

Theoretical insights into on-water catalytic effect in the biogenesis of triterpene dimers: from one-step to two-step a hetero Diels-Alder reaction

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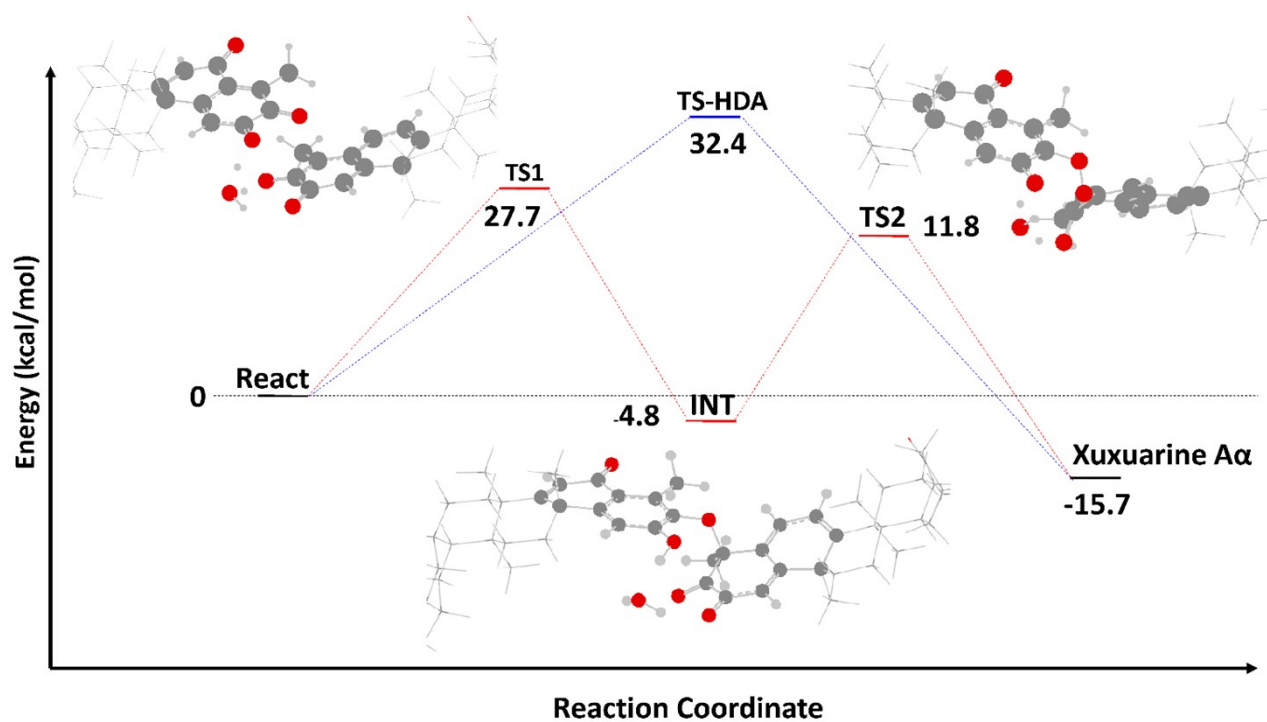


Figure S1. Energy profile of the two-step process with one water molecule (1-wt).

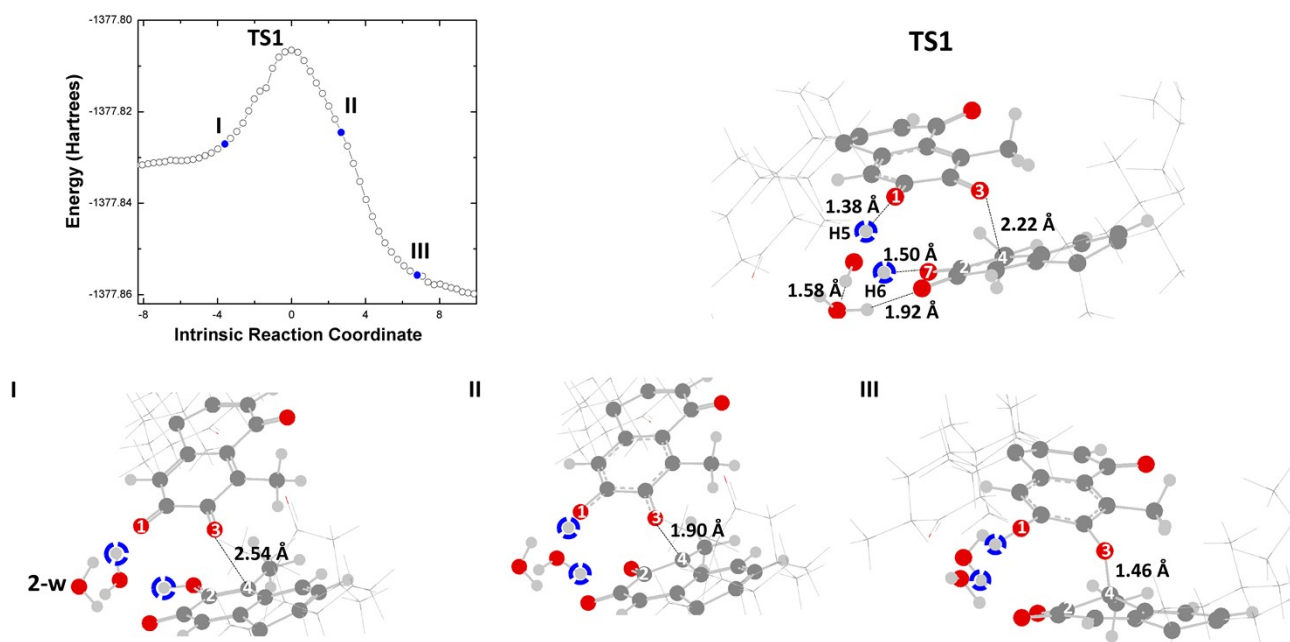


Figure S2. Reaction path calculated employing the IRC method in the first step of the 2-wt-a pathway, illustrating the two-process mechanisms for the first elemental step along with the selected bond distance. The blue circles point out what H atoms are being transferred.

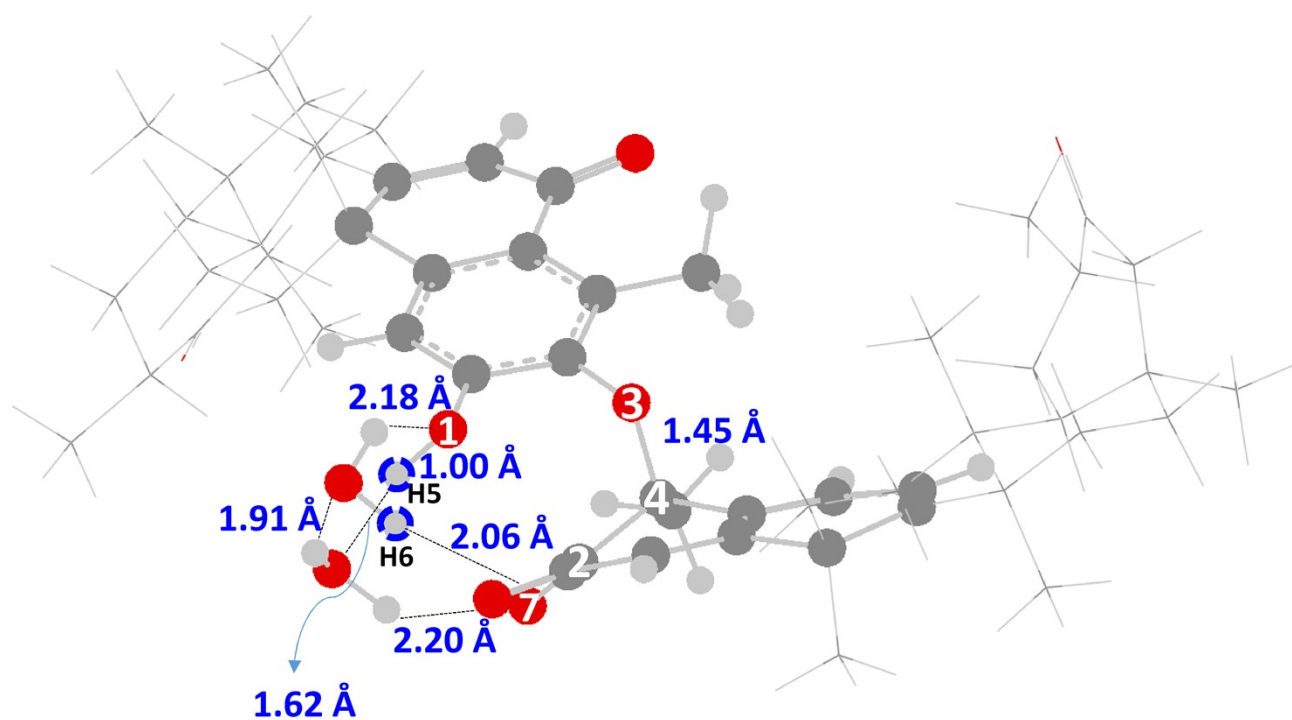


Figure S3. Structure of intermediate for the 2-wt-a pathway, showing the main interatomic distances. The blue circles point out what H atoms are being transferred.

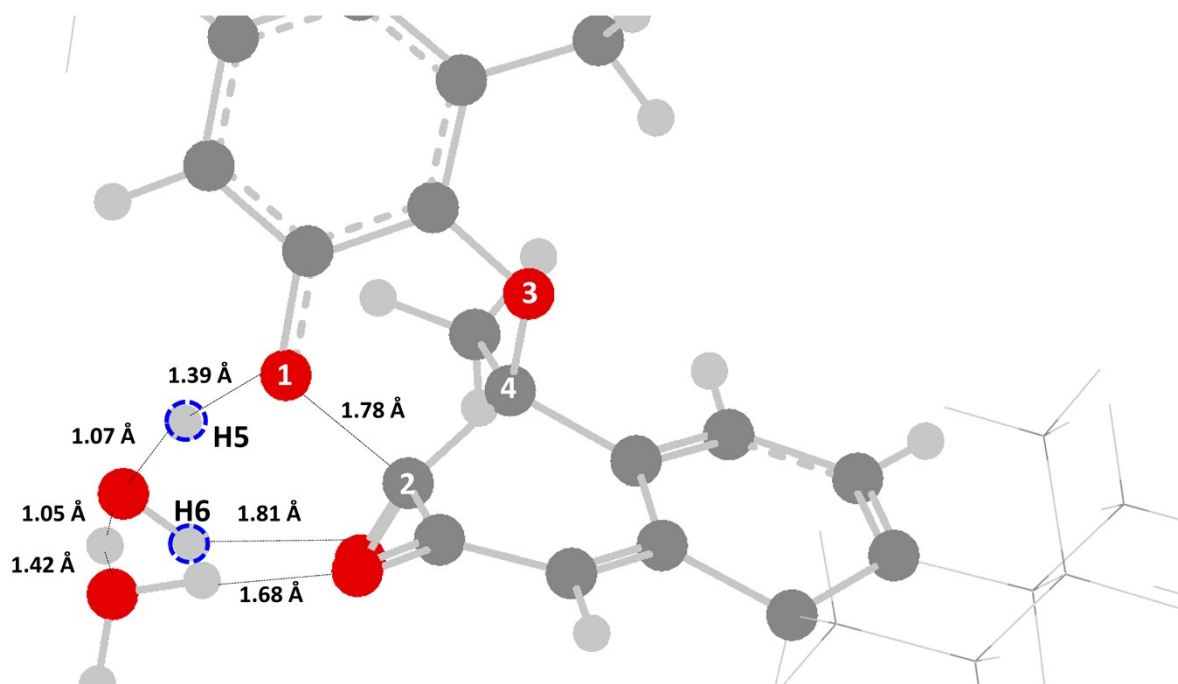


Figure S4. Structure of TS2 for the 2-wt-a pathway, showing the main interatomic distances. The blue circles point out what H atoms are being transferred.

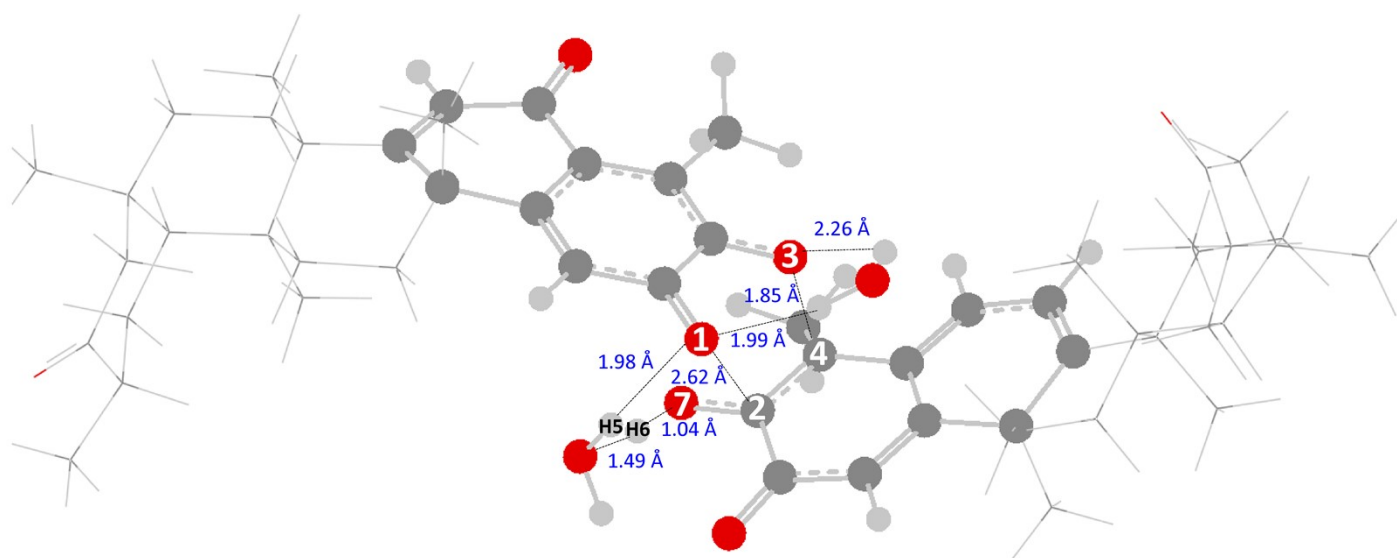


Figure S5. Structure of TS for the 2-wt-b pathway, showing the main interatomic distances.

I. Reactives

Orthoquinone

O	0	-6.46166700	1.24340900	-1.21677600	H		
O	0	-5.14475400	3.16794600	0.15840600	H		
C	0	-5.38303500	0.97612000	-0.73431300	H		
C	0	-4.62800700	2.07493100	0.03861800	H		
C	0	-3.32514700	1.72841300	0.59262700	H		
H	0	-2.82235400	2.51390500	1.14995800	H		
C	0	-2.79930600	0.49556200	0.44243000	H		
C	0	-3.53857300	-0.56679600	-0.28938500	H		
C	0	-4.75662400	-0.37200600	-0.85931100	H		
C	0	-5.55629200	-1.38187400	-1.62841100	H		
H	0	-5.96218400	-2.13940100	-0.95396400	H		
H	0	-4.93186700	-1.91036800	-2.34959400	H		
H	0	-6.37747600	-0.87836000	-2.13566800	H		
C	0	-1.45175700	0.14283500	1.13632400	H		
C	0	-2.85501700	-1.89185800	-0.45126500	H		
O	0	-3.46962200	-2.90028300	-0.76817500	H		
C	0	-1.40557500	-1.93573300	-0.27241200	H		
H	0	-0.93684100	-2.82240600	-0.68701500	H		
C	0	-0.71006200	-1.01546300	0.41733500	H		
C	0	-0.59325800	1.41295900	1.22427800	L H 14	0.0000	
H	0	-0.99252400	2.08208100	2.01669100	L		
H	0	-0.68162700	1.99136900	0.27742100	L		
C	0	0.79147400	-1.19846100	0.62667400	L H 19	0.0000	
C	0	0.88913000	1.16207200	1.50063600	L		
H	0	1.02963700	0.77538200	2.52882900	L		
H	0	1.43123400	2.13175100	1.47950100	L		
C	0	1.51532600	0.19103600	0.46840000	L		
C	0	-1.84335000	-0.34768200	2.53072700	L H 14	0.0000	
H	0	-2.43430000	0.39873700	3.07883000	L		
H	0	-0.95162100	-0.55599900	3.14820200	L		
H	0	-2.43529700	-1.27146800	2.50196900	L		
C	0	1.42702200	-2.17004100	-0.40084100	L		
H	0	1.26847700	-1.79173300	-1.43025900	L		
H	0	0.91594900	-3.15422900	-0.36423800	L		
C	0	3.03483300	0.01443000	0.78487700	L		
H	0	3.07263500	-0.33958600	1.85408800	L		
C	0	2.91894700	-2.38232900	-0.14014600	L		
H	0	3.04052900	-2.95971000	0.80075400	L		
H	0	3.33531100	-3.03925200	-0.92961100	L		
C	0	3.76116400	-1.08574600	-0.04751400	L		
C	0	0.95128500	-1.80623000	2.03550900	L		
H	0	0.52245700	-1.16527500	2.82147900	L		
H	0	2.00805600	-1.95792100	2.29257200	L		
H	0	0.46068100	-2.78413800	2.10404900	L		
C	0	1.27005300	0.74248000	-0.94576400	L		
H	0	1.71231200	1.74310100	-1.06619100	L		
H	0	0.20432900	0.83320000	-1.18281600	L		
H	0	1.71145200	0.09709600	-1.72212300	L		
C	0	4.10108700	-0.58847200	-1.47329100	L		
H	0	3.15739600	-0.46390400	-2.05950100	L		
H	0	4.67805000	-1.36093000	-2.01948700	L		
C	0	3.83022500	1.33461900	0.75787900	L		
H	0	3.24461800	2.13212700	1.26477800	L		
H	0	4.74233000	1.20931700	1.37805100	L		
C	0	4.84667500	0.71809900	-1.46328400	L		
C	0	4.23405700	1.83791300	-0.63741800	L		
H	0	3.29557400	2.15562400	-1.18286400	L		
C	0	5.08806800	-1.45036600	0.65759900	L		
H	0	5.77035400	-0.59604300	0.72088100	L		
H	0	5.61939100	-2.24769200	0.12618000	L		
H	0	4.92227300	-1.80225900	1.68200300	L		
O	0	5.85990000	0.86444700	-2.12672000	L		
C	0	5.16618900	3.04291800	-0.53495400	L		
H	0	4.67775300	3.88447000	-0.02937500	L		
H	0	5.47841700	3.39044500	-1.52789200	L		
H	0	6.07883300	2.80993100	0.02685200	L		

Gibbs Free Energy = -649.037555 hartrees

Quinonemethide triterpenoid

C	0	-3.57336900	1.45021800	0.62190000	H		
C	0	-5.53475000	0.57108700	-0.65061100	H		
C	0	-3.51551300	-0.73468800	-0.45361500	H		
C	0	-4.88050500	-0.57895000	-0.93580800	H		
C	0	-2.89205200	0.30561100	0.35864500	H		
C	0	-4.91919700	1.65537600	0.13121200	H		
H	0	-3.15092600	2.24890600	1.22478200	H		
O	0	-5.58664700	2.67982500	0.33429100	H		
C	0	-2.76561000	-1.82074500	-0.80444000	H		
H	0	-3.21259000	-2.59529000	-1.41926000	H		
C	0	-1.51990100	0.02059000	1.02280900	H		
C	0	-0.71943900	-1.10048500	0.32148100	H		
C	0	-1.37460200	-1.97172300	-0.47785300	H		
H	0	-0.86039200	-2.81491000	-0.92653900	H		
C	0	-1.89420200	-0.48573300	2.42230000	L H 11	0.0000	
H	0	-2.55425200	0.21539900	2.94995900	L		
H	0	-1.00045400	-0.61085500	3.05709200	L		
H	0	-2.40729900	-1.45532500	2.38903600	L		
C	0	-0.71916000	1.32818300	1.11356100	L H 11	0.0000	
H	0	-1.16230200	1.98691200	1.89011200	L		
H	0	-0.82137100	1.89067000	0.16006700	L		
C	0	0.76699500	1.13565700	1.42153200	L		
H	0	0.89801900	0.78050700	2.46257100	L		
C	0	1.27578200	2.12228600	1.38455100	L		
C	0	0.77157500	-1.25374500	0.60085500	L H 12	0.0000	
C	0	1.45426600	0.15846300	0.43326600	L		
C	0	1.47001500	-2.22752700	-0.38303500	L		
H	0	0.98868200	-3.22560900	-0.33786100	L		
H	0	1.33586000	-1.87787400	-1.42601800	L		
C	0	2.96870400	0.03832000	0.79717100	L		
H	0	2.98659700	-0.28686600	1.87546200	L		
C	0	3.75379700	-1.05778300	0.01376100	L		
C	0	2.95872600	-2.38428400	-0.06944200	L		
H	0	3.06746500	-2.93071100	0.89166300	L		
H	0	3.42176900	-3.04816400	-0.82610900	L		
C	0	0.90887100	-1.82963900	2.02395600	L		
H	0	0.49727200	-1.15505700	2.79080500	L		
H	0	1.95875500	-2.00863800	2.29045200	L		
H	0	0.38663100	-2.78925900	2.11400100	L		
C	0	1.23400000	0.67145800	-0.99969000	L		
H	0	0.17270900	0.73200600	-1.26473200	L		
H	0	1.70983400	0.01851000	-1.74865200	L		
H	0	1.65568800	1.67925500	-1.13202200	L		
C	0	4.11631300	-0.58526100	-1.41486600	L		
C	0	3.18478700	-0.50398200	-2.02754300	L		
H	0	4.73010600	-1.35281000	-1.92661500	L		
C	0	3.72407700	1.38196000	0.75883700	L		
H	0	3.09922000	2.17295300	1.22742900	L		
H	0	4.62043600	1.30066700	1.40852500	L		
C	0	4.15468400	1.86339000	-0.63628700	L		
C	0	4.82169600	0.74316500	-1.41818200	L		
C	0	5.07173300	-1.36011100	0.76389200	L		
H	0	4.88845600	-1.69121000	1.79222700	L		
H	0	5.72388300	-0.48235400	0.82331200	L		
H	0	5.64316900	-2.15268300	0.26827000	L		
C	0	5.05006400	3.09632300	-0.53703000	L		
H	0	4.52593100	3.93411100	-0.06202100	L		
H	0	5.37744800	3.43141400	-1.52939800	L		
H	0	5.95447600	2.90081900	0.05161000	L		
H	0	3.22368300	2.14129600	-1.21538200	L		
O	0	5.84678000	0.90444900	-2.05977100	L		
O	0	-6.79817000	0.82881000	-1.05943400	H		
H	0	-6.99151300	1.72000100	-0.71366500	H		
C	0	-5.53926700	-1.65949500	-1.74790000	H		
H	0	-6.57274300	-1.38985700	-1.96325100	H		
H	0	-5.53558700	-2.61361600	-1.21254700	H		
H	0	-5.02061900	-1.81312200	-2.69950500	H		

Gibbs Free Energy = -575.046595 Hartrees

Water

O	0.00000000	0.00000000	0.11903300
H	0.00000000	0.75736500	-0.47613100
H	0.00000000	-0.75736500	-0.47613100

Gibbs Free Energy = -76.387377 Hartrees

II. One-water Case

TS1

C	0	2.38824500	2.60618100	-0.95194300	H	
C	0	0.41418700	2.20854300	0.49207200	H	
C	0	2.65476000	1.84030000	1.37331400	H	
C	0	1.20274300	1.83404900	1.61332300	H	
C	0	3.19194800	2.17383500	0.05697700	H	
C	0	0.95779700	2.70406700	-0.79131700	H	
H	0	2.79331700	2.89825300	-1.91624500	H	
O	0	0.15404500	3.17116100	-1.59980400	H	
C	0	3.50107800	1.42134600	2.35211000	H	
H	0	3.09707900	1.16666900	3.32588100	H	
C	0	4.73296200	2.16902000	-0.14414600	H	
C	0	5.50824700	1.42354000	0.96551200	H	
C	0	4.90128700	1.17086200	2.14549300	H	
H	0	5.43871800	0.71711800	2.97063900	H	
C	0	5.11822100	3.65125600	-0.07728300	L H 11	0.0000
H	0	4.52341000	4.26635500	-0.76528400	L	
H	0	6.17284600	3.80785100	-0.36201500	L	
H	0	4.98824200	4.06762000	0.92966700	L	
O	0	-0.88707800	2.28622300	0.64719200	H	
H	0	-1.24416300	2.59376400	-0.21565900	H	
C	0	0.64118200	2.19708300	2.96839800	H	
H	0	-0.40924000	1.90335400	3.02353500	H	
H	0	0.70935100	3.27850700	3.11472000	H	
H	0	1.18347600	1.69937700	3.77064700	H	
O	0	0.88152100	-0.02151800	1.75692000	H	
O	0	0.39111900	0.25726900	-0.75151600	H	
C	0	-0.27723400	-0.41849700	1.35901100	H	
C	0	-0.52928000	-0.27246600	-0.06389300	H	
C	0	-1.82843100	-0.59215800	-0.55916600	H	
H	0	-2.00101500	-0.46587800	-1.62498300	H	
C	0	-2.79374900	-1.09194100	0.27567900	H	
C	0	-2.51834300	-1.25451900	1.68367500	H	
C	0	-1.30314000	-0.87886900	2.24419600	H	
C	0	-0.96000600	-0.97354800	3.70706000	H	
H	0	-0.92505200	-2.01512200	4.03131300	H	
H	0	-1.72013600	-0.48511600	4.31939000	H	
H	0	0.01016700	-0.50962900	3.88052800	H	
C	0	-4.14368700	-1.55999200	-0.33959100	H	
C	0	-3.60450800	-1.78582800	2.55185400	H	
O	0	-3.40966100	-2.15967500	3.70423300	H	
C	0	-4.96684400	-1.80605000	2.01382700	H	
H	0	-5.72625200	-1.97626400	2.77047300	H	
C	0	-5.27220400	-1.66488200	0.71350500	H	
C	0	-3.86598800	-2.96449400	-0.87966600	L H 38	0.0000
H	0	-3.00608800	-2.97955000	-1.56258600	L	
H	0	-4.72489600	-3.35508900	-1.45216200	L	
H	0	-3.65629800	-3.68436900	-0.07855500	L	
C	0	-4.52423900	-0.60212900	-1.48002700	L H 38	0.0000
H	0	-3.86699500	-0.78388000	-2.35713300	L	
H	0	-4.31586400	0.44529400	-1.16994900	L	
C	0	-5.98160200	-0.70215300	-1.93246000	L	
H	0	-6.17564000	0.07150900	-2.70555000	L	
H	0	-6.15982900	-1.67047300	-2.43993900	L	
C	0	-6.97380100	-0.52307400	-0.75537800	L	

C	0	-6.72985900	-1.70603400	0.25746600	L H 43	0.0000
C	0	-7.73272800	-1.52786700	1.42679700	L	
H	0	-7.55120500	-0.56297800	1.94065900	L	
H	0	-7.56655500	-2.31136100	2.19411600	L	
C	0	-9.18440100	-1.60543000	0.95161000	L	
H	0	-9.85878500	-1.42492400	1.81195600	L	
H	0	-9.40287700	-2.64712400	0.63354100	L	
C	0	-8.43650200	-0.60760000	-1.29749900	L	
H	0	-8.49783300	-1.60184500	-1.82338200	L	
C	0	-9.54746800	-0.64028200	-0.20399400	L	
C	0	-9.82089700	0.77057900	0.37013600	L	
H	0	-8.93782100	1.10713400	0.96787200	L	
H	0	-10.65821800	0.73274000	1.09458800	L	
C	0	-9.09401700	1.85422600	-1.84473800	L	
H	0	-8.14982300	2.29876000	-1.40879900	L	
C	0	-8.76138000	0.44892700	-2.37228500	L	
H	0	-9.61124700	0.07966800	-2.98362200	L	
H	0	-7.90961000	0.53121900	-3.08181800	L	
C	0	-10.85859100	-1.15835000	-0.83902500	L	
H	0	-10.73284800	-2.15388800	-1.27912200	L	
H	0	-11.21876400	-0.50010200	-1.63697100	L	
H	0	-11.66162900	-1.23418500	-0.09771400	L	
C	0	-9.58038500	2.75925400	-2.97447600	L	
H	0	-8.82745400	2.84995300	-3.76658500	L	
H	0	-9.79824600	3.77090700	-2.61095700	L	
H	0	-10.49928900	2.37856400	-3.43707100	L	
C	0	-10.09737700	1.78619000	-0.70439800	L	
O	0	-11.05362700	2.53917200	-0.62061200	L	
C	0	-6.68087400	0.81831200	-0.06236000	L	
H	0	-5.66416400	0.86870900	0.34210100	L	
H	0	-7.36534000	1.00481000	0.78065700	L	
C	0	-6.79010300	1.66081200	-0.76196900	L	
C	0	-6.96130000	-3.09680000	-0.36558200	L	
H	0	-6.32879600	-3.27182200	-1.24988000	L	
H	0	-8.00181800	-3.22741000	-0.69089000	L	
H	0	-6.74875500	-3.89406600	0.35593000	L	
C	0	5.03921700	1.57105100	-1.52330300	L H 11	0.0000
H	0	4.70053500	2.26109000	-2.32280800	L	
H	0	4.43446100	0.64091100	-1.64693100	L	
C	0	6.51645400	1.23873200	-1.74411200	L	
H	0	7.11794000	2.16704700	-1.78945600	L	
H	0	6.63086600	0.76503000	-2.74169900	L	
C	0	7.07387500	0.29174400	-0.64830400	L	
C	0	6.96787800	1.04376400	0.73361400	L H 12	0.0000
C	0	6.21782100	-0.98608000	-0.62530600	L	
H	0	6.33450400	-1.56151800	-1.54907200	L	
H	0	5.14412000	-0.75879300	-0.52478000	L	
H	0	6.48031900	-1.64559100	0.21276900	L	
C	0	7.79251000	2.34547600	0.77835500	L	
H	0	8.87047000	2.14609600	0.71304300	L	
H	0	7.62415900	2.88836500	1.71571300	L	
H	0	7.54658800	3.02696700	-0.05077100	L	
C	0	7.52211500	0.09209600	1.82509400	L	
H	0	6.91432300	-0.83449600	1.86629600	L	
H	0	7.42758500	0.56037900	2.82537200	L	
C	0	8.99081400	-0.25462400	1.57721200	L	
H	0	9.60577400	0.65801000	1.73011700	L	
H	0	9.33546700	-0.96401600	2.35519500	L	
C	0	8.57485700	-0.03328900	-0.95177200	L	
H	0	9.09781500	0.95945200	-0.99768100	L	
C	0	9.29581200	-0.83866500	0.17305200	L	
C	0	10.82512200	-0.72694000	-0.02582000	L	
H	0	11.37375800	-1.22191000	0.78294600	L	
H	0	11.15663900	0.31665600	-0.05131200	L	
H	0	11.15549400	-1.19000300	-0.96639200	L	
C	0	8.74362100	-0.67640400	-2.34894200	L	
H	0	9.41259200	-0.03475900	-2.95736100	L	
H	0	7.77245500	-0.66297700	-2.89069500	L	
C	0	9.30653300	-2.10844400	-2.37291900	L	
H	0	10.42070300	-2.05136800	-2.18766500	L	
C	0	8.89070300	-2.33160900	0.15145700	L	
H	0	9.62941700	-2.93894000	0.71722400	L	
H	0	7.93629900	-2.46807100	0.71322600	L	
C	0	8.72580900	-2.91343700	-1.22478800	L	
O	0	8.16942600	-3.98894600	-1.37927700	L	
C	0	9.07222200	-2.77597800	-3.72478600	L	
H	0	9.52252000	-3.77565800	-3.75937700	L	
H	0	9.51045900	-2.18960800	-4.54135900	L	

H	0	8.00385500	-2.89635200	-3.94232200	L
H	0	2.97745700	-0.75294800	0.77705600	H
O	0	3.01278000	-0.77861800	-0.18687500	H
H	0	2.15617200	-0.37941500	-0.41988300	H

Gibbs Free Energy = -1300.415956 Hartrees

Intermediate

C	0	-2.99091400	2.57217600	-0.09611600	H	
C	0	-0.64769200	1.84194500	-0.74361300	H	
C	0	-2.70702700	0.48687300	-1.37870900	H	
C	0	-1.19024100	0.51591700	-1.30585400	H	
C	0	-3.52681900	1.54219600	-0.81342200	H	
C	0	-1.57291400	2.76145500	0.06050500	H	
H	0	-3.61893200	3.32949700	0.36457400	H	
O	0	-1.07549700	3.66264500	0.72756300	H	
C	0	-3.30847400	-0.62763600	-1.85954700	H	
H	0	-2.68938500	-1.44484200	-2.21733600	H	
C	0	-5.04864000	1.52771800	-1.13408100	H	
C	0	-5.59672300	0.11757800	-1.45813500	H	
C	0	-4.73432900	-0.84413100	-1.84296900	H	
H	0	-5.08181000	-1.82572100	-2.14480000	H	
C	0	-5.13271000	2.37091600	-2.41294800	L H 11	0.0000
H	0	-4.67621700	3.36172400	-2.28603200	L	
H	0	-6.18210600	2.54727700	-2.70702600	L	
H	0	-4.63605600	1.88788000	-3.26432800	L	
O	0	0.49277600	2.18943700	-0.94877100	H	
H	0	2.08621200	2.88789600	0.96726600	H	
C	0	-0.54134600	0.29365300	-2.66984900	H	
H	0	0.54328200	0.24516300	-2.55576400	H	
H	0	-0.78442000	1.12900300	-3.33037300	H	
H	0	-0.90156100	-0.62788800	-3.12592800	H	
O	0	-0.86331800	-0.55887300	-0.38013600	H	
O	0	0.05327400	0.89766400	1.64838600	H	
C	0	0.45754800	-0.72227300	-0.01595200	H	
C	0	0.92832700	0.06090800	1.05046900	H	
C	0	2.25410600	-0.04352600	1.44786400	H	
H	0	2.59723800	0.57337500	2.27567600	H	
C	0	3.12034500	-0.93456100	0.81378200	H	
C	0	2.62289200	-1.76919000	-0.20258300	H	
C	0	1.26877600	-1.68062100	-0.61874200	H	
C	0	0.66216800	-2.58878500	-1.65939200	H	
H	0	0.81678600	-3.63239900	-1.38713300	H	
H	0	1.13395000	-2.44910200	-2.63500400	H	
H	0	-0.40523100	-2.39115700	-1.74182800	H	
C	0	4.57211400	-1.04512400	1.35126800	H	
C	0	3.56004000	-2.71054900	-0.86558400	H	
O	0	3.19975400	-3.57141600	-1.66409300	H	
C	0	4.99392000	-2.55789300	-0.59451200	H	
H	0	5.61701400	-3.15006300	-1.25715600	H	
C	0	5.51101900	-1.77933700	0.36929200	H	
C	0	4.45908200	-1.88217200	2.62788700	L H 38	0.0000
H	0	3.71071000	-1.47790600	3.32211000	L	
H	0	5.41327800	-1.90896000	3.18122100	L	
H	0	4.17781600	-2.92199700	2.41808500	L	
H	0	0.71441400	3.53048700	1.18132600	H	
O	0	1.46791200	3.13860000	1.66597700	H	
H	0	0.55637000	1.70401200	1.92755800	H	
C	0	5.09107300	0.36684100	1.66807000	L H 38	0.0000
H	0	4.59090100	0.75502600	2.58084700	L	
H	0	4.79311000	1.06253300	0.85382400	L	
C	0	6.60554300	0.44856800	1.86743400	L	
H	0	6.89472500	1.50934100	2.02436500	L	
H	0	6.89648800	-0.07285000	2.80063300	L	
C	0	7.39057500	-0.13280100	0.66368700	L	
C	0	7.02421200	-1.66240800	0.54499300	L H 43	0.0000
C	0	7.81853400	-2.23652400	-0.65685500	L	
H	0	7.52731000	-1.71569300	-1.59064900	L	
H	0	7.55520400	-3.30229900	-0.81304800	L	
C	0	9.32970000	-2.12883500	-0.44601000	L	
H	0	9.85076500	-2.50575900	-1.34815700	L	

H	0	9.62874700	-2.82527800	0.36646800	L		
C	0	8.92320600	0.00451500	0.93277400	L		
H	0	9.09878900	-0.52530000	1.91098900	L		
C	0	9.84412100	-0.70855300	-0.10405500	L		
C	0	9.97960000	0.11732500	-1.40606600	L		
H	0	9.00193100	0.12102800	-1.94830700	L		
H	0	10.68924100	-0.37647600	-2.09890900	L		
C	0	9.58719200	2.29989700	-0.10737600	L		
H	0	8.57278400	2.48373900	-0.57288800	L		
C	0	9.38484200	1.45758700	1.16266600	L		
H	0	10.33193700	1.43853000	1.74146600	L		
H	0	8.65594500	1.97969300	1.81964300	L		
C	0	11.25533800	-0.86752500	0.50754900	L		
H	0	11.23208400	-1.43618500	1.44389900	L		
H	0	11.71866200	0.09885000	0.73333100	L		
H	0	11.93077900	-1.39721500	-0.17323200	L		
C	0	10.21938000	3.64910400	0.22680200	L		
H	0	9.58121900	4.23403600	0.89974200	L		
H	0	10.38186700	4.24731300	-0.67858700	L		
H	0	11.19391700	3.53546700	0.71706100	L		
C	0	10.39802300	1.53818800	-1.14369500	L		
O	0	11.30992000	2.04790700	-1.77378900	L		
C	0	6.94999400	0.60468300	-0.61203400	L		
H	0	5.87927700	0.49141800	-0.81356100	L		
H	0	7.48081900	0.23681500	-1.50459100	L		
H	0	7.14953700	1.68448500	-0.53787800	L		
C	0	7.39924900	-2.47755000	1.79763500	L		
H	0	6.95805800	-2.06174800	2.71683700	L		
H	0	8.48569000	-2.50673300	1.95400200	L		
H	0	7.06129400	-3.51661900	1.70965400	L		
C	0	-5.82283200	2.19382700	0.01161800	L	H 11	0.0000
H	0	-5.64451700	3.29020300	0.00103500	L		
H	0	-5.42012400	1.83762800	0.98581200	L		
C	0	-7.33178600	1.94257000	-0.01419900	L		
H	0	-7.79631500	2.47510600	-0.86671600	L		
H	0	-7.78260300	2.39546800	0.89405300	L		
C	0	-7.67745600	0.43168200	-0.07456900	L		
C	0	-7.10035100	-0.13266800	-1.42694400	L	H 12	0.0000
C	0	-7.01519500	-0.27654500	1.12093400	L		
H	0	-7.42558700	0.07962600	2.07232600	L		
H	0	-5.93279700	-0.10800000	1.15626200	L		
H	0	-7.16049700	-1.36583000	1.08552500	L		
C	0	-7.69569300	0.55808100	-2.67038800	L		
H	0	-8.78061800	0.40459800	-2.73893100	L		
H	0	-7.25572800	0.16085500	-3.59233300	L		
H	0	-7.52906700	1.64661100	-2.66629200	L		
C	0	-7.45597700	-1.63974800	-1.49565300	L		
H	0	-6.98481600	-2.18059400	-0.65034200	L		
H	0	-7.03263800	-2.09182400	-2.41538000	L		
C	0	-8.96834500	-1.86323500	-1.48629600	L		
H	0	-9.39425300	-1.48115300	-2.43825100	L		
H	0	-9.17708900	-2.95133400	-1.49901200	L		
C	0	-9.23283100	0.25470000	-0.05114400	L		
H	0	-9.61831100	0.85210000	-0.92110100	L		
C	0	-9.71797700	-1.20707300	-0.29764800	L		
C	0	-11.21513600	-1.18552900	-0.68324200	L		
H	0	-11.58208000	-2.18802000	-0.92945800	L		
H	0	-11.40118200	-0.54927700	-1.55525100	L		
H	0	-11.84791600	-0.80490100	0.13105100	L		
C	0	-9.85323800	0.88473900	1.21846600	L		
H	0	-10.56270200	1.67953500	0.91084400	L		
H	0	-9.06833800	1.41848900	1.79797600	L		
C	0	-10.59645000	-0.07828000	2.16067800	L		
H	0	-11.59877200	-0.32189800	1.69648400	L		
C	0	-9.53167100	-2.08542300	0.96198500	L		
H	0	-10.14779100	-3.00671800	0.88236800	L		
H	0	-8.48103500	-2.46024100	1.00290800	L		
C	0	-9.84579100	-1.39378000	2.25961100	L		
O	0	-9.52281200	-1.89800300	3.32312100	L		
C	0	-10.83573300	0.55721100	3.52707400	L		
H	0	-11.39620700	-0.11608000	4.18718500	L		
H	0	-11.41194300	1.48646100	3.43998300	L		
H	0	-9.89534000	0.80161100	4.03595400	L		

Gibbs Free Energy = -383.694849

TS2

C	0	3.24349500	2.78816500	-1.25361300	H		
C	0	0.96594300	3.10569700	-0.21144600	H		
C	0	2.69686400	1.72367900	0.89612600	H		
C	0	1.20654500	1.82649200	0.59795700	H		
C	0	3.64691200	2.14156400	-0.12484200	H		
C	0	1.89811900	3.30399800	-1.41655800	H		
H	0	3.95352400	3.07270200	-2.02603600	H		
O	0	1.55881400	4.00376100	-2.36323300	H		
C	0	3.14231400	1.08345000	2.00093400	H		
H	0	2.43138200	0.76283400	2.75439100	H		
C	0	5.17136900	1.97182500	0.15550800	H		
C	0	5.48707500	0.99061900	1.30764800	H		
C	0	4.51826100	0.68509000	2.19307100	H		
H	0	4.72424800	0.06619900	3.05941300	H		
C	0	5.60056900	3.37249400	0.60782100	L	H 11	0.0000
H	0	5.32892000	4.14746900	-0.12089300	L		
H	0	6.69599000	3.43577100	0.73045900	L		
H	0	5.15223800	3.65427300	1.56927000	L		
O	0	0.62233800	4.15860100	0.39457400	H		
H	0	-0.20373700	4.91104300	-0.58811600	H		
C	0	0.32106100	1.81491500	1.83725100	H		
H	0	-0.70447900	2.07911600	1.57500100	H		
H	0	0.68396600	2.54391400	2.56186600	H		
H	0	0.31984400	0.81904400	2.28569800	H		
O	0	0.96628000	0.67274300	-0.24076900	H		
O	0	-0.50105900	2.61371600	-1.23341800	H		
C	0	-0.35529100	0.40244400	-0.50602800	H		
C	0	-1.12741800	1.45174100	-1.02339100	H		
C	0	-2.47078700	1.24766100	-1.30647600	H		
H	0	-3.04935500	2.07381200	-1.71220700	H		
C	0	-3.05071700	-0.00574200	-1.09491800	H		
C	0	-2.26037800	-1.05766700	-0.59802800	H		
C	0	-0.89405300	-0.85368500	-0.26865800	H		
C	0	-0.00636600	-1.91053000	0.33962000	H		
H	0	0.19940900	-2.70976800	-0.37513500	H		
H	0	-0.49377000	-2.38004500	1.19514400	H		
H	0	0.93474700	-1.46034400	0.65476900	H		
C	0	-4.53097300	-0.20445800	-1.51658200	H		
C	0	-2.89261000	-2.38178100	-0.39437500	H		
O	0	-2.25223500	-3.40155000	-0.14877800	H		
C	0	-4.35713700	-2.46027100	-0.44944000	H		
H	0	-4.74931400	-3.40623900	-0.08940500	H		
C	0	-5.15338300	-1.48263700	-0.91087400	H		
C	0	-4.49433700	-0.36089200	-3.03924200	L	H 38	0.0000
H	0	-3.94783600	0.45939000	-3.52307800	L		
H	0	-5.50883000	-0.35698200	-3.47217700	L		
H	0	-4.01330600	-1.29768800	-3.34711800	L		
H	0	-0.27695900	5.13608600	-2.15621400	H		
O	0	-0.86368100	4.94336000	-1.40136400	H		
H	0	-0.94850500	3.82918800	-1.43610500	H		
C	0	-5.33116900	1.04583700	-1.11579900	L	H 38	0.0000
H	0	-5.06455700	1.89152800	-1.78482800	L		
H	0	-5.02390500	1.37078000	-0.09821400	L		
C	0	-6.84897600	0.85810700	-1.14383100	L		
H	0	-7.33651800	1.78596100	-0.77689600	L		
H	0	-7.19948600	0.73851400	-2.18792800	L		
C	0	-6.67226600	-1.64999000	-0.90437800	L	H 43	0.0000
C	0	-7.30976200	-0.34719500	-0.28470100	L		
C	0	-8.86650100	-0.46033800	-0.34917500	L		
H	0	-9.11029000	-0.53970500	-1.44579400	L		
C	0	-9.46536900	-1.74052000	0.30957700	L		
C	0	-8.66576200	-3.01030200	-0.07359100	L		
H	0	-8.95688200	-3.84742900	0.59114900	L		
H	0	-8.97219900	-3.33521400	-1.09102000	L		
C	0	-7.14477800	-2.85064300	-0.04407200	L		
H	0	-6.68036300	-3.78796500	-0.41173200	L		
H	0	-6.79551800	-2.73253300	1.00084800	L		
C	0	-6.79423800	-0.15285600	1.15137100	L		
H	0	-7.18415300	0.77682600	1.59276400	L		
H	0	-5.70140400	-0.09492300	1.19977600	L		
H	0	-7.09740100	-0.97981100	1.81305000	L		
C	0	-7.10655400	-1.90692900	-2.36040300	L		

H	0	-6.90505500	-1.04569600	-3.01625100	L		
H	0	-8.18206600	-2.11524400	-2.43370900	L		
H	0	-6.58367400	-2.77326200	-2.78181800	L		
C	0	-9.52083000	-1.61311400	1.85116100	L		
H	0	-8.48168300	-1.62100900	2.26317200	L		
H	0	-10.00965800	-2.50505300	2.29090600	L		
C	0	-9.72885700	0.94142500	1.67181000	L		
H	0	-8.69699900	1.12921900	2.09552100	L		
C	0	-9.60100300	0.80183100	0.14598300	L		
H	0	-9.09165400	1.70733400	-0.24919600	L		
H	0	-10.61413400	0.82059600	-0.30720800	L		
C	0	-10.91053800	-1.93694400	-0.20437700	L		
H	0	-10.94609600	-2.02512900	-1.29598000	L		
H	0	-11.56322000	-1.10118400	0.06912300	L		
H	0	-11.36261400	-2.84634400	0.20665600	L		
C	0	-10.62519600	2.12170400	2.03923400	L		
H	0	-10.22123700	3.06555900	1.65388800	L		
H	0	-10.72266800	2.22531500	3.12714500	L		
H	0	-11.63798100	2.01029300	1.63343500	L		
C	0	-10.21555400	-0.35586300	2.29723400	L		
O	0	-11.08730500	-0.39286700	3.15000700	L		
C	0	7.30095800	1.04749800	-0.95732200	L		
C	0	5.87777600	1.57554700	-1.14854000	L	H 11	0.0000
H	0	5.90932000	2.44397900	-1.84022100	L		
H	0	5.27438800	0.80354000	-1.67441600	L		
H	0	7.97561500	1.86820800	-0.64478600	L		
H	0	7.68889100	0.70821200	-1.94090900	L		
C	0	6.98513600	-0.71941200	2.48354800	L		
H	0	6.30792000	-1.54300200	2.17993600	L		
H	0	6.62304600	-0.38260900	3.47586700	L		
C	0	8.41466600	-1.24129100	2.62943300	L		
H	0	8.42297100	-2.09123900	3.34015900	L		
H	0	9.03568800	-0.45866700	3.11484300	L		
C	0	8.84738600	-0.62614300	0.16921000	L		
H	0	9.45736000	0.27376300	0.45222500	L		
C	0	6.90221500	0.44275300	1.46089300	L	H 12	0.0000
C	0	7.37012900	-0.11795800	0.06440700	L		
C	0	7.78738500	1.59477500	1.97556700	L		
H	0	7.40969100	1.98860100	2.92633600	L		
H	0	7.83794100	2.43508000	1.26569900	L		
H	0	8.82024400	1.26652000	2.15090100	L		
C	0	6.42398400	-1.23987600	-0.40000200	L		
H	0	5.39720500	-0.88447300	-0.54298600	L		
H	0	6.37196500	-2.06205400	0.32815600	L		
H	0	6.75044900	-1.66671000	-1.35484500	L		
C	0	8.56776700	-3.07107300	0.90171700	L		
H	0	7.47159400	-3.13123900	1.10359400	L		
H	0	9.01035200	-3.84909300	1.56010300	L		
C	0	9.38010400	-1.09812100	-1.20477900	L		
H	0	10.25791200	-0.47806700	-1.47802200	L		
H	0	8.62818900	-0.88412900	-1.99567700	L		
C	0	9.79369000	-2.57701600	-1.30141500	L		
H	0	10.79228700	-2.69805900	-0.78401100	L		
C	0	9.09053900	-1.67122200	1.30139000	L		
C	0	10.60667200	-1.76039400	1.59132900	L		
H	0	11.02920000	-0.78372300	1.85077600	L		
H	0	11.17337300	-2.13415000	0.72672900	L		
H	0	10.81773300	-2.43687200	2.42688300	L		
C	0	8.81230700	-3.44399900	-0.53410800	L		
O	0	8.25492800	-4.41296900	-1.02418200	L		
C	0	9.94340800	-3.01794800	-2.75447600	L		
H	0	8.99916500	-2.93718800	-3.30674600	L		
H	0	10.26842700	-4.06351900	-2.82290300	L		
H	0	10.68658900	-2.40767900	-3.28193100	L		

Gibbs Free Energy= -1300.452629 Hartrees

III. Two-water Case

2-wt-a pathway

TS1

C	0	-2.95252300	2.80914600	0.07866700	H		
C	0	-0.58430000	2.25206500	-0.60947300	H		
C	0	-2.54740500	1.06980600	-1.59319900	H		
C	0	-1.11472700	1.23834400	-1.45997100	H		
C	0	-3.44909200	1.88294300	-0.77844000	H		
C	0	-1.53519000	3.09085400	0.19672800	H		
H	0	-3.60572700	3.44007500	0.67589800	H		
O	0	-1.10244800	4.02595500	0.86973200	H		
C	0	-3.08798000	0.08802000	-2.37450400	H		
H	0	-2.43792400	-0.53574100	-2.97702200	H		
C	0	-4.97935100	1.78923900	-1.02922700	H		
C	0	-5.40999100	0.47393800	-1.71375800	H		
C	0	-4.48656800	-0.24535600	-2.38781300	H		
H	0	-4.76570900	-1.12991700	-2.95014200	H		
C	0	-5.25541700	2.93627100	-2.01091600	L H 11	0.0000	
H	0	-4.88818200	3.89942000	-1.63373500	L		
H	0	-6.33757300	3.06138400	-2.18675800	L		
H	0	-4.78594600	2.76639100	-2.98800200	L		
O	0	0.66201700	2.42257300	-0.50935100	H		
C	0	1.18235600	3.25266600	0.63126700	H		
C	0	-0.10870100	0.55824800	-2.31897100	H		
H	0	0.37908000	1.29368100	-2.96701700	H		
H	0	-0.50840200	-0.24723100	-2.93048700	H		
O	0	0.69061500	0.15900700	-1.67822800	H		
O	0	-1.00774700	0.07818700	0.43638900	H		
O	0	0.27457800	1.58700000	2.27898700	H		
C	0	0.18263800	-0.21354700	0.73566500	H		
C	0	0.90143200	0.66252900	1.67555600	H		
C	0	2.29538500	0.42600200	1.85669800	H		
H	0	2.83062900	1.09974100	2.52203500	H		
C	0	2.92971700	-0.64664000	1.28325000	H		
C	0	2.19497000	-1.57832500	0.45976500	H		
C	0	0.85918800	-1.36542600	0.16177500	H		
C	0	0.01637200	-2.27285200	-0.69306400	H		
H	0	-0.14072500	-3.22947600	-0.18961500	H		
H	0	0.51342100	-2.50055900	-1.63697200	H		
H	0	-0.94668600	-1.79717400	-0.87947000	H		
C	0	4.42264700	-0.90114300	1.63925700	H		
C	0	2.92026600	-2.73826000	-0.11302800	H		
O	0	2.34832400	-3.69247400	-0.63377100	H		
C	0	4.38596200	-2.70333900	-0.10147000	H		
H	0	4.84076600	-3.45351600	-0.74067500	H		
C	0	5.11841700	-1.85807100	0.64176400	H		
C	0	4.38349700	-1.58634100	3.00652200	L H 38	0.0000	
H	0	3.81501600	-1.00557400	3.74521700	L		
H	0	5.39800800	-1.71072900	3.42416100	L		
H	0	3.93042700	-2.58512600	2.96004100	L		
O	0	1.18138500	4.41166600	1.83276200	H		
H	0	1.55085900	3.50772200	1.56884200	H		
H	0	1.02677600	2.74142800	2.10614400	H		
C	0	5.14365100	0.45310900	1.72321900	L H 38	0.0000	
H	0	4.83632000	0.98543500	2.64906600	L		
H	0	4.80993400	1.10440400	0.88587600	L		
C	0	6.66973200	0.35921900	1.69774800	L		
H	0	7.09639600	1.38486600	1.69070900	L		
H	0	7.04069100	-0.10241300	2.63396900	L		
C	0	6.64435200	-1.90471800	0.58416900	L H 43	0.0000	
C	0	7.18906000	-0.42989500	0.46899200	L		
C	0	8.75071800	-0.45742500	0.49886000	L		
H	0	9.01775300	-0.90183800	1.49888700	L		
C	0	9.41757900	-1.38265200	-0.56451500	L		
C	0	8.70489000	-2.75438200	-0.65857300	L		
H	0	9.03687100	-3.28345100	-1.57381000	L		
H	0	9.04744400	-3.39708600	0.18031300	L		
C	0	7.17689500	-2.69165400	-0.64125400	L		
H	0	6.77764900	-3.72639000	-0.63324100	L		
H	0	6.80380500	-2.23466900	-1.57929800	L		
C	0	6.63767500	0.22528300	-0.80841300	L		
H	0	6.95653500	1.27568200	-0.88784100	L		
H	0	5.54299300	0.21998700	-0.84486900	L		
H	0	6.98624000	-0.28924800	-1.71832200	L		
C	0	7.11469400	-2.62846900	1.86112700	L		
C	0	6.83512200	-2.08743000	2.77857500	L		
H	0	8.20636100	-2.74455500	1.88345200	L		
H	0	6.68462400	-3.63466800	1.92750100	L		

C	0	9.43960500	-0.71744500	-1.96195000	L		
H	0	8.39636400	-0.64471000	-2.35666800	L		
H	0	9.97458300	-1.36471300	-2.68467800	L		
C	0	9.48890100	1.61796200	-0.89416500	L		
H	0	8.44061300	1.87346100	-1.23308100	L		
C	0	9.39526300	0.94335400	0.48434100	L		
H	0	8.83635200	1.61698300	1.16947800	L		
H	0	10.41250900	0.86752700	0.92223700	L		
C	0	10.88022400	-1.65416400	-0.14304700	L		
H	0	10.93939300	-2.11927200	0.84735900	L		
H	0	11.47481400	-0.73550100	-0.09909100	L		
H	0	11.38177900	-2.32903800	-0.84545200	L		
C	0	10.30078500	2.90887800	-0.81810400	L		
H	0	9.83927300	3.63189500	-0.13500200	L		
H	0	10.37976900	3.38766100	-1.80230800	L		
H	0	11.32307700	2.73119700	-0.46295200	L		
C	0	10.04978900	0.65722400	-1.93038000	L		
O	0	10.91408900	0.97611000	-2.72991000	L		
C	0	-7.19689500	1.60967500	0.27041500	L		
C	0	-5.72215800	2.01674900	0.29573500	L	H 11	0.0000
H	0	-5.65136000	3.08529100	0.58897600	L		
H	0	-5.20821200	1.45529700	1.10628100	L		
H	0	-7.77552100	2.30323300	-0.36998000	L		
H	0	-7.61726100	1.73311200	1.29051300	L		
C	0	-7.08783300	-1.40460800	-2.16989400	L		
H	0	-6.50324000	-2.10132600	-1.53611900	L		
H	0	-6.69318400	-1.53091200	-3.19819200	L		
C	0	-8.56601400	-1.79453900	-2.15578800	L		
H	0	-8.66809800	-2.85282800	-2.46738800	L		
H	0	-9.09786100	-1.21492700	-2.93988800	L		
C	0	-8.92434200	-0.20473300	-0.16451000	L		
H	0	-9.43076100	0.56453700	-0.80777800	L		
C	0	-6.87607200	0.05455600	-1.69094100	L	H 12	0.0000
C	0	-7.39937300	0.14780200	-0.20781400	L		
C	0	-7.63305100	0.98897700	-2.65590200	L		
H	0	-7.22522100	0.92231200	-3.67091300	L		
H	0	-7.57789000	2.04421000	-2.34607500	L		
H	0	-8.69841900	0.73244400	-2.71831800	L		
C	0	-6.58292800	-0.78755200	0.70253000	L		
H	0	-5.52231500	-0.51289900	0.73314600	L		
H	0	-6.62558200	-1.83229800	0.36268000	L		
H	0	-6.95100600	-0.76104800	1.73394900	L		
C	0	-8.92257800	-2.75262100	0.14957000	L		
H	0	-7.83973600	-2.99959700	0.03805500	L		
H	0	-9.44903900	-3.67902800	-0.16504200	L		
C	0	-9.50323500	-0.03020700	1.25979100	L		
H	0	-10.30146900	0.73878200	1.22759400	L		
H	0	-8.72852600	0.39761800	1.93317400	L		
C	0	-10.08593300	-1.29447900	1.91525800	L		
H	0	-11.09035300	-1.50692500	1.44024000	L		
C	0	-9.28455300	-1.58409600	-0.79741300	L		
C	0	-10.80135200	-1.62465300	-1.09548700	L		
H	0	-11.11072700	-0.79633300	-1.74193400	L		
H	0	-11.40641000	-1.55887800	-0.18005800	L		
H	0	-11.08780400	-2.55386000	-1.60022500	L		
C	0	-9.20830000	-2.49282400	1.60284700	L		
O	0	-8.76320800	-3.23598500	2.46277300	L		
C	0	-10.29062600	-1.09759800	3.41437700	L		
H	0	-9.34265500	-0.92494700	3.93819100	L		
H	0	-10.75876100	-1.97772900	3.87191000	L		
H	0	-10.93985200	-0.23740500	3.61884900	L		
H	0	-0.40568700	5.51221600	1.86737700	H		
O	0	0.46958700	5.77136000	2.19823400	H		
H	0	0.36815400	5.89956600	3.14932700	H		

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Intermediate

C	0	-3.19878200	3.01666400	0.28423600	H		
C	0	-0.86044800	2.90527300	-0.68068000	H		
C	0	-2.63608100	1.30200600	-1.39511100	H		
C	0	-1.15191700	1.46129800	-1.10792200	H		
C	0	-3.59245900	2.04330300	-0.59011400	H		

C	0	-1.85467800	3.53570500	0.30055600	H		
H	0	-3.92146600	3.54265000	0.90231700	H		
O	0	-1.49063700	4.50637600	0.95566700	H		
C	0	-3.07968300	0.35419000	-2.25438600	H		
H	0	-2.36427100	-0.20211600	-2.85042500	H		
C	0	-5.11465300	1.82133700	-0.84001800	H		
C	0	-5.43761700	0.53708000	-1.63610500	H		
C	0	-4.46096000	-0.05296000	-2.35379200	H		
H	0	-4.66753700	-0.90699500	-2.98896700	H		
C	0	-5.49696800	3.01878100	-1.71806800	L H 11	0.0000	
H	0	-5.21600500	3.97782200	-1.26294500	L		
H	0	-6.58808300	3.06463300	-1.88096000	L		
H	0	-5.02508600	2.97641800	-2.70836400	L		
O	0	0.08585800	3.54663200	-1.07219700	H		
H	0	0.66415200	4.87796400	0.68513100	H		
C	0	-0.23234100	1.06988300	-2.25208500	H		
H	0	-0.50313800	1.63994500	-3.14286100	H		
H	0	-0.30389900	0.00531500	-2.47340400	H		
H	0	0.80064700	1.30559700	-1.99509600	H		
O	0	-0.96852800	0.64286000	0.08514200	H		
O	0	0.42692300	2.34277200	1.60593200	H		
C	0	0.32683400	0.30900500	0.42595100	H		
C	0	1.06452900	1.22713700	1.18808000	H		
C	0	2.38600000	0.95053600	1.50813800	H		
H	0	2.93968600	1.67912800	2.09590600	H		
C	0	2.98176800	-0.24441600	1.10311700	H		
C	0	2.20874900	-1.19674600	0.41560000	H		
C	0	0.85953200	-0.92877900	0.07148500	H		
C	0	-0.02555900	-1.91767200	-0.64726800	H		
H	0	-0.12701300	-2.83174700	-0.06113600	H		
H	0	0.40805300	-2.21488700	-1.60482900	H		
H	0	-1.01215300	-1.48358600	-0.80929100	H		
C	0	4.44512400	-0.51576900	1.54277700	H		
C	0	2.85200100	-2.47651800	0.02242700	H		
O	0	2.22592700	-3.43636200	-0.41854800	H		
C	0	4.31277800	-2.56855400	0.12025700	H		
H	0	4.71998200	-3.44553300	-0.37281300	H		
C	0	5.09071300	-1.68061800	0.76015900	H		
C	0	4.35057200	-0.92034500	3.01609300	L H 38	0.0000	
H	0	3.78909200	-0.18749100	3.61032800	L		
H	0	5.34853600	-0.99707600	3.48028600	L		
H	0	3.85679300	-1.89147100	3.14811300	L		
H	0	0.88914500	4.93988600	2.19467500	H		
O	0	1.35284500	4.73870400	1.35767600	H		
H	0	0.99171100	3.16676500	1.51649600	H		
C	0	5.25493300	0.78111000	1.38322600	L H 38	0.0000	
H	0	4.96369400	1.50525600	2.17363800	L		
H	0	4.98388000	1.27152300	0.42323000	L		
C	0	6.77103000	0.58498300	1.43380000	L		
H	0	7.26991600	1.55864800	1.24256900	L		
H	0	7.08432900	0.29374700	2.45582400	L		
C	0	6.60913500	-1.84933200	0.77915000	L H 43	0.0000	
C	0	7.26441700	-0.46424600	0.40481700	L		
C	0	8.81813400	-0.59122600	0.50454800	L		
H	0	9.02346500	-0.85091900	1.58106300	L		
C	0	9.44356600	-1.74726200	-0.33445700	L		
C	0	8.63381700	-3.06014300	-0.19508400	L		
H	0	8.94987300	-3.77655700	-0.97891300	L		
H	0	8.90552800	-3.55056200	0.76423200	L		
C	0	7.11434000	-2.89310500	-0.25043800	L		
H	0	6.64001000	-3.87690300	-0.05896200	L		
H	0	6.80104800	-2.60312000	-1.27305500	L		
C	0	6.79893100	-0.03542600	-0.99695500	L		
H	0	7.20069900	0.95332300	-1.26568400	L		
H	0	5.70833000	0.03172900	-1.07451100	L		
H	0	7.12879200	-0.74282500	-1.77444700	L		
C	0	6.99241100	-2.34362800	2.18732400	L		
H	0	6.76398100	-1.60245700	2.96893100	L		
H	0	8.06569900	-2.56247200	2.26361500	L		
H	0	6.45926900	-3.26724500	2.44110400	L		
C	0	9.55485100	-1.36772500	-1.83096100	L		
H	0	8.53160100	-1.30523400	-2.27642200	L		
H	0	10.06286600	-2.17629600	-2.39314500	L		
C	0	9.74577400	1.12184400	-1.22623400	L		
H	0	8.72856900	1.37782200	-1.64979900	L		
C	0	9.56566800	0.73329500	0.25030500	L		
H	0	9.04049500	1.56271900	0.77162600	L		
H	0	10.56239500	0.67405800	0.73532700	L		

C	0	10.86963800	-2.03070100	0.19191400	L
H	0	10.86598900	-2.29859900	1.25440800	L
H	0	11.52947200	-1.16330200	0.08458000	L
H	0	11.33898100	-2.86092000	-0.34736300	L
C	0	10.64932600	2.34485700	-1.36423300	L
H	0	10.21890600	3.21899200	-0.86131500	L
H	0	10.80064700	2.61105000	-2.41801500	L
H	0	11.64156800	2.17399700	-0.92942600	L
C	0	10.26052000	-0.05562300	-2.03841100	L
O	0	11.16341500	0.04713600	-2.85238900	L
C	0	-7.28740000	1.33539900	0.45223000	L
C	0	-5.85356700	1.86678100	0.50470200	L H 11 0.0000
H	0	-5.87285700	2.90812300	0.89068000	L
H	0	-5.28063800	1.28508100	1.25979300	L
H	0	-7.93421300	2.03249100	-0.11533500	L
H	0	-7.70078300	1.32647400	1.48299000	L
C	0	-6.96319700	-1.41989800	-2.26204200	L
H	0	-6.31435700	-2.12268800	-1.70133000	L
H	0	-6.57557400	-1.41566500	-3.30077800	L
C	0	-8.40410300	-1.93065600	-2.27378900	L
H	0	-8.42452600	-2.95865600	-2.68662800	L
H	0	-8.99533200	-1.32413700	-2.99242300	L
C	0	-8.86094800	-0.57215100	-0.13806600	L
H	0	-9.44016100	0.20733900	-0.70292700	L
C	0	-6.86501200	0.00036100	-1.64835800	L H 12 0.0000
C	0	-7.37216100	-0.08813100	-0.15869700	L
C	0	-7.70765100	0.95409600	-2.51749500	L
H	0	-7.30031800	1.02788700	-3.53256300	L
H	0	-7.75081100	1.97333600	-2.10283900	L
H	0	-8.74524700	0.60766300	-2.61191800	L
C	0	-6.46547700	-1.02953800	0.65424200	L
H	0	-5.43239600	-0.66765100	0.70834600	L
H	0	-6.42066500	-2.03714700	0.21667200	L
H	0	-6.82148200	-1.13383600	1.68517600	L
C	0	-8.63356100	-3.12914200	-0.06719500	L
H	0	-7.53826700	-3.27708900	-0.22170100	L
H	0	-9.09359600	-4.06298900	-0.45578900	L
C	0	-9.43267600	-0.58092900	1.29974100	L
H	0	-10.30334200	0.10462600	1.34060000	L
H	0	-8.69392100	-0.13817200	2.00318100	L
C	0	-9.87857600	-1.94930800	1.84427300	L
H	0	-10.86996800	-2.21254800	1.36738800	L
C	0	-9.11283300	-1.91293500	-0.89447400	L
C	0	-10.62581800	-2.05756500	-1.17804900	L
H	0	-11.01843300	-1.20140600	-1.73720000	L
H	0	-11.21588100	-2.13343200	-0.25369600	L
H	0	-10.84107700	-2.95552800	-1.76769800	L
O	0	-8.90133400	-3.02586500	1.40887900	L
C	0	-8.36556100	-3.79548300	2.19002500	L
C	0	-10.06361100	-1.91152300	3.35827300	L
H	0	-9.13042300	-1.66587200	3.87945200	L
H	0	-10.40255200	-2.88153200	3.74299800	L
H	0	-10.80998400	-1.16272600	3.65024100	L
H	0	-1.12446400	4.58829100	2.92703900	H
O	0	-0.37913800	4.39175300	3.51418000	H
H	0	-0.23682700	3.44504100	3.36819000	H

Gibbs Free Energy= -1376.862759 Hartrees

TS2

C	0	3.18845500	2.58077700	-1.19534500	H
C	0	1.04296700	3.08761600	0.02155900	H
C	0	2.76840100	1.65322500	1.03970500	H
C	0	1.26937000	1.79736000	0.81692400	H
C	0	3.66002200	1.99526400	-0.05981400	H
C	0	1.84027800	3.10793300	-1.29186600	H
H	0	3.84335900	2.79700400	-2.03570200	H
O	0	1.44660700	3.69841300	-2.29678500	H
C	0	3.27080300	1.06506500	2.14829700	H

H	0	2.60440800	0.80298100	2.96261500	H		
C	0	5.19509900	1.81404800	0.13396600	H		
C	0	5.56762700	0.89283700	1.31849600	H		
C	0	4.65085000	0.65178800	2.27584400	H		
H	0	4.90142000	0.07671900	3.16054400	H		
C	0	5.67017100	3.23086600	0.47876300	L H 27	0.0000	
H	0	5.36429100	3.96772900	-0.27532400	L		
H	0	6.77181300	3.28236000	0.53049400	L		
H	0	5.28659300	3.57303200	1.44843600	L		
O	0	1.00564100	4.18807100	0.62984100	H		
H	0	-0.56646500	5.08860900	0.51692300	H		
C	0	0.44448800	1.80035200	2.09394000	H		
H	0	-0.59463200	2.05054600	1.87301500	H		
H	0	0.83577400	2.54977300	2.78232300	H		
H	0	0.47207900	0.81638700	2.56689200	H		
O	0	0.96289000	0.66258800	-0.02546700	H		
O	0	-0.59396600	2.79092700	-0.63596600	H		
C	0	-0.35929400	0.45836800	-0.32764600	H		
C	0	-1.15087400	1.56958600	-0.64790800	H		
C	0	-2.49288700	1.38954900	-0.96102400	H		
H	0	-3.08523500	2.26684100	-1.21003600	H		
C	0	-3.05424900	0.11276000	-0.98340300	H		
C	0	-2.24090200	-0.99787300	-0.69636500	H		
C	0	-0.87995700	-0.83092900	-0.33487400	H		
C	0	0.02630100	-1.96800200	0.06737900	H		
H	0	0.28299600	-2.58954900	-0.79331000	H		
H	0	-0.46917000	-2.62348500	0.78430500	H		
H	0	0.94129000	-1.56903500	0.50357900	H		
C	0	-4.53383600	-0.03042000	-1.42630300	H		
C	0	-2.84423700	-2.34949800	-0.75877200	H		
O	0	-2.18073600	-3.38366200	-0.74017000	H		
C	0	-4.30811300	-2.44455300	-0.80882300	H		
H	0	-4.68018700	-3.44958600	-0.63522200	H		
C	0	-5.12690300	-1.41187700	-1.06586700	H		
C	0	-4.51254500	0.09963000	-2.95176000	L H 38	0.0000	
H	0	-3.98948800	1.00789700	-3.27859600	L		
H	0	-5.53207300	0.16006500	-3.36824100	L		
H	0	-4.01492000	-0.75210200	-3.43200500	L		
H	0	-1.10318700	5.35567000	-0.97794100	H		
O	0	-1.38600100	4.98522000	-0.02626100	H		
H	0	-1.25837200	3.94279400	-0.24383300	H		
C	0	-5.35125900	1.10796700	-0.79381200	L H 38	0.0000	
H	0	-5.10727100	2.06814600	-1.29588600	L		
H	0	-5.03825500	1.24446600	0.26392700	L		
C	0	-6.86560700	0.89866800	-0.84433800	L		
H	0	-7.36569800	1.73289800	-0.30844100	L		
H	0	-7.22557400	0.96681300	-1.88983000	L		
C	0	-6.64250200	-1.60668400	-1.07513800	L H 43	0.0000	
C	0	-7.29454600	-0.45352900	-0.21925500	L		
C	0	-8.84974400	-0.58299900	-0.28986500	L		
H	0	-9.10535600	-0.46457500	-1.38030000	L		
C	0	-9.41820300	-1.97369800	0.12759300	L		
C	0	-8.60083500	-3.13584200	-0.48888500	L		
H	0	-8.86789300	-4.08578400	0.01485400	L		
H	0	-8.91512700	-3.27606500	-1.54535700	L		
C	0	-7.08260200	-2.95426700	-0.44635700	L		
H	0	-6.60712800	-3.79855400	-0.98545300	L		
H	0	-6.72053800	-3.02395000	0.59858200	L		
C	0	-6.76451100	-0.51860500	1.22327300	L		
H	0	-7.16405100	0.30621800	1.83259100	L		
H	0	-5.67225000	-0.45062300	1.27129700	L		
H	0	-7.04568800	-1.45906900	1.72333200	L		
C	0	-7.09129800	-1.59884900	-2.54931100	L		
H	0	-6.90956100	-0.62884300	-3.03781000	L		
H	0	-8.16476800	-1.80667300	-2.64892500	L		
H	0	-6.56211700	-2.36503500	-3.12755800	L		
C	0	-9.45831700	-2.13229100	1.66682200	L		
H	0	-8.41451000	-2.19740300	2.06136800	L		
H	0	-9.92758800	-3.09835200	1.93961600	L		
C	0	-9.70906300	0.40746600	1.96187900	L		
H	0	-8.67438500	0.53229100	2.40146500	L		
C	0	-9.59998300	0.55237200	0.43511900	L		
H	0	-9.11245400	1.52500100	0.20741900	L		
H	0	-10.61939800	0.63336700	0.00341100	L		
C	0	-10.86558700	-2.10055200	-0.40182000	L		
H	0	-10.91225000	-1.98792500	-1.49074100	L		
H	0	-11.52958700	-1.34198800	0.02592000	L		
H	0	-11.29677700	-3.07856800	-0.16118200	L		

C	0	-10.61790200	1.48448000	2.54939700	L		
H	0	-10.22495800	2.48941500	2.35371900	L		
H	0	-10.71575900	1.37525800	3.63666000	L		
H	0	-11.62979600	1.44241900	2.12852100	L		
C	0	-10.16781800	-0.99104000	2.34235800	L		
O	0	-11.02973400	-1.19903000	3.18048900	L		
C	0	7.24294200	0.80176400	-1.05048300	L		
C	0	5.81506000	1.33459600	-1.18586300	L	H 27	0.0000
H	0	5.81081100	2.16094800	-1.92776800	L		
H	0	5.17361300	0.54073100	-1.62716900	L		
H	0	7.94158500	1.63059100	-0.82422000	L		
H	0	7.56863500	0.40452200	-2.03490100	L		
C	0	7.11390300	-0.77412400	2.49392700	L		
H	0	6.41190600	-1.60349000	2.27411800	L		
H	0	6.81325800	-0.38081500	3.48597500	L		
C	0	8.54425600	-1.30605600	2.58541300	L		
H	0	8.58466900	-2.11907100	3.33704700	L		
H	0	9.19907100	-0.50758500	2.99472900	L		
C	0	8.84041700	-0.82415400	0.07516600	L		
H	0	9.47248600	0.08286900	0.27466100	L		
C	0	6.98328800	0.33365900	1.41733000	L	H 26	0.0000
C	0	7.36339100	-0.30664100	0.02844700	L		
C	0	7.90947200	1.49908000	1.81745700	L		
H	0	7.59065600	1.94940700	2.76464300	L		
H	0	7.92914300	2.29857600	1.06052000	L		
H	0	8.94675700	1.16603100	1.95263000	L		
C	0	6.38334000	-1.44195900	-0.31835600	L		
H	0	5.35281400	-1.08337500	-0.42063800	L		
H	0	6.36792400	-2.22310100	0.45522700	L		
H	0	6.65013200	-1.92296200	-1.26593300	L		
C	0	8.58721900	-3.22488500	0.95010100	L		
H	0	7.50472600	-3.26512500	1.21908500	L		
H	0	9.06377000	-3.97194400	1.62054600	L		
C	0	9.28979000	-1.37298700	-1.30005000	L		
H	0	10.15329900	-0.77541400	-1.65633800	L		
H	0	8.49415800	-1.19604900	-2.05654600	L		
C	0	9.68996200	-2.85825900	-1.34018700	L		
H	0	10.71412600	-2.95998700	-0.87084700	L		
C	0	9.14052800	-1.81082000	1.24553400	L		
C	0	10.67013300	-1.89870500	1.45413000	L		
H	0	11.11273400	-0.91374900	1.63769300	L		
H	0	11.18480000	-2.32206000	0.57984400	L		
H	0	10.92388000	-2.53272200	2.31082700	L		
C	0	8.74455300	-3.67305600	-0.47650400	L		
O	0	8.14800800	-4.65654900	-0.88477600	L		
C	0	9.75987200	-3.37585200	-2.77374000	L		
H	0	8.78010100	-3.35106800	-3.26624400	L		
H	0	10.11200900	-4.41414400	-2.80718500	L		
H	0	10.44932500	-2.77688900	-3.38119600	L		
H	0	-0.12617500	6.29844600	-2.47338400	H		
O	0	-0.56511300	5.45797700	-2.29253000	H		
H	0	0.14118100	4.75982400	-2.32278400	H		

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2-wt-b pathway

TS

C	0	2.64039300	2.81965200	-0.72851700	H		
C	0	0.53628600	2.35691700	0.52276500	H		
C	0	2.74307000	1.77499200	1.48183500	H		
C	0	1.27498700	1.77254700	1.60241900	H		
C	0	3.37390200	2.23817300	0.25614800	H		
C	0	1.21121200	2.99619900	-0.64347900	H		
H	0	3.10901400	3.21344400	-1.62584000	H		
O	0	0.56539800	3.68908000	-1.43232600	H		
C	0	3.50780400	1.18662500	2.43995800	H		

H	0	3.03931200	0.81961700	3.34615000	H		
C	0	4.92092200	2.18584900	0.13009200	H		
C	0	5.59921800	1.27999000	1.18232900	H		
C	0	4.91007900	0.90747900	2.28236000	H		
H	0	5.37775800	0.33042900	3.07199500	H		
C	0	5.36422200	3.62989900	0.38784400	L H 11	0.0000	
H	0	4.83059400	4.34854000	-0.24799700	L		
H	0	6.43728900	3.76755300	0.16965700	L		
H	0	5.20344100	3.93280700	1.43036500	L		
O	0	-0.75331600	2.34489500	0.62628500	H		
H	0	-1.22247700	2.50219000	-0.29313900	H		
C	0	0.61107900	1.85769000	2.95271400	H		
H	0	-0.42482000	1.52241800	2.87241300	H		
H	0	0.60988000	2.89779000	3.29006700	H		
H	0	1.12174400	1.25066900	3.69729800	H		
O	0	0.98485400	-0.01336000	1.20251000	H		
O	0	0.21264000	0.48104500	-1.27832200	H		
C	0	-0.21107200	-0.37650300	0.86901400	H		
C	0	-0.59983500	-0.11372800	-0.51007500	H		
C	0	-1.93166900	-0.47015700	-0.89122500	H		
H	0	-2.21556300	-0.29665600	-1.92690400	H		
C	0	-2.80153200	-1.05510400	-0.00972100	H		
C	0	-2.39231500	-1.31901300	1.34840400	H		
C	0	-1.12239300	-0.97539000	1.79839000	H		
C	0	-0.60455400	-1.27316800	3.18136800	H		
H	0	-0.64107600	-2.34546500	3.37727400	H		
H	0	-1.22534700	-0.80108100	3.94598600	H		
H	0	0.42185300	-0.92201300	3.27120500	H		
C	0	-4.18547600	-1.53278100	-0.53470600	H		
C	0	-3.38359300	-1.91977700	2.27732400	H		
O	0	-3.08816800	-2.34059700	3.39264400	H		
C	0	-4.78885000	-1.94549300	1.85974000	H		
H	0	-5.47333100	-2.18208400	2.66843900	H		
C	0	-5.21368500	-1.73385800	0.60371200	H		
C	0	-3.91190400	-2.89654000	-1.17308900	L H 38	0.0000	
H	0	-3.12020100	-2.84389300	-1.93226900	L		
H	0	-4.80766600	-3.29060000	-1.68356800	L		
H	0	-3.60409400	-3.64756700	-0.43462700	L		
H	0	-1.35067900	3.25398500	-2.01739600	H		
O	0	-1.75849200	2.43616400	-1.69055200	H		
H	0	-1.13334500	1.74757600	-1.99356200	H		
C	0	-4.69217900	-0.53096500	-1.58415900	L H 38	0.0000	
H	0	-4.10510300	-0.64021900	-2.52107600	L		
H	0	-4.49525400	0.50529600	-1.23261800	L		
C	0	-6.17818800	-0.66469200	-1.91882600	L		
H	0	-6.46329000	0.13583300	-2.63415100	L		
H	0	-6.36643700	-1.61459200	-2.45649300	L		
C	0	-7.07104400	-0.57727500	-0.65506600	L		
C	0	-6.70437700	-1.79605800	0.27444200	L H 43	0.0000	
C	0	-7.60489500	-1.70219000	1.53345300	L		
H	0	-7.40547800	-0.75604300	2.07475200	L		
H	0	-7.34997700	-2.51321300	2.24591300	L		
C	0	-9.09037700	-1.80496000	1.18342100	L		
H	0	-9.69044100	-1.67929300	2.10634500	L		
H	0	-9.30719900	-2.83997600	0.84322900	L		
C	0	-8.57119900	-0.69023500	-1.07580400	L		
H	0	-8.64596300	-1.66326300	-1.63860300	L		
C	0	-9.58287900	-0.80822400	0.10483800	L		
C	0	-9.85577300	0.56761000	0.75954700	L		
H	0	-8.93818700	0.91292900	1.29681500	L		
H	0	-10.62863400	0.46967500	1.54743600	L		
C	0	-9.34659300	1.76743700	-1.45464600	L		
H	0	-8.38378000	2.22091200	-1.07200300	L		
C	0	-9.01891800	0.39805600	-2.07169900	L		
H	0	-9.90666500	0.02628300	-2.62488300	L		
H	0	-8.23432700	0.53878600	-2.84647300	L		
C	0	-10.92496500	-1.34939900	-0.44022000	L		
H	0	-10.80327200	-2.32100000	-0.93194700	L		
H	0	-11.37396800	-0.67372600	-1.17608800	L		
H	0	-11.65886800	-1.48537900	0.36169200	L		
C	0	-9.94403000	2.70770300	-2.49873100	L		
H	0	-9.24599800	2.88210100	-3.32619300	L		
H	0	-10.18933100	3.68387800	-2.06249000	L		
H	0	-10.86949500	2.30665300	-2.92993100	L		
C	0	-10.25560700	1.61305800	-0.24563900	L		
O	0	-11.23249100	2.31948900	-0.05904500	L		
C	0	-6.76354600	0.74024900	0.07643900	L		
H	0	-5.71930500	0.80617700	0.40040600	L		

H	0	-7.38241800	0.86417700	0.97958100	L		
H	0	-6.95589000	1.60972200	-0.57021200	L		
C	0	-6.95057300	-3.16389200	-0.39275700	L		
H	0	-6.38665900	-3.28082600	-1.33133300	L		
H	0	-8.01016600	-3.30956000	-0.64070200	L		
H	0	-6.66081900	-3.98618400	0.27143500	L		
C	0	5.27154900	1.73295800	-1.29299400	L	H 11	0.0000
H	0	5.01673000	2.52994400	-2.02081900	L		
H	0	4.62205300	0.86197900	-1.55714900	L		
C	0	6.73766500	1.33797500	-1.48008100	L		
H	0	7.39001200	2.22883900	-1.39847300	L		
H	0	6.87764500	0.96556600	-2.51675800	L		
C	0	7.18828100	0.25042600	-0.46896700	L		
C	0	7.05123600	0.85776300	0.98035700	L	H 12	0.0000
C	0	6.26697100	-0.97255500	-0.62230800	L		
H	0	6.41797200	-1.46682100	-1.58768700	L		
H	0	5.20325100	-0.69587800	-0.57212100	L		
H	0	6.43809800	-1.72053300	0.16382000	L		
C	0	7.93130400	2.10369000	1.19967400	L		
H	0	9.00092500	1.85783200	1.15981600	L		
H	0	7.74301500	2.55296100	2.18178700	L		
H	0	7.75741900	2.88047500	0.43889600	L		
C	0	7.50687300	-0.22904800	1.98795500	L		
H	0	6.85487800	-1.12244000	1.90474200	L		
H	0	7.38685400	0.13778700	3.02703700	L		
C	0	8.96732000	-0.62500800	1.76763900	L		
H	0	9.61775000	0.23415000	2.03812100	L		
H	0	9.24121800	-1.42582400	2.48247600	L		
C	0	8.68395200	-0.12468700	-0.73867000	L		
H	0	9.25800700	0.83710300	-0.65625400	L		
C	0	9.30727200	-1.08062600	0.32472700	L		
C	0	10.84792400	-1.03757700	0.20237100	L		
H	0	11.33069600	-1.64371800	0.97675900	L		
H	0	11.23521200	-0.01773700	0.30064600	L		
H	0	11.19756900	-1.41975800	-0.76713000	L		
C	0	8.88967600	-0.62880100	-2.18693500	L		
H	0	9.62560200	0.02948200	-2.69154400	L		
H	0	7.95106700	-0.49825200	-2.76901800	L		
C	0	9.37078500	-2.08284900	-2.33726000	L		
H	0	10.47655000	-2.11323300	-2.10119500	L		
C	0	8.82409100	-2.53735500	0.13074000	L		
H	0	9.50194400	-3.24092200	0.66028200	L		
H	0	7.83874800	-2.67511800	0.63534900	L		
O	0	8.69458600	-2.96582100	-1.30444200	L		
C	0	8.09246800	-3.98784500	-1.59269500	L		
C	0	9.16438700	-2.59214900	-3.76064500	L		
H	0	9.52795700	-3.62110300	-3.87276900	L		
H	0	9.70216300	-1.97191700	-4.48792700	L		
H	0	8.10575100	-2.59156900	-4.04768700	L		
H	0	2.87934600	-0.62558000	0.13272300	H		
O	0	2.94886100	-0.51483500	-0.82369100	H		
H	0	2.10202700	-0.07717400	-1.02052000	H		

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IV. Non-water HDA Case

TS

C	0	-2.41911600	-0.44233500	2.48925300	H		
C	0	-0.45799500	0.98044200	1.93112500	H		
C	0	-2.70043400	1.73908700	1.38857900	H		
C	0	-1.25952900	2.04146200	1.44937600	H		
C	0	-3.23500900	0.49792500	1.94763700	H		
C	0	-0.98379500	-0.25792400	2.53951300	H		
H	0	-2.80495700	-1.35533100	2.93204200	H		
O	0	-0.17405500	-1.01285300	3.08015300	H		
C	0	-3.53403200	2.57657300	0.71802000	H		
H	0	-3.12354500	3.47391600	0.26660800	H		
C	0	-4.77935800	0.35856600	2.05221700	H		
C	0	-5.54347200	1.22371900	1.02083900	H		
C	0	-4.92338300	2.28881800	0.47037500	H		

H	0	-5.44966700	2.96218300	-0.19727200	H		
C	0	-5.09651300	0.91544400	3.44623400	L H 11	0.0000	
H	0	-4.51925700	0.41088300	4.23204300	L		
H	0	-6.16123300	0.77527900	3.70080400	L		
H	0	-4.88439200	1.98960900	3.52243700	L		
C	0	-5.16205500	-1.12577000	1.95926700	L H 11	0.0000	
H	0	-4.87576700	-1.64710800	2.89726100	L		
H	0	-4.56340700	-1.61284700	1.15889500	L		
C	0	-6.64627200	-1.37945500	1.69051400	L		
H	0	-7.24834600	-1.09966100	2.57708700	L		
H	0	-6.81009400	-2.47024800	1.55973800	L		
C	0	-7.00717200	0.92201200	0.71760600	L H 12	0.0000	
C	0	-7.15552100	-0.62248700	0.43717400	L		
C	0	-7.52766700	1.67330300	-0.53494400	L		
H	0	-7.39690800	2.76700200	-0.40564100	L		
H	0	-6.92058500	1.40292100	-1.42157800	L		
C	0	-8.66473200	-0.95776900	0.21234000	L		
H	0	-9.17470900	-0.67737800	1.17688900	L		
C	0	-9.37138800	-0.11936000	-0.89627600	L		
C	0	-9.00549100	1.38264800	-0.80106400	L		
H	0	-9.61369000	1.85172800	0.00130500	L		
H	0	-9.31615500	1.89984200	-1.73045300	L		
C	0	-7.82229000	1.39706000	1.93708500	L		
H	0	-7.53966200	0.86980500	2.86159000	L		
H	0	-8.89837700	1.23281300	1.79547300	L		
H	0	-7.68087700	2.46964300	2.11343600	L		
C	0	-6.28148300	-1.01523400	-0.76580100	L		
H	0	-5.22776600	-0.75374800	-0.62110400	L		
H	0	-6.60671100	-0.51504800	-1.69197100	L		
H	0	-6.32119200	-2.09934000	-0.95082400	L		
C	0	-9.02662500	-0.64399600	-2.31101400	L		
H	0	-7.95037100	-0.43799100	-2.53262400	L		
H	0	-9.58960500	-0.07572800	-3.07747800	L		
C	0	-8.94342400	-2.46207400	0.01996200	L		
H	0	-8.34540600	-3.04729700	0.75178800	L		
H	0	-10.00189900	-2.66148600	0.28847400	L		
C	0	-8.66758300	-3.01472600	-1.38808700	L		
C	0	-9.28223600	-2.11951700	-2.45193900	L		
C	0	-10.90199800	-0.23077300	-0.70678900	L		
H	0	-11.21621800	0.11777500	0.28337200	L		
H	0	-11.25657700	-1.26201400	-0.80812100	L		
H	0	-11.44273800	0.37011900	-1.44624200	L		
C	0	-9.15037800	-4.45794000	-1.51380400	L		
H	0	-8.64238600	-5.11319900	-0.79625000	L		
H	0	-8.95888500	-4.85593500	-2.51822300	L		
H	0	-10.22838500	-4.54709800	-1.33244700	L		
O	0	0.84329800	1.17070000	2.02282500	H		
H	0	1.20871100	0.34887300	2.41651400	H		
C	0	-0.79917500	3.44852500	1.75597500	H		
H	0	0.27174800	3.54241000	1.56819700	H		
H	0	-0.99464500	3.67138800	2.80882600	H		
H	0	-1.32824500	4.17716000	1.14227800	H		
H	0	-7.55022400	-2.99349700	-1.56169700	L		
O	0	-9.91331700	-2.55678400	-3.40001700	L		
O	0	-0.78408900	2.14046200	-0.39871200	H		
C	0	-0.47855700	-0.36238400	0.10446100	H		
O	0	0.35160100	1.63386700	-0.70851600	H		
C	0	0.49844600	0.20971700	-0.44789500	H		
C	0	1.77302900	-0.39589300	-0.68455800	H		
H	0	1.86698100	-1.45786700	-0.47100900	H		
C	0	2.80712400	0.32741500	-1.21472500	H		
C	0	2.63515400	1.73569500	-1.49196200	H		
C	0	1.45850600	2.40834600	-1.19148700	H		
C	0	1.22924100	3.88331600	-1.38597800	H		
H	0	1.19270600	4.13771600	-2.44722800	H		
H	0	2.04615700	4.46582200	-0.95704300	H		
H	0	0.28568500	4.16366700	-0.91852400	H		
C	0	4.12663400	-0.40989500	-1.58344600	H		
C	0	3.78909500	2.48043600	-2.06501600	H		
O	0	3.67751500	3.60260200	-2.54916100	H		
C	0	5.11280700	1.85763800	-1.99418100	H		
H	0	5.92569900	2.54632800	-2.20245900	H		
C	0	5.32567200	0.55694300	-1.73463400	H		
C	0	4.40133000	-1.48501400	-0.51965300	L H 81	0.0000	
H	0	3.69344400	-2.33114300	-0.65076100	L		
H	0	4.18144200	-1.07294900	0.48956000	L		
C	0	6.75028700	0.00644200	-1.68630000	L H 86	0.0000	
C	0	5.82799500	-2.03547300	-0.52718100	L		

H	0	6.00211900	-2.63612200	-1.44147200	L
H	0	5.94645600	-2.74842400	0.31638300	L
C	0	6.89024700	-0.91257600	-0.41334300	L
C	0	3.85848500	-1.04968900	-2.94708000	L H 81 0.0000
H	0	2.95459600	-1.67341900	-2.93745000	L
H	0	4.68806200	-1.70865400	-3.25581500	L
H	0	3.72684300	-0.30173400	-3.73902300	L
C	0	7.82370300	1.11996800	-1.57325700	L
H	0	7.64887200	1.72677700	-0.66260600	L
H	0	7.73274900	1.82485700	-2.42478000	L
C	0	8.31526500	-1.55262500	-0.39814000	L
H	0	8.37092300	-2.16787300	-1.33999600	L
C	0	9.24172200	0.54710000	-1.55899500	L
H	0	9.46839800	0.12508000	-2.56132500	L
H	0	9.96703700	1.37459400	-1.42975300	L
C	0	9.49777400	-0.54013100	-0.48612300	L
C	0	6.98088600	-0.74931700	-3.00969700	L
H	0	6.29903100	-1.60575300	-3.12911100	L
H	0	8.00209900	-1.14704000	-3.07712300	L
H	0	6.83697500	-0.08928900	-3.87285300	L
C	0	6.60371100	-0.08689100	0.85214200	L
H	0	6.64076600	-0.71478000	1.75524500	L
H	0	5.61506000	0.38423400	0.83130300	L
H	0	7.33699600	0.72388000	0.98973600	L
C	0	9.76825800	0.13726000	0.87890100	L
H	0	8.91740900	0.81684600	1.13223800	L
H	0	10.65265300	0.80059700	0.80751000	L
C	0	8.53487800	-2.54770900	0.75897900	L
H	0	7.63482100	-3.19018900	0.87239700	L
H	0	9.35186700	-3.24348200	0.47491000	L
C	0	9.94405100	-0.86086400	1.99060600	L
C	0	8.86056000	-1.91913200	2.12381800	L
H	0	7.93655300	-1.38127800	2.49287200	L
C	0	10.77763900	-1.30164400	-0.90172200	L
H	0	11.06385900	-2.06032500	-0.16536900	L
H	0	11.63075000	-0.62332500	-1.01259700	L
H	0	10.65176400	-1.81823400	-1.85978000	L
O	0	10.88623200	-0.77845500	2.76115900	L
C	0	9.23617700	-2.99211800	3.14328600	L
H	0	8.41926000	-3.70923600	3.28810200	L
H	0	9.46440900	-2.55140900	4.12153100	L
H	0	10.12085400	-3.56096200	2.83223500	L

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