.32434100	3.10470100	0.74391800	H	-0.41071400	3.12624200	0.68245800
C	-1.58036000	0.30166800	-0.20922300	C	-1.61006100	0.27182400	-0.17863000
H	-2.75143200	-1.44811600	1.29827600	H	-2.57564400	-1.57420800	1.30406900
C	-2.67504300	-0.66944900	-0.50064600	C	-2.68894700	-0.72412300	-0.45522400
H	-3.64037400	-0.16112900	-0.45289600	H	-3.66532600	-0.24025000	-0.35451200
H	-2.55879000	-1.10124000	-1.49449600	H	-2.60829500	-1.11108000	-1.47189000
O	-2.66458200	-1.79185000	0.40054500	O	-2.60941600	-1.87654900	0.38960100
O	2.15511400	-1.99690600	1.18568500	O	2.35780900	-1.90688400	1.06465500
H	1.61602500	-1.32166700	1.62889000	H	1.72394700	-1.41012200	1.60573700
Frequency and Energy							

Zero-point correction=	0.176142 (Hartree/Particle)	Zero-point correction=	0.176974 (Hartree/Particle)
Thermal correction to Energy=	0.187248	Thermal correction to Energy=	0.187798
Thermal correction to Enthalpy=	0.188192	Thermal correction to Enthalpy=	0.188742
Thermal correction to Gibbs Free Energy=	0.138242	Thermal correction to Gibbs Free Energy=	0.139554
Sum of electronic and zero-point Energies=	-553.908846	Sum of electronic and zero-point Energies=	-553.898334
Sum of electronic and thermal Energies=	-553.897741	Sum of electronic and thermal Energies=	-553.887510
Sum of electronic and thermal Enthalpies=	-553.896797	Sum of electronic and thermal Enthalpies=	-553.886566
Sum of electronic and thermal Free Energies=	-553.946746	Sum of electronic and thermal Free Energies=	-553.935753
<b>Name: TS-C7-OH-RAF</b>			
Cartesian Coordinates			
C	1.90742100 1.00674100 -0.30834000	C	1.88686800 1.02325700 -0.29133000
C	2.50137000 -0.23689100 -0.57356900	C	2.48801800 -0.22807300 -0.52615300
C	1.70245300 -1.39693600 -0.79203800	C	1.67724700 -1.38565100 -0.75489700
C	0.33131300 -1.34899800 -0.68067100	C	0.30837300 -1.33427300 -0.64446600
C	-0.28378000 -0.11376400 -0.37147100	C	-0.30623500 -0.09549900 -0.34199700
C	0.52251900 1.03924500 -0.19042800	C	0.50283400 1.05651300 -0.16938600
H	2.51050900 1.89629600 -0.17813500	H	2.49326400 1.91127600 -0.16782400
H	3.56231800 -0.28096400 -0.77648100	H	3.53344300 -0.26287500 -0.79539900
H	2.19705600 -2.33085700 -1.02721500	H	2.17157000 -2.32212700 -0.97989800
H	-0.27056200 -2.23774000 -0.82979100	H	-0.29493400 -2.22302700 -0.78555800
C	-1.60970600 1.64374100 0.08454300	C	-1.63073000 1.66486600 0.11239000
H	-2.42820600 2.32089000 0.27619400	H	-2.44846500 2.34291900 0.30550700
N	-0.32138400 2.09225600 0.08817400	N	-0.34047800 2.11192600 0.10424800
H	-0.03585800 3.04540600 0.25220900	H	-0.05185100 3.06182500 0.27434700
C	-1.64322600 0.29299000 -0.19370000	C	-1.66556700 0.31348700 -0.15973400
H	-3.01971500 -0.93704900 1.65191800	H	-2.75855100 -1.15084500 1.62146200
C	-2.86056300 -0.56752800 -0.26858900	C	-2.88490100 -0.54753100 -0.23549600
H	-3.75363600 0.05819500 -0.32571800	H	-3.78015000 0.07739300 -0.15938900
H	-2.82895200 -1.20701900 -1.15023200	H	-2.92591500 -1.07981800 -1.18657700
O	-2.96634900 -1.46976800 0.84876800	O	-2.90156600 -1.57088300 0.76574600
O	3.06459000 -0.56509000 1.58075200	O	3.14295400 -0.57585000 1.41484400
H	2.12399400 -0.60569700 1.81945400	H	2.25837900 -0.76691100 1.76529500
Frequency and Energy			
Zero-point correction=	0.175937 (Hartree/Particle)	Zero-point correction=	0.176467 (Hartree/Particle)
Thermal correction to Energy=	0.187066	Thermal correction to Energy=	0.187451
Thermal correction to Enthalpy=	0.188010	Thermal correction to Enthalpy=	0.188395
Thermal correction to Gibbs Free Energy=	0.137889	Thermal correction to Gibbs Free Energy=	0.138858
Sum of electronic and zero-point Energies=	-553.908755	Sum of electronic and zero-point Energies=	-553.899022
Sum of electronic and thermal Energies=	-553.897626	Sum of electronic and thermal Energies=	-553.888038
Sum of electronic and thermal Enthalpies=	-553.896682	Sum of electronic and thermal Enthalpies=	-553.887093

Sum of electronic and thermal Free Energies= -553.946803				Sum of electronic and thermal Free Energies= -553.936630			
<b>Name: TS-C8-OH-RAF</b>							
Cartesian Coordinates							
C	2.07674800	0.52573000	-0.43977900	C	2.09129700	0.41699200	-0.41485000
C	2.48517700	-0.81620500	-0.49145100	C	2.43297000	-0.94895900	-0.45246800
C	1.55622400	-1.86643600	-0.43942300	C	1.45918700	-1.95140800	-0.36843300
C	0.19026500	-1.61131000	-0.36476200	C	0.10422300	-1.63507600	-0.29598300
C	-0.25679500	-0.27941300	-0.35007200	C	-0.28240100	-0.28416500	-0.31155200
C	0.69092700	0.76700100	-0.40659100	C	0.71085000	0.71542000	-0.39624800
H	2.78458400	1.33375400	-0.56473500	H	2.82486800	1.17818100	-0.63753600
H	3.54322700	-1.03773300	-0.54882900	H	3.47953200	-1.21919600	-0.51251500
H	1.91122100	-2.88896500	-0.45790800	H	1.76710300	-2.98967700	-0.36573400
H	-0.52019500	-2.42876000	-0.32072100	H	-0.64084000	-2.41856200	-0.22710100
C	-1.34329200	1.69034200	-0.31812400	C	-1.27856500	1.73359100	-0.31880400
H	-2.05668400	2.49990500	-0.29994400	H	-1.95480500	2.57493100	-0.31411300
N	0.00472300	1.94970900	-0.38551200	N	0.08035600	1.92631200	-0.40031000
H	0.41888500	2.86860400	-0.42188100	H	0.53903500	2.82329300	-0.41604000
C	-1.55806600	0.33527000	-0.29712500	C	-1.55522600	0.39105400	-0.27005300
H	-3.04557900	-0.31512700	1.74389100	H	-2.89852300	-0.42044000	1.75741200
C	-2.87663200	-0.35786700	-0.21092900	C	-2.90774300	-0.23858000	-0.19031500
H	-3.68318700	0.35361500	-0.40006200	H	-3.67643500	0.53531500	-0.27917900
H	-2.94162000	-1.15982600	-0.94595400	H	-3.05288100	-0.95230800	-1.00227500
O	-3.07740100	-0.99872200	1.06327100	O	-3.09581200	-0.99620800	1.01002100
O	2.54533100	0.62225900	1.79600700	O	2.62439900	0.77391000	1.60873300
H	2.02551900	-0.18439100	1.95003700	H	2.17420800	-0.01056000	1.96145700
Frequency and Energy							
Zero-point correction= 0.176142 (Hartree/Particle)				Zero-point correction= 0.176576 (Hartree/Particle)			
Thermal correction to Energy= 0.187222				Thermal correction to Energy= 0.187625			
Thermal correction to Enthalpy= 0.188167				Thermal correction to Enthalpy= 0.188569			
Thermal correction to Gibbs Free Energy= 0.138054				Thermal correction to Gibbs Free Energy= 0.138557			
Sum of electronic and zero-point Energies= -553.909534				Sum of electronic and zero-point Energies= -553.901123			
Sum of electronic and thermal Energies= -553.898453				Sum of electronic and thermal Energies= -553.890074			
Sum of electronic and thermal Enthalpies= -553.897509				Sum of electronic and thermal Enthalpies= -553.889130			
Sum of electronic and thermal Free Energies= -553.947622				Sum of electronic and thermal Free Energies= -553.939142			