

Supporting Information (SI)

Thermodynamic and Kinetic Studies of the Antiradical Activity of 5-Hydroxymethylfurfural: Computational Insights

Housseem Boulebd^{1*}, Adam Mechler², Nguyen Thi Hoa³ and Quan V. Vo^{4*}

¹Laboratory of Synthesis of Molecules with Biological Interest, University of Frères Mentouri Constantine 1, Constantine, Algeria.

²Department of Chemistry and Physics, La Trobe University, Victoria 3086, Australia.

³Academic Affairs, The University of Danang - University of Technology and Education, 48 Cao Thang, Danang 550000, Vietnam.

⁴Institute of Research and Development, Duy Tan University, Danang 550000, Vietnam.

*Corresponding author: boulebd.housseem@umc.edu.dz; vovanquan2@duytan.edu.vn

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Name				TS-5-HMF-C1-H-OH-FHT (gas phase)	
Cartesian Coordinates				Frequency and Energy	
C	-0.97329600	-1.26801200	-0.07209900	Zero-point correction=	0.121510 (Hartree/Particle)
C	0.44750600	-1.19086400	-0.11182400	Thermal correction to Energy=	0.132351
C	0.75784000	0.13831500	-0.06573100	Thermal correction to Enthalpy=	0.133295
O	-0.37873600	0.88500700	0.00016200	Thermal correction to Gibbs Free Energy=	0.082872
C	-1.40799600	0.02188300	-0.00558700	Sum of electronic and zero-point Energies=	-533.436686
C	-2.77184500	0.61637800	0.05916100	Sum of electronic and thermal Energies=	-533.425846
O	-3.68912700	-0.45432900	0.06468900	Sum of electronic and thermal Enthalpies=	-533.424902
C	2.05083400	0.79185300	-0.07607300	Sum of electronic and thermal Free Energies=	-533.475324
O	2.27596800	1.96554200	-0.00062700		
H	-1.60444400	-2.14018400	-0.08800900		
H	1.17013700	-1.99091600	-0.15992800		
H	-2.85062300	1.22881600	0.96585600		
H	-2.91432600	1.27402200	-0.80727000		
H	-4.58141400	-0.10269500	0.07383800		
H	2.88994000	0.01824700	-0.17480600		
O	3.66914300	-1.38154400	0.06700200		
H	4.25448300	-1.06201700	0.77342500		
Name				TS-5-HMF-C1-H-OH-FHT (water)	
Cartesian Coordinates				Frequency and Energy	
C	-0.99995900	-1.28454400	-0.03899400	Zero-point correction=	0.120447 (Hartree/Particle)
C	0.41887100	-1.22704700	-0.05547300	Thermal correction to Energy=	0.130919
C	0.75155300	0.09805400	-0.02699900	Thermal correction to Enthalpy=	0.131864
O	-0.38382700	0.86562300	0.00496100	Thermal correction to Gibbs Free Energy=	0.082329
C	-1.42709500	0.01218600	-0.00336500	Sum of electronic and zero-point Energies=	-533.460237
C	-2.78132300	0.62595800	0.02485600	Sum of electronic and thermal Energies=	-533.449764
O	-3.72475300	-0.42874200	0.02715100	Sum of electronic and thermal Enthalpies=	-533.448820
C	2.03368000	0.74466200	-0.02687300	Sum of electronic and thermal Free Energies=	-533.498355
O	2.24454300	1.93430100	0.00297700		
H	-1.62710600	-2.16068800	-0.05210800		
H	1.11641600	-2.05118200	-0.08443300		
H	-2.87272900	1.25021200	0.92021100		
H	-2.90002000	1.26972500	-0.85337900		
H	-4.60632500	-0.04064600	0.02883900		
H	2.90613200	-0.00234500	-0.06329000		
O	3.94089800	-1.16099700	0.00519900		
H	3.39437300	-1.76216300	0.54294400		
Name				TS-5-HMF-C1-H-OH-FHT (pentyl ethanoate)	
Cartesian Coordinates				Frequency and Energy	
C	-0.99616500	-1.27561200	-0.09743600	Zero-point correction=	0.120512 (Hartree/Particle)
C	0.42285700	-1.21158300	-0.15053300	Thermal correction to Energy=	0.131472
C	0.74817200	0.11413100	-0.08376600	Thermal correction to Enthalpy=	0.132416
O	-0.38162600	0.86952500	0.00657200	Thermal correction to Gibbs Free Energy=	0.081411
C	-1.42065600	0.01804400	-0.00345300	Sum of electronic and zero-point Energies=	-533.454070
C	-2.77647600	0.62536000	0.08639800	Sum of electronic and thermal Energies=	-533.443110
O	-3.70924100	-0.43372600	0.07489200	Sum of electronic and thermal Enthalpies=	-533.442166
C	2.04149800	0.75539500	-0.09940000	Sum of electronic and thermal Free Energies=	-533.493171
O	2.27667300	1.93058500	-0.02150700		
H	-1.62823000	-2.14764600	-0.12308000		

H	1.12858800	-2.02528600	-0.22521200	
H	-2.84237200	1.21746600	1.00737800	
H	-2.91964300	1.30479400	-0.76276700	
H	-4.59457100	-0.05897900	0.10321000	
H	2.88426900	-0.01809800	-0.20516700	
O	3.78091700	-1.29563800	0.10609600	
H	4.12280200	-0.99263300	0.96634500	
Name				TS-5-HMF-O-H-OH-FHT (gas phase)
Cartesian Coordinates				Frequency and Energy
C	0.34959600	1.22753100	-0.54582300	Zero-point correction= 0.119701 (Hartree/Particle)
C	-1.01520800	1.54270400	-0.28601700	Thermal correction to Energy= 0.129909
C	-1.64120000	0.35808500	-0.02574700	Thermal correction to Enthalpy= 0.130853
O	-0.74962300	-0.66314100	-0.10325100	Thermal correction to Gibbs Free Energy= 0.081773
C	0.44161900	-0.12579300	-0.41741800	Sum of electronic and zero-point Energies= -533.432596
C	1.58269100	-1.07785400	-0.55875300	Sum of electronic and thermal Energies= -533.422388
O	2.81267900	-0.42223500	-0.65807600	Sum of electronic and thermal Enthalpies= -533.421444
C	-3.03321000	0.06878000	0.30056600	Sum of electronic and thermal Free Energies= -533.470524
O	-3.47894300	-1.03026400	0.50724200	
H	1.15505900	1.89986200	-0.79092000	
H	-1.48026500	2.51619300	-0.28913000	
H	1.56819400	-1.79376300	0.27154900	
H	1.47934400	-1.66009700	-1.48282900	
H	-3.66828900	0.97369100	0.34305900	
H	2.95399400	0.23012800	0.18651000	
O	3.15775300	0.36975000	1.42456300	
H	3.95130700	-0.15960800	1.59708900	
Name				TS-5-HMF-O-H-OH-FHT (water)
Cartesian Coordinates				Frequency and Energy
C	-0.31688100	-1.65342200	0.41450900	Zero-point correction= 0.118849 (Hartree/Particle)
C	1.09390800	-1.61464800	0.58810000	Thermal correction to Energy= 0.129085
C	1.51277100	-0.41365800	0.09106700	Thermal correction to Enthalpy= 0.130029
O	0.44254700	0.29473000	-0.38244400	Thermal correction to Gibbs Free Energy= 0.081256
C	-0.64967100	-0.47128100	-0.18088900	Sum of electronic and zero-point Energies= -533.454458
C	-1.93997700	0.11453900	-0.60384900	Sum of electronic and thermal Energies= -533.444222
O	-2.97338800	-0.77954800	-0.29616000	Sum of electronic and thermal Enthalpies= -533.443278
C	2.83201300	0.16440600	-0.00310800	Sum of electronic and thermal Free Energies= -533.492051
O	3.06523800	1.26043100	-0.48487400	
H	-0.99764400	-2.44351600	0.68621900	
H	1.72964700	-2.37107100	1.02315300	
H	-2.07508100	1.09359000	-0.02785400	
H	-1.92077800	0.39847800	-1.66062900	
H	-3.77162900	-0.49402000	-0.75563500	
H	3.63418100	-0.47058500	0.40060700	
O	-1.89288300	2.36526900	0.87796700	
H	-0.92378800	2.40445400	0.78324600	
Name				TS-5-HMF-O-H-OH-FHT (pentyl ethanoate)
Cartesian Coordinates				Frequency and Energy
C	0.33951800	1.24116500	-0.53612500	Zero-point correction= 0.119392 (Hartree/Particle)
C	-1.02449500	1.54650000	-0.26620200	Thermal correction to Energy= 0.129597
C	-1.64416100	0.35477700	-0.02073800	Thermal correction to Enthalpy= 0.130541
O	-0.74723000	-0.66271600	-0.11711200	Thermal correction to Gibbs Free Energy= 0.081755
C	0.44047200	-0.11477300	-0.42854600	Sum of electronic and zero-point Energies= -533.450302
C	1.58544400	-1.05739700	-0.59564900	Sum of electronic and thermal Energies= -533.440098
O	2.81239100	-0.39367800	-0.66664700	Sum of electronic and thermal Enthalpies= -533.439154

C	-3.02896900	0.06140400	0.30781300	Sum of electronic and thermal Free Energies= -533.487940	
O	-3.47311900	-1.04594400	0.50655600		
H	1.13749600	1.92495200	-0.77765000		
H	-1.49491700	2.51810000	-0.25342700		
H	1.57170900	-1.80687100	0.20496700		
H	1.48644300	-1.60734600	-1.54073200		
H	-3.66552200	0.96187800	0.36253600		
H	2.95869400	0.21501000	0.20278200		
O	3.16809300	0.33496100	1.45288100		
H	3.91815200	-0.25676700	1.63277500		
Name					TS-5-HMF-C6-H-OH-FHT (gas phase)
Cartesian Coordinates					Frequency and Energy
C	0.07114200	1.57669200	0.32083400	Zero-point correction= 0.121014 (Hartree/Particle)	
C	-1.33357000	1.50395100	0.52465700	Thermal correction to Energy= 0.131458	
C	-1.71674700	0.25253700	0.12832600	Thermal correction to Enthalpy= 0.132402	
O	-0.64112200	-0.44545300	-0.31132700	Thermal correction to Gibbs Free Energy= 0.083360	
C	0.42909600	0.36189200	-0.19089200	Sum of electronic and zero-point Energies= -533.435955	
C	1.73297500	-0.19521800	-0.59225500	Sum of electronic and thermal Energies= -533.425511	
O	2.67740500	0.82021200	-0.69455500	Sum of electronic and thermal Enthalpies= -533.424566	
C	-3.03181900	-0.38050100	0.11452400	Sum of electronic and thermal Free Energies= -533.473609	
O	-3.24942300	-1.50411000	-0.25868900		
H	0.74245000	2.39785300	0.50730000		
H	-1.98644900	2.27073400	0.91178800		
H	2.08873300	-0.91594000	0.23429400		
H	1.64423300	-0.81011700	-1.49547700		
H	3.52439500	0.44905500	-0.42289200		
H	-3.83845000	0.27760600	0.48823600		
O	3.41185200	-1.37645600	0.90663500		
H	3.32892900	-2.33885100	0.80907400		
Name				TS-5-HMF-C6-H-OH-FHT (water)	
Cartesian Coordinates				Frequency and Energy	
C	-0.99995900	-1.28454400	-0.03899400	Zero-point correction= 0.120447 (Hartree/Particle)	
C	0.41887100	-1.22704700	-0.05547300	Thermal correction to Energy= 0.130919	
C	0.75155300	0.09805400	-0.02699900	Thermal correction to Enthalpy= 0.131864	
O	-0.38382700	0.86562300	0.00496100	Thermal correction to Gibbs Free Energy= 0.082329	
C	-1.42709500	0.01218600	-0.00336500	Sum of electronic and zero-point Energies= -533.460237	
C	-2.78132300	0.62595800	0.02485600	Sum of electronic and thermal Energies= -533.449764	
O	-3.72475300	-0.42874200	0.02715100	Sum of electronic and thermal Enthalpies= -533.448820	
C	2.03368000	0.74466200	-0.02687300	Sum of electronic and thermal Free Energies= -533.498355	
O	2.24454300	1.93430100	0.00297700		
H	-1.62710600	-2.16068800	-0.05210800		
H	1.11641600	-2.05118200	-0.08443300		
H	-2.87272900	1.25021200	0.92021100		
H	-2.90002000	1.26972500	-0.85337900		
H	-4.60632500	-0.04064600	0.02883900		
H	2.90613200	-0.00234500	-0.06329000		
O	3.94089800	-1.16099700	0.00519900		
H	3.39437300	-1.76216300	0.54294400		
Name				TS-5-HMF-C6-H-OH-FHT (pentyl ethanoate)	
Cartesian Coordinates				Frequency and Energy	
C	0.06237400	1.58065400	0.33408500	Zero-point correction= 0.120483 (Hartree/Particle)	
C	-1.34212700	1.49938400	0.53352600	Thermal correction to Energy= 0.131014	
C	-1.71661900	0.24796800	0.12961500	Thermal correction to Enthalpy= 0.131958	
O	-0.63414000	-0.44268400	-0.31103100	Thermal correction to Gibbs Free Energy= 0.082678	

C	0.43091400	0.37044900	-0.18284700	Sum of electronic and zero-point Energies=	-533.453529
C	1.73914300	-0.18264200	-0.57906300	Sum of electronic and thermal Energies=	-533.442998
O	2.67021200	0.84351800	-0.70742200	Sum of electronic and thermal Enthalpies=	-533.442054
C	-3.02602800	-0.38533400	0.10868600	Sum of electronic and thermal Free Energies=	-533.491334
O	-3.24012200	-1.51174000	-0.27538800		
H	0.72135100	2.40959400	0.53398200		
H	-2.00147900	2.26018900	0.92343300		
H	2.10041100	-0.88378500	0.26086200		
H	1.65469100	-0.81691400	-1.46886700		
H	3.53998700	0.46645000	-0.52956600		
H	-3.83442300	0.26549200	0.48438500		
O	3.40622100	-1.40600400	0.92319500		
H	3.31615900	-2.34861300	0.69692600		
Name				TS-5-HMF-C2-OH-RAF (gas phase)	
Cartesian Coordinates				Frequency and Energy	
C	-1.23138500	0.41322100	-0.05710300	Zero-point correction=	0.124502 (Hartree/Particle)
C	-0.63606800	1.54526700	-0.54598300	Thermal correction to Energy=	0.134873
C	0.73798800	1.24521300	-0.67165700	Thermal correction to Enthalpy=	0.135817
C	0.89331100	-0.04862800	-0.20937100	Thermal correction to Gibbs Free Energy=	0.087396
O	-0.32189900	-0.56317900	0.11644400	Sum of electronic and zero-point Energies=	-533.439320
C	2.03545700	-0.97642700	-0.28049200	Sum of electronic and thermal Energies=	-533.428949
O	3.10599200	-0.64712700	-0.71799700	Sum of electronic and thermal Enthalpies=	-533.428005
C	-2.63149900	0.07007200	0.32727500	Sum of electronic and thermal Free Energies=	-533.476425
O	-3.09420700	-1.09755700	-0.31572800		
H	-1.13777600	2.46834600	-0.78631000		
H	1.53700600	1.86777900	-1.04212500		
H	1.82966700	-1.98862200	0.10612500		
H	-2.68427100	-0.03160200	1.41820100		
H	-3.28942500	0.88524700	0.02821000		
H	-2.54396700	-1.83667000	-0.04101100		
O	1.44715700	0.33198200	1.82185100		
H	2.18559600	0.95025300	1.70432800		
Name				TS-5-HMF-C2-OH-RAF (water)	
Cartesian Coordinates				Frequency and Energy	
C	-1.23640200	0.38420200	-0.06314400	Zero-point correction=	0.123702 (Hartree/Particle)
C	-0.65461300	1.43518300	-0.72284800	Thermal correction to Energy=	0.134298
C	0.71311300	1.11444600	-0.85474200	Thermal correction to Enthalpy=	0.135242
C	0.88271200	-0.11200800	-0.24455200	Thermal correction to Gibbs Free Energy=	0.085599
O	-0.31951800	-0.56437100	0.21936400	Sum of electronic and zero-point Energies=	-533.465182
C	2.01218400	-1.03193400	-0.17565100	Sum of electronic and thermal Energies=	-533.454586
O	3.09789100	-0.77630100	-0.65715300	Sum of electronic and thermal Enthalpies=	-533.453642
C	-2.63521500	0.11559700	0.37559100	Sum of electronic and thermal Free Energies=	-533.503286
O	-3.15695300	-1.06727100	-0.21218100		
H	-1.16485600	2.32037800	-1.06795500		
H	1.49423300	1.69089900	-1.32686900		
H	1.81133000	-1.98045300	0.34441900		
H	-2.66753700	0.05166700	1.46747300		
H	-3.26046000	0.94745100	0.05483500		
H	-2.72934700	-1.82597100	0.20137100		
O	1.60023400	0.66684800	1.77766800		
H	2.25271500	1.29186800	1.41721800		
Name				TS-5-HMF-C2-OH-RAF (pentyl ethanoate)	
Cartesian Coordinates				Frequency and Energy	
C	-1.23199400	0.39594300	-0.05664100	Zero-point correction=	0.124075 (Hartree/Particle)

C	-0.64995000	1.48701800	-0.64710100	Thermal correction to Energy=	0.134558
C	0.72235700	1.18265300	-0.77338300	Thermal correction to Enthalpy=	0.135503
C	0.89102700	-0.07160600	-0.21599800	Thermal correction to Gibbs Free Energy=	0.086360
O	-0.31379300	-0.55751500	0.18309500	Sum of electronic and zero-point Energies=	-533.457726
C	2.02649100	-1.00365100	-0.21468900	Sum of electronic and thermal Energies=	-533.447243
O	3.09497000	-0.73251900	-0.70444200	Sum of electronic and thermal Enthalpies=	-533.446299
C	-2.63068800	0.08457500	0.35587400	Sum of electronic and thermal Free Energies=	-533.495441
O	-3.12545200	-1.08520600	-0.27070800		
H	-1.16133000	2.38594600	-0.95300800		
H	1.50676100	1.78505400	-1.20584700		
H	1.82505900	-1.97377100	0.26923000		
H	-2.67349700	-0.00502300	1.44752800		
H	-3.27302200	0.91166400	0.05531600		
H	-2.65437700	-1.84605900	0.08524900		
O	1.53015800	0.51238100	1.79832300		
H	2.17988800	1.19547100	1.56300800		
Name				TS-5-HMF-C3-OH-RAF (gas phase)	
Cartesian Coordinates				Frequency and Energy	
C	-1.20610800	0.03262100	-0.50277800	Zero-point correction=	0.125193 (Hartree/Particle)
C	-0.58472700	1.16852100	-0.90158100	Thermal correction to Energy=	0.135288
C	0.82234500	0.94911100	-0.72050800	Thermal correction to Enthalpy=	0.136232
C	0.92606900	-0.37224500	-0.29856700	Thermal correction to Gibbs Free Energy=	0.088392
O	-0.29744100	-0.91290700	-0.13747000	Sum of electronic and zero-point Energies=	-533.433566
C	2.09102600	-1.16721800	0.06408500	Sum of electronic and thermal Energies=	-533.423471
O	3.20487500	-0.69740200	0.08270400	Sum of electronic and thermal Enthalpies=	-533.422526
C	-2.64515300	-0.32141000	-0.34369200	Sum of electronic and thermal Free Energies=	-533.470367
O	-2.99956400	-0.52106800	1.00871200		
H	-1.06457900	2.07585100	-1.22959000		
H	1.63634400	1.54286700	-1.10183600		
H	1.88717700	-2.21795200	0.33060900		
H	-3.24082200	0.47001800	-0.81088200		
H	-2.85944000	-1.26163600	-0.85426900		
H	-2.72921900	0.25003400	1.51636900		
O	1.08493300	1.63697800	1.17921700		
H	2.00739700	1.35974800	1.30254800		
Name				TS-5-HMF-C3-OH-RAF (water)	
Cartesian Coordinates				Frequency and Energy	
C	-1.20965700	0.06193800	-0.48471600	Zero-point correction=	0.124538 (Hartree/Particle)
C	-0.57924400	1.18355700	-0.90906400	Thermal correction to Energy=	0.134730
C	0.82359000	0.95673400	-0.73038000	Thermal correction to Enthalpy=	0.135675
C	0.92746600	-0.35049200	-0.26190100	Thermal correction to Gibbs Free Energy=	0.087789
O	-0.30087700	-0.88193800	-0.08423100	Sum of electronic and zero-point Energies=	-533.459608
C	2.07957100	-1.16983600	0.07316500	Sum of electronic and thermal Energies=	-533.449416
O	3.21668200	-0.74430400	-0.00704400	Sum of electronic and thermal Enthalpies=	-533.448472
C	-2.64640300	-0.31240200	-0.37157100	Sum of electronic and thermal Free Energies=	-533.496357
O	-3.02375200	-0.56214000	0.97530400		
H	-1.05580700	2.07806300	-1.27685500		
H	1.64101100	1.54958400	-1.10884000		
H	1.85921500	-2.19447300	0.40486200		
H	-3.24384400	0.48599500	-0.81644200		
H	-2.82771300	-1.23728500	-0.92138500		
H	-2.96171100	0.26608900	1.46614900		
O	1.12710100	1.62108500	1.24632100		
H	2.06367300	1.37340400	1.31651500		

Name				TS-5-HMF-C3-OH-RAF (pentyl ethanoate)	
Cartesian Coordinates				Frequency and Energy	
C	-1.20836500	0.05112700	-0.48250700	Zero-point correction=	0.124894 (Hartree/Particle)
C	-0.58173800	1.18126500	-0.89068700	Thermal correction to Energy=	0.135052
C	0.82400500	0.95329700	-0.71940800	Thermal correction to Enthalpy=	0.135996
C	0.92347200	-0.36483500	-0.28182600	Thermal correction to Gibbs Free Energy=	0.088082
O	-0.30224700	-0.89506300	-0.10978600	Sum of electronic and zero-point Energies=	-533.451198
C	2.07959200	-1.17834800	0.06269000	Sum of electronic and thermal Energies=	-533.441040
O	3.20720000	-0.73457400	0.04368300	Sum of electronic and thermal Enthalpies=	-533.440096
C	-2.64838800	-0.31162000	-0.35696000	Sum of electronic and thermal Free Energies=	-533.488010
O	-3.03002200	-0.54090600	0.98794800		
H	-1.05916900	2.08451700	-1.23555300		
H	1.63537200	1.54212200	-1.11587100		
H	1.86237100	-2.22058800	0.34759500		
H	-3.23952700	0.48440800	-0.81925800		
H	-2.84370700	-1.24251600	-0.89265000		
H	-2.87939200	0.26842200	1.48908600		
O	1.14084600	1.63827300	1.19751100		
H	2.06636500	1.35647300	1.28399100		
Name				TS-5-HMF-C4-OH-RAF (gas phase)	
Cartesian Coordinates				Frequency and Energy	
C	0.79113700	-0.48845200	0.24109200	Zero-point correction=	0.125956 (Hartree/Particle)
C	0.56380400	0.81183400	0.71348800	Thermal correction to Energy=	0.135579
C	-0.86888300	0.97405800	0.65524100	Thermal correction to Enthalpy=	0.136523
C	-1.36138200	-0.15036100	0.08460000	Thermal correction to Gibbs Free Energy=	0.090316
O	-0.34639800	-1.04386000	-0.18228500	Sum of electronic and zero-point Energies=	-533.439470
C	-2.71949000	-0.57847600	-0.26502200	Sum of electronic and thermal Energies=	-533.429847
O	-3.68439400	0.11989500	-0.09515000	Sum of electronic and thermal Enthalpies=	-533.428903
C	2.08465900	-1.18664900	-0.01406600	Sum of electronic and thermal Free Energies=	-533.475110
O	3.15661900	-0.29715600	0.11007800		
H	1.24117900	1.35229700	1.35358800		
H	-1.45134400	1.82522600	0.96845800		
H	-2.79198800	-1.59339800	-0.69502000		
H	2.23140100	-1.99012800	0.71394400		
H	2.02874600	-1.65145200	-1.00796500		
H	2.93810600	0.48419200	-0.42233000		
O	1.39632400	1.67777500	-0.82305200		
H	0.68761900	1.62830500	-1.47939900		
Name				TS-5-HMF-C4-OH-RAF (water)	
Cartesian Coordinates				Frequency and Energy	
C	-0.79205600	-0.49027900	-0.23319400	Zero-point correction=	0.125679 (Hartree/Particle)
C	-0.56074400	0.80619200	-0.72169700	Thermal correction to Energy=	0.135403
C	0.86938100	0.96980300	-0.66378000	Thermal correction to Enthalpy=	0.136347
C	1.36279000	-0.14992800	-0.08598700	Thermal correction to Gibbs Free Energy=	0.089762
O	0.34038800	-1.04574800	0.19258800	Sum of electronic and zero-point Energies=	-533.460786
C	2.70829900	-0.57916500	0.27061200	Sum of electronic and thermal Energies=	-533.451063
O	3.68387000	0.12148600	0.09010100	Sum of electronic and thermal Enthalpies=	-533.450118
C	-2.07845400	-1.19612500	0.00664800	Sum of electronic and thermal Free Energies=	-533.496703
O	-3.15884900	-0.29409800	-0.11112600		
H	-1.23298300	1.33945900	-1.37438300		
H	1.44317700	1.82231600	-0.99192700		
H	2.78541700	-1.58305600	0.71342200		
H	-2.21463200	-1.98822800	-0.73461700		
H	-2.03665500	-1.66504600	0.99625400		

H	-2.91737800	0.49594800	0.40214800	
O	-1.38058300	1.71451600	0.83175000	
H	-0.76085900	1.44637900	1.52698600	
Name				TS-5-HMF-C4-OH-RAF (pentyl ethanoate)
Cartesian Coordinates				Frequency and Energy
C	-0.78934700	-0.48961800	-0.24543000	Zero-point correction= 0.125754 (Hartree/Particle)
C	-0.56337300	0.81243200	-0.71857100	Thermal correction to Energy= 0.135346
C	0.86798600	0.97881500	-0.65567300	Thermal correction to Enthalpy= 0.136291
C	1.36173100	-0.14605500	-0.08650200	Thermal correction to Gibbs Free Energy= 0.090155
O	0.34689800	-1.04162700	0.17747200	Sum of electronic and zero-point Energies= -533.455566
C	2.71426500	-0.57865900	0.26774300	Sum of electronic and thermal Energies= -533.445974
O	3.68569000	0.11909200	0.10548900	Sum of electronic and thermal Enthalpies= -533.445030
C	-2.07765600	-1.19596900	0.00330000	Sum of electronic and thermal Free Energies= -533.491166
O	-3.15394400	-0.30121100	-0.08773100	
H	-1.23274000	1.34953500	-1.37087400	
H	1.44111700	1.83614600	-0.97186700	
H	2.78552600	-1.59380900	0.69388900	
H	-2.22604700	-1.98254500	-0.74306300	
H	-2.01671900	-1.68331600	0.98548300	
H	-2.90267600	0.48446600	0.42555200	
O	-1.40478000	1.69001100	0.81709500	
H	-0.72100800	1.57372800	1.49307000	
Name				TS-5-HMF-C5-OH-RAF (gas phase)
Cartesian Coordinates				Frequency and Energy
C	-0.85868700	0.22140900	-0.48130200	Zero-point correction= 0.125032 (Hartree/Particle)
C	-0.27098500	1.47452100	-0.56370600	Thermal correction to Energy= 0.135064
C	1.11430800	1.28163000	-0.35110700	Thermal correction to Enthalpy= 0.136009
C	1.27707400	-0.06312300	-0.16873900	Thermal correction to Gibbs Free Energy= 0.088718
O	0.08755300	-0.70695700	-0.27592800	Sum of electronic and zero-point Energies= -533.444464
C	2.45668600	-0.88155600	0.12378900	Sum of electronic and thermal Energies= -533.434432
O	3.56195200	-0.41378500	0.22314600	Sum of electronic and thermal Enthalpies= -533.433487
C	-2.24622000	-0.25057800	-0.79092300	Sum of electronic and thermal Free Energies= -533.480778
O	-2.71864200	-1.20694500	0.11410000	
H	-0.79540800	2.39829100	-0.75360400	
H	1.90315800	2.01542400	-0.31831000	
H	2.25611300	-1.96025200	0.24606200	
H	-2.88758600	0.63782600	-0.83704100	
H	-2.24674000	-0.72089400	-1.77787900	
H	-2.59380500	-0.83678900	0.99692800	
O	-1.33954100	0.60517800	1.68870900	
H	-1.19936200	1.55264200	1.83555700	
Name				TS-5-HMF-C5-OH-RAF (water)
Cartesian Coordinates				Frequency and Energy
C	-0.85294200	0.18218500	-0.51887000	Zero-point correction= 0.124535 (Hartree/Particle)
C	-0.28209400	1.43524900	-0.63057500	Thermal correction to Energy= 0.134656
C	1.10357600	1.26646800	-0.39600500	Thermal correction to Enthalpy= 0.135600
C	1.28797800	-0.06695600	-0.16155900	Thermal correction to Gibbs Free Energy= 0.088134
O	0.09766800	-0.73521700	-0.25286800	Sum of electronic and zero-point Energies= -533.466791
C	2.46011400	-0.86170000	0.16385400	Sum of electronic and thermal Energies= -533.456670
O	3.57326800	-0.38052700	0.26055800	Sum of electronic and thermal Enthalpies= -533.455726
C	-2.23207500	-0.31519400	-0.79920900	Sum of electronic and thermal Free Energies= -533.503192
O	-2.68141700	-1.23063900	0.18216800	
H	-0.81515800	2.34750400	-0.85038100	
H	1.87313500	2.02267500	-0.38500600	

H	2.27722600	-1.93571900	0.31755900	
H	-2.89021400	0.55402700	-0.88050100	
H	-2.23485900	-0.84383400	-1.75490900	
H	-2.57432100	-0.78408800	1.03503900	
O	-1.35101800	0.73884300	1.68306900	
H	-1.65116500	1.65944100	1.58895800	
Name				TS-5-HMF-C5-OH-RAF (pentyl ethanoate)
Cartesian Coordinates				Frequency and Energy
C	-0.85336600	0.19230800	-0.50300100	Zero-point correction= 0.124651 (Hartree/Particle)
C	-0.28075600	1.44873300	-0.60580200	Thermal correction to Energy= 0.134716
C	1.10502900	1.27605100	-0.37856200	Thermal correction to Enthalpy= 0.135660
C	1.28343700	-0.06213800	-0.16398100	Thermal correction to Gibbs Free Energy= 0.088324
O	0.09917800	-0.72181900	-0.26210000	Sum of electronic and zero-point Energies= -533.461762
C	2.46153200	-0.86854000	0.14795900	Sum of electronic and thermal Energies= -533.451697
O	3.57068800	-0.39890500	0.24455600	Sum of electronic and thermal Enthalpies= -533.450753
C	-2.23386500	-0.29964200	-0.80220600	Sum of electronic and thermal Free Energies= -533.498089
O	-2.71710800	-1.20065400	0.16145600	
H	-0.81249700	2.36377800	-0.81942600	
H	1.87800700	2.02821900	-0.35920500	
H	2.26659700	-1.94518000	0.28879200	
H	-2.87807000	0.58026600	-0.91042600	
H	-2.22150300	-0.82892200	-1.75878400	
H	-2.58612800	-0.77087900	1.01719100	
O	-1.34714100	0.67256900	1.68747900	
H	-1.38340600	1.64255500	1.72429400	
Name				TS-5-HMF-C1-H-OOH-FHT (gas phase)
Cartesian Coordinates				Frequency and Energy
C	1.19219100	-1.21105300	-0.25036600	Zero-point correction= 0.125101 (Hartree/Particle)
C	-0.20821600	-0.98138100	-0.33338400	Thermal correction to Energy= 0.136786
C	-0.38636200	0.35908900	-0.13776200	Thermal correction to Enthalpy= 0.137730
O	0.81708800	0.97008300	0.06508300	Thermal correction to Gibbs Free Energy= 0.085081
C	1.75109800	0.00912600	-0.00862500	Sum of electronic and zero-point Energies= -608.576586
C	3.16410600	0.44112600	0.17796100	Sum of electronic and thermal Energies= -608.564902
O	3.96372000	-0.71604900	0.08899600	Sum of electronic and thermal Enthalpies= -608.563958
C	-1.60314100	1.13663700	-0.11404500	Sum of electronic and thermal Free Energies= -608.616606
O	-1.74731500	2.30255000	0.07236000	
H	1.73213500	-2.13718900	-0.34975200	
H	-1.00141600	-1.69351000	-0.50260100	
H	3.41571000	1.17513700	-0.59756100	
H	3.25954800	0.93293000	1.15386700	
H	4.88672200	-0.46720400	0.16742800	
H	-2.58381700	0.36017400	-0.32807300	
O	-3.26133000	-1.39842200	0.64598400	
H	-3.93913800	-1.08219800	1.25808000	
O	-3.42563800	-0.60933600	-0.47293100	
Name				TS-5-HMF-C1-H-OOH-FHT (water)
Cartesian Coordinates				Frequency and Energy
C	1.23811100	-1.23279200	-0.26128200	Zero-point correction= 0.124430 (Hartree/Particle)
C	-0.16085900	-1.02087400	-0.35631500	Thermal correction to Energy= 0.136166
C	-0.36402900	0.31520300	-0.14751000	Thermal correction to Enthalpy= 0.137110
O	0.83666200	0.94334400	0.07553900	Thermal correction to Gibbs Free Energy= 0.084153
C	1.78626600	-0.00854400	0.00168100	Sum of electronic and zero-point Energies= -608.600533
C	3.18594700	0.44550900	0.21359100	Sum of electronic and thermal Energies= -608.588797
O	4.02955000	-0.68191100	0.07870900	Sum of electronic and thermal Enthalpies= -608.587853

C	-1.57180800	1.08291300	-0.13449000	Sum of electronic and thermal Free Energies= -608.640811	
O	-1.71644700	2.26004300	0.03746100		
H	1.77565200	-2.16022900	-0.37018800		
H	-0.93415300	-1.74832900	-0.55345300		
H	3.42447400	1.21748000	-0.52582500		
H	3.26749900	0.89206500	1.21056200		
H	4.93877100	-0.38576700	0.19666900		
H	-2.57785000	0.32943300	-0.32848100		
O	-3.43704100	-1.35060200	0.64239900		
H	-3.96228900	-0.92289300	1.33683200		
O	-3.53945700	-0.50965400	-0.44162800		
Name					TS-5-HMF-C1-H-OOH-FHT (pentyl ethanoate)
Cartesian Coordinates					Frequency and Energy
C	1.22494400	-1.22013800	-0.26312300		Zero-point correction= 0.124374 (Hartree/Particle)
C	-0.17435800	-1.00145300	-0.35207000	Thermal correction to Energy= 0.136238	
C	-0.36631000	0.33667200	-0.14530100	Thermal correction to Enthalpy= 0.137183	
O	0.83158200	0.95455700	0.06935300	Thermal correction to Gibbs Free Energy= 0.083211	
C	1.77542100	0.00340900	-0.00665900	Sum of electronic and zero-point Energies= -608.597023	
C	3.18246600	0.44596100	0.19263600	Sum of electronic and thermal Energies= -608.585159	
O	3.99684600	-0.70225800	0.10026000	Sum of electronic and thermal Enthalpies= -608.584215	
C	-1.58274300	1.10363600	-0.12564900	Sum of electronic and thermal Free Energies= -608.638187	
O	-1.73867800	2.27200600	0.05589900		
H	1.76476100	-2.14617900	-0.37011000		
H	-0.95344100	-1.72504600	-0.53902200		
H	3.43391300	1.18834700	-0.57462500		
H	3.26848000	0.93076200	1.17273900		
H	4.91547700	-0.43164600	0.18992100		
H	-2.57441400	0.33374300	-0.33374900		
O	-3.37276300	-1.36608800	0.65100300		
H	-3.98027400	-0.97793000	1.29900700		
O	-3.49586600	-0.55578800	-0.45691000		
Name				TS-5-HMF-O-H-OOH-FHT (gas phase)	
Cartesian Coordinates				Frequency and Energy	
C	0.17582100	1.50535000	-0.16233800	Zero-point correction= 0.123316 (Hartree/Particle)	
C	1.52815500	1.46857200	-0.60691900	Thermal correction to Energy= 0.134471	
C	2.03437600	0.26616100	-0.20307700	Thermal correction to Enthalpy= 0.135416	
O	1.08216600	-0.43859800	0.45879200	Thermal correction to Gibbs Free Energy= 0.082820	
C	-0.02910500	0.31894100	0.47554500	Sum of electronic and zero-point Energies= -608.565484	
C	-1.22445100	-0.27029100	1.14392100	Sum of electronic and thermal Energies= -608.554329	
O	-2.31289400	0.55149700	1.16155800	Sum of electronic and thermal Enthalpies= -608.553385	
C	3.36318600	-0.31292600	-0.37182800	Sum of electronic and thermal Free Energies= -608.605980	
O	3.70110900	-1.39181100	0.04145000		
H	-0.55295000	2.28826000	-0.29008700		
H	2.06457700	2.22790900	-1.15433300		
H	-1.49192800	-1.22839300	0.64665300		
H	-0.99399400	-0.56762300	2.18118100		
H	4.05826400	0.34326600	-0.92860500		
H	-2.93345800	0.43315200	0.03680300		
O	-3.07743100	-1.27241900	-0.93441800		
H	-3.91502100	-1.65082800	-0.63100800		
O	-3.30837200	0.08875700	-0.91643500		
Name				TS-5-HMF-O-H-OOH-FHT (water)	
Cartesian Coordinates				Frequency and Energy	
C	0.17582100	1.50535000	-0.16233800	Zero-point correction= 0.121696 (Hartree/Particle)	

C	1.52815500	1.46857200	-0.60691900	Thermal correction to Energy=	0.130611
C	2.03437600	0.26616100	-0.20307700	Thermal correction to Enthalpy=	0.131555
O	1.08216600	-0.43859800	0.45879200	Thermal correction to Gibbs Free Energy=	0.086217
C	-0.02910500	0.31894100	0.47554500	Sum of electronic and zero-point Energies=	-608.590375
C	-1.22445100	-0.27029100	1.14392100	Sum of electronic and thermal Energies=	-608.581460
O	-2.31289400	0.55149700	1.16155800	Sum of electronic and thermal Enthalpies=	-608.580516
C	3.36318600	-0.31292600	-0.37182800	Sum of electronic and thermal Free Energies=	-608.625854
O	3.70110900	-1.39181100	0.04145000		
H	-0.55295000	2.28826000	-0.29008700		
H	2.06457700	2.22790900	-1.15433300		
H	-1.49192800	-1.22839300	0.64665300		
H	-0.99399400	-0.56762300	2.18118100		
H	4.05826400	0.34326600	-0.92860500		
H	-2.90294495	0.43897101	0.09210705		
O	-3.07743100	-1.27241900	-0.93441800		
H	-3.91502100	-1.65082800	-0.63100800		
O	-3.30837200	0.08875700	-0.91643500		
Name				TS-5-HMF-O-H-OOH-FHT (pentyl ethanoate)	
Cartesian Coordinates				Frequency and Energy	
C	0.08946100	1.47337000	-0.25934800	Zero-point correction=	0.122974 (Hartree/Particle)
C	1.43133400	1.41638000	-0.72968300	Thermal correction to Energy=	0.134150
C	1.97024200	0.27030900	-0.21806200	Thermal correction to Enthalpy=	0.135094
O	1.04620800	-0.38179100	0.53492900	Thermal correction to Gibbs Free Energy=	0.082766
C	-0.07953100	0.35406800	0.50125800	Sum of electronic and zero-point Energies=	-608.587381
C	-1.24738700	-0.18113000	1.25742900	Sum of electronic and thermal Energies=	-608.576205
O	-2.36982500	0.58225200	1.15930300	Sum of electronic and thermal Enthalpies=	-608.575261
C	3.30287500	-0.29270800	-0.36457800	Sum of electronic and thermal Free Energies=	-608.627589
O	3.67689900	-1.32299600	0.14616100		
H	-0.65239100	2.23158800	-0.45169300		
H	1.94076100	2.12559400	-1.36455000		
H	-1.45949600	-1.22078900	0.92504900		
H	-1.00753300	-0.30585200	2.32934000		
H	3.96788900	0.31695900	-1.00064400		
H	-2.89429500	0.36716900	0.00327100		
O	-2.74730400	-1.32116100	-1.01064400		
H	-3.48830800	-1.88123400	-0.72812700		
O	-3.25705200	-0.04070000	-0.93409200		
Name				TS-5-HMF-C6-H-OOH-FHT (gas phase)	
Cartesian Coordinates				Frequency and Energy	
C	-0.09369700	-2.02958800	0.26093000	Zero-point correction=	0.125262 (Hartree/Particle)
C	1.31563400	-1.88421400	0.38433800	Thermal correction to Energy=	0.136417
C	1.60710300	-0.59921400	0.02224800	Thermal correction to Enthalpy=	0.137362
O	0.46783300	0.05235000	-0.32544700	Thermal correction to Gibbs Free Energy=	0.086811
C	-0.55196100	-0.81854200	-0.17955700	Sum of electronic and zero-point Energies=	-608.577117
C	-1.88335400	-0.27564300	-0.42627800	Sum of electronic and thermal Energies=	-608.565961
O	-2.85551100	-1.22222500	-0.19119000	Sum of electronic and thermal Enthalpies=	-608.565017
C	2.85065800	0.15853300	-0.00557700	Sum of electronic and thermal Free Energies=	-608.615567
O	2.91228000	1.33005200	-0.28541000		
H	-0.70216800	-2.89474500	0.46382400		
H	2.02932900	-2.62714300	0.70478000		
H	-1.91864100	0.73558500	0.37826700		
H	-1.96928000	0.27912100	-1.36824500		
H	-3.71780400	-0.85943500	-0.40864000		
H	3.74736400	-0.42732000	0.26422500		

O	-1.01312600	2.52662100	-0.12820400	
H	-0.07575300	2.28152500	-0.05974200	
O	-1.61889500	1.83875500	0.89136300	
Name				TS-5-HMF-C6-H-OOH-FHT (water)
Cartesian Coordinates				Frequency and Energy
C	-0.07115700	-1.97584800	0.37516300	Zero-point correction= 0.124546 (Hartree/Particle)
C	1.32920700	-1.80664400	0.53141400	Thermal correction to Energy= 0.135779
C	1.62467200	-0.55741300	0.06038900	Thermal correction to Enthalpy= 0.136723
O	0.48942700	0.05505700	-0.38519200	Thermal correction to Gibbs Free Energy= 0.085834
C	-0.52573500	-0.81544100	-0.19158400	Sum of electronic and zero-point Energies= -608.604040
C	-1.85902500	-0.32601200	-0.53589700	Sum of electronic and thermal Energies= -608.592808
O	-2.82616200	-1.28193800	-0.28093100	Sum of electronic and thermal Enthalpies= -608.591864
C	2.87307400	0.16455400	-0.01495600	Sum of electronic and thermal Free Energies= -608.642753
O	2.97255400	1.30090800	-0.44683900	
H	-0.67067800	-2.83258700	0.63699200	
H	2.04021500	-2.50908100	0.93950800	
H	-1.98619300	0.67192200	0.20984200	
H	-1.92223100	0.14969500	-1.51949100	
H	-3.65331000	-1.01259400	-0.69868200	
H	3.74535200	-0.39215200	0.35687300	
O	-1.04517100	2.57880500	0.04879800	
H	-0.12781700	2.29336500	0.19777400	
O	-1.79709200	1.78870000	0.88041500	
Name				TS-5-HMF-C6-H-OOH-FHT (pentyl ethanoate)
Cartesian Coordinates				Frequency and Energy
C	-0.07652700	-2.01769100	0.28839300	Zero-point correction= 0.124938 (Hartree/Particle)
C	1.32957900	-1.85701200	0.42288900	Thermal correction to Energy= 0.136215
C	1.61326900	-0.57770600	0.03663200	Thermal correction to Enthalpy= 0.137159
O	0.47000400	0.05948000	-0.33514400	Thermal correction to Gibbs Free Energy= 0.085892
C	-0.54236700	-0.82127700	-0.18247900	Sum of electronic and zero-point Energies= -608.598270
C	-1.87989200	-0.30369700	-0.46483100	Sum of electronic and thermal Energies= -608.586993
O	-2.84357600	-1.24737900	-0.20174300	Sum of electronic and thermal Enthalpies= -608.586049
C	2.86173200	0.16449100	-0.00676400	Sum of electronic and thermal Free Energies= -608.637316
O	2.94469200	1.32725900	-0.33280400	
H	-0.67231800	-2.88978200	0.50343400	
H	2.04809000	-2.58676700	0.76443500	
H	-1.95110800	0.70825400	0.30608400	
H	-1.96587100	0.20347900	-1.43307600	
H	-3.69222000	-0.94125200	-0.54061500	
H	3.74524700	-0.42312300	0.29378500	
O	-1.03952200	2.55612700	-0.07448500	
H	-0.11096400	2.28028400	-0.00246000	
O	-1.68604900	1.82029400	0.88734900	
Name				TS-5-HMF-C5-OOH-RAF (gas phase)
Cartesian Coordinates				Frequency and Energy
C	0.61503400	-0.15719200	0.53714100	Zero-point correction= 0.130138 (Hartree/Particle)
C	0.07621900	0.95157600	1.22076600	Thermal correction to Energy= 0.140838
C	-1.28434800	0.99233400	0.90885200	Thermal correction to Enthalpy= 0.141782
C	-1.52627000	-0.10258800	0.10554400	Thermal correction to Gibbs Free Energy= 0.092832
O	-0.39313200	-0.82597400	-0.06667900	Sum of electronic and zero-point Energies= -608.583516
C	-2.74008500	-0.57901900	-0.55149500	Sum of electronic and thermal Energies= -608.572816
O	-3.79978600	-0.01203600	-0.44301600	Sum of electronic and thermal Enthalpies= -608.571872
C	1.87303800	-0.92193800	0.82933500	Sum of electronic and thermal Free Energies= -608.620822
O	2.27879400	-1.72555300	-0.23936400	

H	0.64734700	1.64657200	1.81642400	
H	-2.02619700	1.71736100	1.20303200	
H	-2.61691100	-1.49614100	-1.15277900	
H	2.63413500	-0.18410200	1.11368300	
H	1.69587400	-1.58215000	1.68198100	
H	2.28169500	-1.16354000	-1.02394500	
H	1.91505100	2.42760300	-0.79660200	
O	1.27281700	0.70861000	-1.09405200	
O	2.31474200	1.54687300	-0.79972200	
Name				TS-5-HMF- C5-OOH-RAF (water)
Cartesian Coordinates				Frequency and Energy
C	0.60862400	-0.16689700	0.54691800	Zero-point correction= 0.129702 (Hartree/Particle)
C	0.07418500	0.94296400	1.22812700	Thermal correction to Energy= 0.140503
C	-1.28352300	0.99043600	0.91240300	Thermal correction to Enthalpy= 0.141448
C	-1.53453000	-0.09989500	0.10348300	Thermal correction to Gibbs Free Energy= 0.092472
O	-0.39661100	-0.83348500	-0.07232400	Sum of electronic and zero-point Energies= -608.608989
C	-2.73495500	-0.57384200	-0.55486600	Sum of electronic and thermal Energies= -608.598188
O	-3.80714800	-0.00280800	-0.45220800	Sum of electronic and thermal Enthalpies= -608.597244
C	1.86010700	-0.93146900	0.83877700	Sum of electronic and thermal Free Energies= -608.646219
O	2.27608900	-1.72286600	-0.25430100	
H	0.64830200	1.63711800	1.82254900	
H	-2.01283700	1.72595200	1.21473000	
H	-2.61872500	-1.48824900	-1.15454900	
H	2.62522700	-0.21002800	1.14124500	
H	1.67129600	-1.60686100	1.67577900	
H	2.34406300	-1.13342200	-1.01795800	
H	1.98152000	2.40862500	-0.63504500	
O	1.25988800	0.74485800	-1.09260800	
O	2.34549600	1.52668500	-0.81553500	
Name				TS-5-HMF- C5-OOH-RAF (pentyl ethanoate)
Cartesian Coordinates				Frequency and Energy
C	0.61259500	-0.16297700	0.53734300	Zero-point correction= 0.129719 (Hartree/Particle)
C	0.07790900	0.94346200	1.22854800	Thermal correction to Energy= 0.140476
C	-1.28116200	0.99032200	0.91677800	Thermal correction to Enthalpy= 0.141421
C	-1.52871500	-0.09928300	0.10547100	Thermal correction to Gibbs Free Energy= 0.092353
O	-0.39612000	-0.82571200	-0.07192400	Sum of electronic and zero-point Energies= -608.603795
C	-2.73680900	-0.57469400	-0.55456700	Sum of electronic and thermal Energies= -608.593038
O	-3.80346500	-0.01142200	-0.44856500	Sum of electronic and thermal Enthalpies= -608.592093
C	1.86325100	-0.93389300	0.83335400	Sum of electronic and thermal Free Energies= -608.641161
O	2.28768100	-1.71748500	-0.24853200	
H	0.64950700	1.63299600	1.83106200	
H	-2.01364700	1.72139100	1.22179300	
H	-2.61340900	-1.48882600	-1.15884600	
H	2.62265800	-0.20855400	1.14866100	
H	1.66936600	-1.60919900	1.67075400	
H	2.28928100	-1.13898400	-1.02176200	
H	1.91854000	2.42573100	-0.72405900	
O	1.26999000	0.71815200	-1.09465700	
O	2.32132500	1.54744300	-0.80746900	

