Electronic Supplementary Material (ESI) for RSC Advances.

Influence of the double bond on the hydrogen abstraction reactions of methyl esters with hydrogen radical: an *ab initio* and chemical kinetic study

Quan-De Wang[a,*], Weidong Zhang[b]

[a]Low Carbon Energy Institute, China University of Mining and Technology, Xuzhou 221008, Jiangsu, People's Republic of China

[b]Wuhan Institute of Marine Electric Propulsion, CSIC, Wuhan 430064, Hubei, People's Republic of China

*Corresponding author. Email address: wqd198686@126.com (Q.-D. Wang)

Optimized geometries and vibrational frequenices at the B3LYP/6-311G(2d,d,p) level for all the stationary points on the potential energy surfaces.

Optimized geometries at the B3LYP/6-311G(2d,d,p) level.

(1)methyl valerate

C	-0.09614800	-0.64997200	-0.00000800
C	1.19845500	0.13471200	-0.00000500
O	2.26355400	-0.69887800	0.00000600
O	1.29859100	1.33591200	-0.00001300
C	-1.34252900	0.23408800	0.00001100
C	3.55336700	-0.06200400	0.00000700
C	-2.64416000	-0.57462100	-0.00001100
C	-3.89486500	0.30859300	0.00000900
H	-0.08056400	-1.31385300	-0.87174700
H	-0.08055500	-1.31388000	0.87171100
H	-1.31556900	0.89432500	0.87294500
H	-1.31556400	0.89436600	-0.87289200
H	3.67400700	0.56081700	-0.88787800
H	3.67398000	0.56087100	0.88785800
H	4.27877500	-0.87261900	0.00004200
H	-2.66288600	-1.23424200	0.87627700
H	-2.66288300	-1.23419800	-0.87633200
H	-3.92123500	0.95489700	-0.88261700
H	-3.92124000	0.95484800	0.88267000
H	-4.80813900	-0.29238300	-0.00001000

TS at α'

C	0.15900500	-0.64043300	-0.00839800
C	-1.12765500	0.14724400	-0.07326000
O	-2.20248300	-0.70201400	-0.09554800
O	-1.23704400	1.34299500	-0.10671100
C	1.40932700	0.23824300	-0.01808200
C	-3.47557900	-0.12357300	-0.12191000
C	2.70556900	-0.57572500	0.05654600
C	3.96057300	0.30120600	0.04704000
H	0.11740600	-1.26209100	0.89340300
H	0.15974800	-1.34535900	-0.84742000
H	1.40980600	0.85470100	-0.92294900
H	1.36221800	0.93975700	0.82096100
H	-3.83457500	0.16323700	1.11923900
H	-3.51156600	0.83501000	-0.63459500
H	-4.19472200	-0.86835700	-0.45003600
H	2.74399300	-1.27751500	-0.78560000
H	2.69678000	-1.19118200	0.96444300
H	3.96614300	0.99107200	0.89634100
H	4.01563800	0.90151700	-0.86616700
H	4.86962600	-0.30332700	0.10326300
H	-4.07172300	0.35291800	2.03557200

TS at α

C	2.63946000	-0.54209600	-0.00234500

H	2.65772900	-1.07944600	0.95267400
H	2.65452600	-1.30966200	-0.78536500
C	1.33961000	0.26390600	-0.10361700
H	1.30581500	1.03533300	0.67146100
H	1.31874600	0.80466200	-1.05964100
C	0.09009100	-0.58725800	-0.00591000
H	0.13009600	-1.17931300	1.10033900
H	0.04846600	-1.42863300	-0.69898800
C	-1.20419100	0.16049700	0.03892900
O	-2.24845900	-0.65919200	-0.21730800
O	-1.32443300	1.33393100	0.29933300
C	-3.54942300	-0.04982200	-0.14229400
H	-3.72631700	0.35377900	0.85598800
H	-3.63670100	0.75732700	-0.87138100
H	-4.25684300	-0.84550000	-0.36481400
H	0.22262900	-1.66524500	2.01259800
C	3.88941200	0.33378300	-0.12069700
H	4.80162500	-0.26322000	-0.04177500
H	3.91659000	0.85776300	-1.08107100
H	3.91700400	1.09018000	0.66938100

TS at β

C	2.63406100	-0.56901100	-0.15955100
H	2.67784500	-1.43785200	0.50878900
H	2.67854900	-0.97633500	-1.18074100
C	1.31052100	0.14339800	0.02198200
H	1.28423500	0.51871300	1.28852000
H	1.24441500	1.10561600	-0.48732700
C	0.06696400	-0.69674600	-0.16047200
H	0.00192400	-1.49663900	0.58279600
H	0.09039900	-1.20234600	-1.13753300
C	-1.21485200	0.11234500	-0.12466600
O	-2.27548900	-0.68178900	0.13156300
O	-1.30185400	1.29798800	-0.32118800
C	-3.55688600	-0.02563800	0.14603500
H	-3.57796800	0.75299300	0.90977300
H	-3.76808500	0.42376100	-0.82561800
H	-4.28023500	-0.80556500	0.37283400
H	1.26001300	0.70965300	2.23280800
C	3.84829800	0.33269400	0.08092500
H	4.78195900	-0.21402700	-0.07306100
H	3.84456500	1.18738200	-0.60188800
H	3.85249500	0.72280900	1.10214000

TS at γ

C	2.59871200	-0.45000800	-0.16549100
H	2.63138700	-1.32729600	0.81777300
H	2.61440400	-1.11142700	-1.03632800

C	1.29048400	0.29533400	-0.00421400
H	1.27144400	0.80855700	0.96294400
H	1.22781600	1.09214800	-0.75719300
C	0.06313600	-0.60749400	-0.12795600
H	0.07078800	-1.39344700	0.63392200
H	0.05297800	-1.13090300	-1.09066100
C	-1.24303500	0.14760500	-0.00489100
O	-2.29330600	-0.69888800	-0.07765800
O	-1.35905400	1.33928200	0.13605300
C	-3.59352100	-0.09077100	0.02377100
H	-3.70249700	0.42332100	0.98000700
H	-3.74515700	0.62716600	-0.78385000
H	-4.30482600	-0.91000100	-0.05361800
H	2.66404100	-1.93617200	1.57048400
C	3.86212200	0.36782800	-0.01596200
H	3.87372300	0.90938700	0.93452000
H	4.75459600	-0.26141100	-0.05857600
H	3.94279400	1.11196000	-0.81812800

TS at δ

C	2.57282800	-0.62974400	-0.09017000
H	2.56007200	-1.27557900	-0.98176600
C	1.28226600	0.19713600	-0.04831700
H	1.28932800	0.84675100	0.83214500
H	1.24055900	0.86496200	-0.91396000
C	0.02745900	-0.67450900	-0.02511800
H	0.00440000	-1.32196300	0.85744500
H	0.00439100	-1.35225900	-0.88705800
C	-1.25707100	0.12672600	-0.05094100
O	-2.32744000	-0.67849800	0.13062500
O	-1.34367000	1.31720600	-0.21820800
C	-3.60987200	-0.02644700	0.10389900
H	-3.67278400	0.72730200	0.89027900
H	-3.77572200	0.45442300	-0.86153900
H	-4.34093000	-0.81471800	0.26933600
C	3.82507700	0.21263900	-0.11350200
H	3.89282100	0.86355500	1.08952200
H	4.76615500	-0.33589200	-0.11382200
H	3.82591800	1.04136900	-0.82174600
H	2.60697400	-1.31313200	0.76751000
H	3.92358000	1.27070900	1.91920800

(2)methyl-2-pentenoate

C	-3.64656900	0.15116000	0.62888100
C	-2.69407100	-0.39538700	-0.44885300
H	-4.65133600	-0.25908600	0.50118300
H	-3.71931500	1.24098400	0.57534300
H	-3.29631400	-0.11179500	1.63009200

C	-1.31687700	0.18134100	-0.34235000
H	-3.10110100	-0.14443800	-1.43699400
H	-2.64880200	-1.48716600	-0.39372000
C	-0.19365600	-0.51656300	-0.16141700
C	1.11661900	0.16425800	-0.06541500
O	1.30995800	1.35596000	-0.13494700
O	2.10955700	-0.73944200	0.11642400
C	3.43288300	-0.19082700	0.22373200
H	4.09218900	-1.04406600	0.36811800
H	3.49764600	0.49268900	1.07210900
H	3.69897000	0.35046300	-0.68589200
H	-1.22634000	1.26442300	-0.40893200
H	-0.19168600	-1.59804500	-0.08059600

TS at α'

C	3.73413300	0.13066900	-0.56600900
C	2.74592800	-0.40238100	0.48632600
H	4.73056800	-0.28825900	-0.40640400
H	3.81546400	1.21995200	-0.51521100
H	3.41126100	-0.13433900	-1.57578200
C	1.37900700	0.18772100	0.33865200
H	3.12625100	-0.14999100	1.48465400
H	2.69132700	-1.49378800	0.43510100
C	0.25354200	-0.50140000	0.13126200
C	-1.04161300	0.19026600	-0.00234800
O	-1.24045200	1.37808100	0.05406800
O	-2.04241400	-0.72443200	-0.21726800
C	-3.34251800	-0.22884500	-0.33114100
H	-3.96509100	-0.97710000	-0.81336600
H	-3.39369300	0.77510400	-0.74677600
H	-3.85214800	-0.10089900	0.87315500
H	1.29872200	1.27198700	0.39700500
H	0.24226900	-1.58304400	0.05813300
H	-4.21287800	-0.02498700	1.77463900

TS at α

C	3.66082900	-0.15722600	0.63738000
C	2.70294300	0.34089000	-0.45776000
H	4.65507300	0.27618800	0.50461500
H	3.76234600	-1.24580600	0.60997700
H	3.29821800	0.12093100	1.62989000
C	1.33943700	-0.27619800	-0.34492000
H	3.11800800	0.07750900	-1.43872800
H	2.62350500	1.42973000	-0.42653700
C	0.19249800	0.36186400	-0.17643900
C	-1.14950800	-0.23138000	-0.06020300
O	-1.37674100	-1.41930700	-0.10364400
O	-2.09872200	0.70906500	0.10067600

C	-3.44511800	0.21751500	0.22226100
H	-4.06654200	1.10178300	0.34296100
H	-3.53615800	-0.43830900	1.08961300
H	-3.73256700	-0.33580300	-0.67322400
H	1.29371500	-1.36829500	-0.39722400
H	0.24430200	1.83967600	-0.09145900
H	0.33732200	2.69154700	-0.04805800

TS at β

C	-3.62022300	0.02041500	0.67865700
C	-2.70358700	-0.41119600	-0.47995700
H	-4.63707400	-0.34421700	0.51569000
H	-3.65853300	1.10886200	0.76268300
H	-3.26088000	-0.37916900	1.62964100
C	-1.31545200	0.08529400	-0.33241800
H	-3.11436700	-0.03089700	-1.42337300
H	-2.68852000	-1.50670700	-0.56158700
C	-0.15715500	-0.53780700	-0.18771700
C	1.14812300	0.15455100	-0.04705800
O	1.34127200	1.34504900	-0.03276500
O	2.13964900	-0.76352900	0.06837100
C	3.46405100	-0.22553800	0.21193800
H	4.12267600	-1.08794800	0.28884700
H	3.53246300	0.39139500	1.10963000
H	3.72706900	0.38291400	-0.65505400
H	-1.28670400	1.52929400	-0.38571500
H	-0.11501400	-1.62727200	-0.16879200
H	-1.36303100	2.39726400	-0.45747800

TS at γ

C	3.68569000	0.31794900	-0.55778400
C	2.61101100	-0.47745800	0.17797400
H	4.67027700	-0.13381900	-0.41685200
H	3.73054300	1.34866500	-0.19609200
H	3.47805900	0.34903300	-1.63152800
C	1.26149100	0.12411700	0.17858200
H	2.96846500	-0.53238500	1.31773100
H	2.59102800	-1.52777000	-0.12427500
C	0.11514500	-0.54634400	0.00640400
C	-1.18564900	0.15579900	0.04726800
O	-1.35108400	1.33953700	0.23218100
O	-2.20242500	-0.71510900	-0.15604600
C	-3.52029900	-0.14270700	-0.13717400
H	-4.20140000	-0.97189400	-0.31576900
H	-3.62125000	0.61304300	-0.91800800
H	-3.72344300	0.32006000	0.83010200
H	1.19176300	1.19690600	0.34955100
H	0.09201500	-1.61568700	-0.17165700

H	3.44768400	-0.62971400	2.37608800
TS at δ			
C	-3.47532200	0.14297800	0.66733600
C	-2.61340100	-0.28453600	-0.50725100
H	-4.72311400	-0.36242800	0.44130700
H	-3.67248300	1.21177700	0.74354000
H	-3.20885400	-0.30102600	1.62536500
C	-1.22115500	0.26119800	-0.37281400
H	-3.05807400	0.09023600	-1.43722300
H	-2.58413600	-1.37560000	-0.57681400
C	-0.11917500	-0.47338600	-0.20252300
C	1.20626200	0.16965200	-0.05990600
O	1.42724900	1.35840300	-0.07034700
O	2.17383300	-0.76590300	0.08780600
C	3.50974800	-0.25711200	0.23439300
H	4.14577500	-1.13315600	0.34108900
H	3.58269000	0.38057800	1.11704000
H	3.79789600	0.32235900	-0.64436100
H	-1.10719000	1.34301300	-0.39403100
H	-0.14593600	-1.55691900	-0.16761000
H	-5.55697300	-0.71160300	0.25661400
(3)methyl-3-pentenoate			
C	0.13555800	-0.69995900	0.56999700
C	-1.08024200	0.12570800	0.18680800
O	-2.12283300	-0.67448400	-0.12446900
O	-1.14060500	1.32886400	0.18365100
C	1.42799200	0.04612400	0.40089800
C	-3.35086900	0.00178100	-0.45114100
C	2.49970400	-0.44121400	-0.21893000
C	3.80295300	0.28351000	-0.38449300
H	-0.01335800	-0.97413600	1.62458700
H	0.12691700	-1.63542200	0.00718700
H	-3.20991900	0.65485200	-1.31356600
H	-4.06518100	-0.78616500	-0.67920200
H	3.76783200	1.27765500	0.06670300
H	4.05841500	0.39868500	-1.44373400
H	4.62630500	-0.27222100	0.07821800
H	2.44961500	-1.44233200	-0.64687600
H	1.45176400	1.04849000	0.82034200
H	-3.69545800	0.59986000	0.39405000
TS at α'			
C	0.19373900	-0.70724000	0.49805100
C	-1.00085000	0.13044400	0.09014700
O	-2.07626300	-0.67723200	-0.16303200
O	-1.04294000	1.32752500	0.01166500
C	1.49486300	0.03664500	0.41008500

C	-3.28739300	-0.05171500	-0.47896600
C	2.58432400	-0.43162200	-0.19317800
C	3.89884000	0.28591400	-0.27740800
H	-0.00467800	-1.02291000	1.53263500
H	0.20492300	-1.62289000	-0.09764800
H	-3.16810100	0.90183500	-0.98813500
H	-3.94179500	-0.77259100	-0.96007500
H	3.85713800	1.25824400	0.21845800
H	4.19302100	0.44726200	-1.32034200
H	4.69925500	-0.30041900	0.18753200
H	2.54096800	-1.41075000	-0.66994000
H	1.51316800	1.01742000	0.87794400
H	-3.90606500	0.26049100	0.65002100
H	-4.33534800	0.46740600	1.48810000

TS at α

C	0.14921800	-0.71087900	0.27998100
C	-1.09171600	0.13440000	0.12886600
O	-2.13248500	-0.61626100	-0.28804300
O	-1.17158900	1.31145900	0.37769900
C	1.42234400	0.05163300	0.26596100
C	-3.38995200	0.07450800	-0.40780800
C	2.55658500	-0.39317600	-0.27934200
C	3.85618700	0.35288800	-0.28910600
H	0.00567600	-1.21873100	1.33445800
H	0.13247800	-1.55657400	-0.40853600
H	-3.31424200	0.88165200	-1.13794200
H	-4.10345300	-0.67653500	-0.73904200
H	3.76679700	1.32245000	0.20556500
H	4.20584700	0.52194900	-1.31369700
H	4.64128300	-0.21898800	0.21861800
H	2.55972500	-1.37006300	-0.76199100
H	1.39277900	1.02690900	0.74421900
H	-3.68971000	0.49246300	0.55439800
H	-0.18059100	-1.82236000	2.39538300

TS at β

C	0.06866400	-0.92728700	0.17596300
C	-1.08108200	0.05508900	-0.00801400
O	-2.26009400	-0.60137400	0.05705300
O	-0.98211700	1.23837300	-0.19478200
C	1.39373500	-0.27904700	0.31890800
C	-3.43432800	0.21052200	-0.12742200
C	2.49138100	-0.32756900	-0.40760700
C	3.78806300	0.37685700	-0.12444300
H	-0.16697700	-1.55479300	1.04251900
H	0.06496100	-1.60284400	-0.69141800
H	-3.42387500	0.68072700	-1.11202700

H	-4.27675900	-0.47155600	-0.03758600
H	3.73679400	0.95425100	0.79926200
H	4.04263500	1.05859600	-0.94261700
H	4.61091800	-0.34079400	-0.03987200
H	2.46799500	-0.93443400	-1.32000300
H	1.47755900	0.51674600	1.52507700
H	-3.48507800	0.98772700	0.63651800
H	1.53091100	0.95898600	2.27767500

TS at γ

C	-0.10075400	0.58669400	0.63150400
C	1.13339400	-0.16429100	0.16371600
O	2.16066900	0.68707300	-0.03593200
O	1.21580200	-1.35702400	0.01438100
C	-1.36845000	-0.19268300	0.41101900
C	3.40459800	0.08110700	-0.43423000
C	-2.48590700	0.28434200	-0.09910800
C	-3.81339700	-0.31420700	-0.37463300
H	0.04842600	0.77300300	1.70437500
H	-0.13343400	1.56554600	0.15236500
H	3.28133600	-0.46153700	-1.37249700
H	4.10333500	0.90557000	-0.55637300
H	-3.82805800	-1.37328500	-0.09052300
H	-4.06735000	-0.24341200	-1.43713500
H	-4.60429000	0.19870500	0.18233800
H	-2.43799300	1.65698700	-0.49109600
H	-1.32590600	-1.24504500	0.70171500
H	3.75634000	-0.61062200	0.33287900
H	-2.42107500	2.50792600	-0.74325200

TS at δ

C	-0.06796600	-0.69581800	-0.51610900
C	1.16745800	0.12315700	-0.18123700
O	2.20947900	-0.68314300	0.10908800
O	1.23692200	1.32559300	-0.19702500
C	-1.34428800	0.06980700	-0.33278400
C	3.45460700	-0.01610900	0.38992000
C	-2.42364500	-0.40493900	0.29939600
C	-3.69436700	0.32446800	0.44698100
H	0.04936300	-0.99164200	-1.56920700
H	-0.05704200	-1.62106000	0.06317600
H	3.34562800	0.65047400	1.24649300
H	4.16616600	-0.80910000	0.60833200
H	-3.63680800	1.38300600	0.19146800
H	-4.19455500	0.17497800	1.40519200
H	-4.52635100	-0.11927800	-0.34781100
H	-2.38762400	-1.41018700	0.71684200
H	-1.35538700	1.07530900	-0.74443300

H	3.78021100	0.56549400	-0.47396200
H	-5.30560100	-0.44099000	-1.02959600

(4)methyl-4-pentenoate

C	3.79125600	-0.14961400	-0.48335400
C	2.77419600	-0.20295400	0.37125500
C	1.44717500	0.47582900	0.18123900
C	0.28377700	-0.52306900	0.14262700
C	-1.06918600	0.14889700	0.03799400
O	-1.26982000	1.33742400	0.04745600
O	-2.05290600	-0.77137600	-0.06589400
C	-3.38977000	-0.24769400	-0.16362500
H	-4.03856500	-1.11769900	-0.23628200
H	-3.49106000	0.38169800	-1.04918600
H	-3.63607100	0.34241800	0.72054200
H	0.27180200	-1.15053600	1.04103800
H	0.38666200	-1.21606700	-0.69808300
H	1.45438000	1.06728000	-0.73809600
H	1.26958300	1.18267700	0.99933200
H	4.72764200	-0.65981800	-0.28748300
H	3.72560700	0.41357000	-1.40967400
H	2.88713800	-0.78027500	1.28858000

TS at α'

C	3.86839000	-0.16891200	-0.41418500
C	2.82827600	-0.20850600	0.41277700
C	1.51313100	0.48109200	0.18206900
C	0.34358100	-0.50939300	0.11611400
C	-0.99669500	0.17096000	-0.03275100
O	-1.20177000	1.35461000	-0.04063400
O	-1.98876800	-0.76206800	-0.16547000
C	-3.30176600	-0.29094200	-0.27400100
H	-3.92704800	-1.08070900	-0.67969900
H	-3.38097000	0.67957200	-0.75844600
H	-3.77540800	-0.08131800	0.94499900
H	0.29805100	-1.12946900	1.01865800
H	0.46523500	-1.21067300	-0.71541000
H	1.55104400	1.06693000	-0.74005400
H	1.31891100	1.19331300	0.99162400
H	4.79464100	-0.68549700	-0.18936500
H	3.83330200	0.38903600	-1.34531500
H	2.91083300	-0.78029200	1.33665000
H	-4.09379100	0.05297900	1.84506000

TS at α

C	3.78213300	-0.19189200	-0.53691400
C	2.77002600	-0.11889200	0.32154100
C	1.44258700	0.52732300	0.03669800

C	0.27661800	-0.44425400	0.12971800
C	-1.08164800	0.17580400	0.04749300
O	-1.32399900	1.34681600	0.21923300
O	-2.02562800	-0.75485900	-0.21145300
C	-3.38024000	-0.27082100	-0.25560100
H	-3.99494900	-1.14527400	-0.45643300
H	-3.49575900	0.47049900	-1.04788200
H	-3.65585400	0.18273600	0.69773500
H	0.30449200	-0.95178200	1.28299500
H	0.36789300	-1.33015800	-0.49841400
H	1.45426200	0.97331000	-0.96503900
H	1.25929100	1.35109100	0.73468300
H	4.72017600	-0.66573400	-0.27095700
H	3.71191800	0.22593000	-1.53697600
H	2.88467100	-0.55109100	1.31427800
H	0.38402800	-1.35878700	2.22616800

TS at β

C	3.84214000	0.15001700	-0.34532900
C	2.74459400	-0.43170300	0.14214100
C	1.42328700	0.22607600	0.25802000
C	0.22740300	-0.63560900	-0.12574100
C	-1.08349500	0.12433600	-0.08659300
O	-1.20009300	1.32264700	-0.13690300
O	-2.12842600	-0.72633500	-0.01966200
C	-3.43213500	-0.11479200	-0.02802000
H	-4.13986900	-0.93898200	0.02366400
H	-3.57865600	0.46167900	-0.94269900
H	-3.54839200	0.54669800	0.83162800
H	0.14402100	-1.52210300	0.50825100
H	0.34689200	-1.00730900	-1.15186200
H	1.38806200	1.20285100	-0.22609000
H	1.25332000	0.50362500	1.43206800
H	4.79016700	-0.37345500	-0.38971300
H	3.82646100	1.17014800	-0.71633300
H	2.80898200	-1.45633000	0.50576300
H	1.00640300	0.73273200	2.49097500

TS at γ

C	3.78416000	-0.04167700	-0.56608500
C	2.71725800	-0.12078300	0.20050200
C	1.37791300	0.51878400	0.17034800
C	0.24121400	-0.49849500	0.00260500
C	-1.12629700	0.15063300	0.04226600
O	-1.34469800	1.31768600	0.25130700
O	-2.09423400	-0.76113000	-0.18596500
C	-3.44367000	-0.25985600	-0.15977800
H	-4.07728500	-1.12059900	-0.36099400

H	-3.58203900	0.50654800	-0.92389100
H	-3.67426900	0.16707100	0.81744300
H	0.27528000	-1.25632800	0.79187800
H	0.33698100	-1.04574600	-0.93956000
H	1.34283000	1.25157000	-0.64610800
H	1.21255800	1.08517900	1.09267400
H	4.68725900	-0.60577300	-0.35465600
H	3.80444800	0.60189800	-1.44640700
H	2.87742400	-0.99221300	1.30641100
H	3.00480600	-1.53568600	2.00132800

TS at δ

C	-3.68670000	-0.00214800	0.49295500
C	-2.68492200	-0.13439100	-0.34876800
C	-1.33311600	0.52859700	-0.20822100
C	-0.20029900	-0.49905100	-0.10319400
C	1.16908800	0.14424600	-0.02918400
O	1.39293900	1.32839100	-0.05385900
O	2.13303400	-0.79558800	0.07018300
C	3.48264200	-0.30060300	0.14836500
H	4.11276800	-1.18429100	0.21875700
H	3.60804000	0.33172100	1.02865900
H	3.73033200	0.27829600	-0.74267500
H	-0.20274400	-1.18220200	-0.95940500
H	-0.32595500	-1.13290600	0.78021100
H	-1.31946500	1.18451000	0.66472600
H	-1.15178800	1.16817700	-1.07866900
H	-4.92052300	-0.74666000	0.14995600
H	-3.79368500	0.56509800	1.41011700
H	-2.81388800	-0.77109700	-1.22566300
H	-5.61103200	-1.19297400	-0.08832600

(5)methyl 2-methylbutanoate

C	3.12488400	-0.28264000	-0.41523300
C	1.73025700	-0.73373700	0.02850600
H	3.13802900	-0.01417400	-1.47668500
H	3.85183200	-1.08585300	-0.27011100
H	3.47958800	0.58222400	0.15118800
C	0.62780300	0.30672600	-0.22596400
H	1.73568100	-0.98976100	1.09240900
H	1.46489700	-1.65633900	-0.49629000
C	-0.74271300	-0.28656500	0.06460400
O	-1.72152700	0.45073900	-0.51036600
O	-0.96396600	-1.26809100	0.72927500
C	-3.06637600	0.00469600	-0.26231400
H	-3.70831000	0.70202100	-0.79621900
H	-3.28577700	0.02236200	0.80653200
H	-3.20794200	-1.01081500	-0.63548600

C	0.80120000	1.59813000	0.59991300
H	0.62726100	0.58477800	-1.28635500
H	1.74371500	2.09120600	0.35526500
H	0.80359100	1.37309000	1.67062900
H	-0.00893600	2.30041400	0.39677300

TS at α'

C	-3.15846000	-0.36385000	0.46004000
C	-1.77801500	-0.74139900	-0.08462100
H	-3.12945300	-0.20574400	1.54301800
H	-3.87846000	-1.16218300	0.26352300
H	-3.55102300	0.54704200	0.00083100
C	-0.68187600	0.28937200	0.23039500
H	-1.82610300	-0.88761100	-1.16824100
H	-1.47637100	-1.70682200	0.33154300
C	0.68353700	-0.25683800	-0.14747400
O	1.67735200	0.50802400	0.40740800
O	0.90959300	-1.20919100	-0.84458800
C	2.99834300	0.12926900	0.14916500
H	3.65495800	0.96693200	0.36557500
H	3.13664700	-0.35062500	-0.81704500
H	3.34736200	-0.80195500	1.02193300
C	-0.90066600	1.65060900	-0.46207100
H	-0.65035100	0.46626600	1.31229300
H	-1.84469100	2.09536200	-0.14308400
H	-0.93225900	1.53009400	-1.54896900
H	-0.09874500	2.34765900	-0.21486600
H	3.57575200	-1.47206000	1.67832300

TS at α

C	-3.13355000	-0.28209700	0.19413200
C	-1.72717600	-0.71191500	-0.23335800
H	-3.18657300	-0.11882800	1.27466300
H	-3.85957700	-1.05848900	-0.05916000
H	-3.45521800	0.63806500	-0.29982700
C	-0.61724500	0.26620600	0.15077600
H	-1.69730700	-0.85195200	-1.32184000
H	-1.48841400	-1.68727000	0.19524700
C	0.75506600	-0.34891200	-0.01594600
O	1.74005600	0.55820100	0.16539500
O	0.97008600	-1.51497500	-0.24529600
C	3.08160500	0.04601300	0.07849500
H	3.73123800	0.90106000	0.25168600
H	3.26420400	-0.38260200	-0.90802300
H	3.24704500	-0.72241800	0.83519900
C	-0.75051800	1.67725800	-0.41464600
H	-0.69530100	0.39934300	1.35635300

H	-1.69816800	2.12782400	-0.11469500
H	-0.72231000	1.65364600	-1.50984900
H	0.06014400	2.31760500	-0.06978200
H	-0.82999200	0.55889500	2.45252100

TS at β

C	3.08461400	-0.40813700	-0.33253000
C	1.66930000	-0.66984600	0.13132500
H	3.12468200	-0.21101800	-1.40833200
H	3.72540100	-1.26876900	-0.12476800
H	3.52532700	0.45448100	0.18007000
C	0.60337800	0.33364500	-0.28053700
H	1.58571900	-0.94886700	1.18249600
H	1.32051300	-1.79220900	-0.45579500
C	-0.76820100	-0.12623600	0.19272700
O	-1.72455200	0.17814200	-0.70967800
O	-0.99635100	-0.65806000	1.25058700
C	-3.07061800	-0.16838400	-0.33264100
H	-3.69542600	0.14287200	-1.16671100
H	-3.35883600	0.35424000	0.58076300
H	-3.15470700	-1.24350100	-0.16855500
C	0.86094900	1.74649100	0.29655800
H	0.56971800	0.41035600	-1.37144400
H	1.80963300	2.14474800	-0.06758900
H	0.89269100	1.71571900	1.38839500
H	0.06799300	2.43420600	-0.00764400
H	1.07798500	-2.59812100	-0.93756400

TS at γ

C	2.80393300	-0.83314800	-0.10025600
C	1.37950800	-0.67241000	0.37187200
H	2.92225300	-1.17568400	-1.12856900
H	3.32805200	-1.87624500	0.59977200
H	3.49605200	-0.03187600	0.15249700
C	0.57620800	0.40234800	-0.42002700
H	1.36522500	-0.40386000	1.43397800
H	0.85489200	-1.62693900	0.27392700
C	-0.87625800	0.34691800	0.03100100
O	-1.49900500	-0.74271900	-0.47284700
O	-1.41852800	1.13956600	0.75984900
C	-2.86833900	-0.92311600	-0.06805800
H	-3.20072000	-1.83343000	-0.56199900
H	-3.47468000	-0.07204900	-0.38172400
H	-2.93718000	-1.02689300	1.01596800
C	1.13656300	1.81666200	-0.25786900
H	0.59020000	0.11048500	-1.47551400
H	2.16578200	1.86979900	-0.61824300
H	1.11577700	2.12241400	0.79032400

H	0.54274800	2.53936200	-0.82131300
H	3.66218000	-2.59337800	1.08490200

TS at δ

C	2.82870500	-1.12570000	-0.04082500
C	1.40478500	-0.85754400	0.45168000
H	2.83600000	-1.38985700	-1.10270500
H	3.27265100	-1.95826800	0.51103200
H	3.48024300	-0.25918200	0.09459600
C	0.66394400	0.26304000	-0.33787100
H	1.41601200	-0.58893000	1.51310000
H	0.81442500	-1.77490100	0.36200500
C	-0.78989600	0.27405500	0.11410900
O	-1.51236200	-0.64952000	-0.55565900
O	-1.24848200	0.97574300	0.98045900
C	-2.89336300	-0.76495100	-0.16482500
H	-3.31260700	-1.53946700	-0.80305800
H	-3.41235200	0.18235400	-0.31720100
H	-2.97181400	-1.04786600	0.88607700
C	1.28369200	1.62757400	-0.15298600
H	0.67689100	-0.02008500	-1.39552900
H	2.32308900	1.71721500	-0.45997700
H	1.06490400	2.10347400	0.80017500
H	0.66658300	2.46690800	-1.03826900
H	0.24552200	2.99998000	-1.66433700

(6)methyl tiglate

C	-3.17500100	-0.33110800	0.00000100
C	-1.71096700	-0.63179000	0.00000100
H	-3.65392200	-0.78248300	0.87635300
H	-3.65392200	-0.78248700	-0.87635000
H	-3.40340600	0.73463400	-0.00000200
C	-0.68465200	0.23191900	0.00000000
C	0.68089000	-0.38036700	0.00000000
O	1.64859900	0.56806000	0.00000100
O	0.93118600	-1.56384600	-0.00000200
C	2.99813900	0.07554700	0.00000100
H	3.63172300	0.95999300	0.00000500
H	3.18458100	-0.53151900	-0.88741600
H	3.18457900	-0.53152600	0.88741300
C	-0.78817800	1.73495500	-0.00000100
H	-1.82518300	2.06952500	-0.00000200
H	-0.29073200	2.16013100	-0.87575800
H	-0.29073400	2.16013200	0.87575600
H	-1.44265300	-1.68505200	0.00000100

TS at α'

C	-3.23163700	-0.31967300	0.07813400

C	-1.77155700	-0.62970100	0.01664300
H	-3.67710900	-0.77865400	0.96800800
H	-3.74753200	-0.75943600	-0.78296100
H	-3.45319800	0.74709900	0.09892500
C	-0.73969000	0.22865200	-0.01487100
C	0.61426800	-0.39419100	-0.07280700
O	1.59553500	0.56482300	-0.10939100
O	0.86746100	-1.57320000	-0.09324600
C	2.91914500	0.12128100	-0.13262300
H	3.55672900	0.93208300	-0.47337300
H	3.05252200	-0.83521600	-0.63285800
H	3.30852000	-0.10911200	1.10441000
C	-0.83445300	1.73238600	0.00615400
H	-1.86930400	2.06980100	0.05078100
H	-0.37169200	2.16623800	-0.88413100
H	-0.30230900	2.14539200	0.86699300
H	-1.51198000	-1.68485600	-0.00419800
H	3.57491900	-0.25885800	2.02572500

TS at β

C	-3.18596700	-0.20095600	0.00022200
C	-1.73220800	-0.47148200	0.00011200
H	-3.65849300	-0.65371000	0.87860100
H	-3.65845900	-0.65290000	-0.87859900
H	-3.41856600	0.86852100	0.00070400
C	-0.64405800	0.29171700	-0.00011800
C	0.70410300	-0.36577300	-0.00019100
O	1.69107000	0.56510200	0.00037000
O	0.92791500	-1.55104600	-0.00068500
C	3.02970300	0.04307700	0.00032000
H	3.68222600	0.91359600	0.00074400
H	3.20271400	-0.56755800	-0.88733700
H	3.20250800	-0.56826200	0.88753200
C	-0.68614200	1.80886600	-0.00030400
H	-1.71113200	2.17913500	-0.00018300
H	-0.17277100	2.20833600	-0.87827600
H	-0.17245700	2.20856000	0.87737600
H	-1.55556700	-1.90475400	0.00058700
H	-1.60446900	-2.77610700	0.00112300

TS at γ

C	3.08381400	-0.29162500	-0.16011400
C	1.65182200	-0.62054400	-0.12080000
H	3.67887500	-1.01745400	-0.71573000
H	3.54853700	-0.37428400	0.95551400
H	3.32968500	0.72474300	-0.46445300
C	0.61523000	0.23966800	-0.06030800
C	-0.74455700	-0.37959800	-0.01571400

O	-1.71589700	0.56257400	0.03093700
O	-0.98459500	-1.56536500	-0.01999500
C	-3.06255300	0.06274900	0.07590600
H	-3.69970100	0.94390500	0.10842300
H	-3.21246200	-0.55382600	0.96360200
H	-3.27824000	-0.53624100	-0.81029400
C	0.71811300	1.74033800	-0.03437800
H	1.75267800	2.07783200	-0.09053600
H	0.27903300	2.14207300	0.88312200
H	0.16162400	2.18524600	-0.86351800
H	1.39350100	-1.67550500	-0.11266400
H	4.07919700	-0.40009400	1.95145400

TS at δ

C	3.15827800	-0.39998100	0.01227700
C	1.69503400	-0.69467500	0.02218100
H	3.65759900	-0.98050400	-0.77172100
H	3.61172200	-0.71393800	0.95969100
H	3.39149900	0.65394500	-0.13862700
C	0.67472300	0.18035000	-0.08850900
C	-0.70055500	-0.41188400	-0.01444800
O	-1.65909800	0.54055400	-0.06843900
O	-0.95487700	-1.58965000	0.08478400
C	-3.01310900	0.06405500	0.00937700
H	-3.63788700	0.95315300	-0.03954200
H	-3.17626500	-0.47037200	0.94639500
H	-3.23078400	-0.60671700	-0.82322900
C	0.81319800	1.64514700	-0.22732800
H	1.79625300	1.97885900	-0.55351500
H	0.68293400	2.18569000	0.87757100
H	0.02029100	2.11384200	-0.80480900
H	1.41488600	-1.73860400	0.13154200
H	0.61614200	2.71933800	1.80417700

(7)methyl 2-methylbut-3-enoate

C	-2.46217100	-1.51373700	-0.01643800
C	-1.72167100	-0.49839500	-0.44799000
C	-0.78530300	0.31111200	0.41888200
C	0.62134100	0.21725200	-0.16260900
O	1.45031900	-0.47024500	0.64879500
O	0.96038100	0.68792700	-1.22005600
C	2.79819100	-0.63334000	0.16760100
H	3.31716200	-1.19429700	0.94150600
H	3.26894700	0.33870100	0.01390200
H	2.80216000	-1.18307600	-0.77474000
C	-1.21771600	1.78932100	0.48005800
H	-0.76542100	-0.11593900	1.42342300
H	-2.23443100	1.86597100	0.87041900

H	-1.18888500	2.23496500	-0.51610500
H	-0.55299800	2.36503800	1.12967700
H	-2.43022000	-1.84537400	1.01698800
H	-3.12989700	-2.04954600	-0.68155300
H	-1.76805000	-0.19117900	-1.49044800

TS at α'

C	2.22818000	-1.75588600	0.01841600
C	1.65348500	-0.64287600	0.46101800
C	0.88248400	0.32968700	-0.40522500
C	-0.55041800	0.38662200	0.10622900
O	-1.38071500	-0.36264300	-0.67730000
O	-0.92395900	0.98885100	1.07724700
C	-2.72064300	-0.45652200	-0.28304400
H	-3.31342100	-0.79380300	-1.12805000
H	-3.08579500	0.42506800	0.23863500
H	-2.82974100	-1.42852300	0.61185800
C	1.51025400	1.73405400	-0.37010800
H	0.85767400	-0.05178100	-1.42804900
H	2.54897300	1.68634700	-0.70247000
H	1.48285900	2.13854700	0.64317000
H	0.96824100	2.42237200	-1.02369500
H	2.16761800	-2.05433700	-1.02360000
H	2.78167300	-2.40893900	0.68345500
H	1.72442200	-0.37143400	1.51220000
H	-2.88516300	-2.14365600	1.25325200

TS at α

C	1.04327100	2.10255200	-0.46800000
C	1.61782800	1.00123700	0.01252900
C	0.97031200	-0.30171300	0.38116800
C	-0.46206200	-0.47670600	-0.09015800
O	-1.29975700	0.39299200	0.51103000
O	-0.82633500	-1.30560900	-0.88620200
C	-2.68729000	0.27709200	0.14189600
H	-3.20590200	1.03708000	0.72166800
H	-3.06360400	-0.71717000	0.38623000
H	-2.81526600	0.45231500	-0.92729900
C	1.82929300	-1.51071800	0.00914900
H	0.89463900	-0.30513000	1.56108300
H	2.83176700	-1.40482300	0.43015600
H	1.91324700	-1.59990300	-1.07601200
H	1.38923600	-2.43475300	0.38682400
H	-0.02364700	2.17781500	-0.63529000
H	1.64065400	2.97630800	-0.70132200
H	2.69427600	1.00590900	0.17201600
H	0.88522100	-0.43717000	2.76381900

TS at β

C	2.17463600	-1.74777700	0.01089000
C	1.57416400	-0.61777600	0.31807700
C	0.78368200	0.36530900	-0.48327100
C	-0.66333000	0.38678100	0.01971100
O	-1.35892900	-0.65201400	-0.48115200
O	-1.12695100	1.20737300	0.76862200
C	-2.72289800	-0.76387500	-0.03257200
H	-3.12218000	-1.64260600	-0.53370900
H	-3.28923700	0.12736200	-0.30671800
H	-2.75817900	-0.88941000	1.05057200
C	1.39425900	1.77373000	-0.44500200
H	0.75360500	-0.00895000	-1.51539000
H	2.42917000	1.74340400	-0.79042600
H	1.37084900	2.17255100	0.56952700
H	0.83011600	2.45445000	-1.08618000
H	2.14258600	-2.15255700	-1.00086700
H	2.72395600	-2.32234900	0.75017100
H	1.71975000	-0.24422400	1.69112700
H	1.84352300	-0.05889600	2.54513900

TS at γ

C	2.45900500	-1.29181100	-0.22328300
C	1.68706600	-0.37505300	0.31566100
C	0.67247700	0.46289100	-0.45071600
C	-0.70176100	0.21787300	0.16383000
O	-1.48998700	-0.50392000	-0.65628800
O	-1.04330500	0.60483200	1.25369800
C	-2.79946000	-0.81861000	-0.14334100
H	-3.28662500	-1.39584800	-0.92574600
H	-3.35679600	0.09553100	0.06582600
H	-2.71796300	-1.40371100	0.77370200
C	1.02446300	1.95883900	-0.37094700
H	0.64449200	0.13294500	-1.49019900
H	2.02437000	2.13181500	-0.77346000
H	0.99680300	2.29979300	0.66543500
H	0.31172500	2.55685700	-0.94504000
H	2.55018900	-1.65797700	-1.23885900
H	3.38850500	-1.97701100	0.69749200
H	1.74984700	-0.15962700	1.38188900
H	3.91105300	-2.35482700	1.26244600

TS at δ

C	2.43585400	-1.58398900	-0.09383300
C	1.68175500	-0.62928900	0.44197500
C	0.79127800	0.30705700	-0.35278100
C	-0.63227500	0.19750800	0.18754200
O	-1.42017400	-0.51151000	-0.64092100

O	-1.00303800	0.66300600	1.23609600
C	-2.77716700	-0.70570000	-0.19618200
H	-3.25861100	-1.28651600	-0.97939700
H	-3.27568900	0.25575200	-0.06653000
H	-2.79329500	-1.24696300	0.75083900
C	1.29531800	1.73345900	-0.22290300
H	0.79013900	-0.00593400	-1.39896900
H	2.29682000	1.89364600	-0.61699700
H	1.13036700	2.18671600	0.75227400
H	0.52652600	2.51159300	-1.04445500
H	2.44666900	-1.77146200	-1.16298300
H	3.07013600	-2.21275300	0.52062400
H	1.68474500	-0.46175500	1.51616900
H	-0.00069700	3.01142700	-1.61488900

(8)methyl 2-methylenebutyrate

C	-3.17913900	-0.13256400	0.00000400
C	-1.76401900	-0.70694100	-0.00000100
C	-0.64488500	0.30850200	-0.00000100
C	0.72491700	-0.29547400	-0.00000100
O	1.71837200	0.61991900	0.00000300
O	0.93137600	-1.48751600	-0.00000300
C	3.05227100	0.08577600	0.00000200
H	3.71204200	0.95071700	0.00000700
H	3.22079200	-0.52594500	-0.88782900
H	3.22078900	-0.52595300	0.88782800
C	-0.80726900	1.63403300	-0.00000400
H	-3.91364800	-0.94119400	0.00000600
H	-3.36566800	0.48340900	-0.88434000
H	-3.36566200	0.48340700	0.88435100
H	-1.62550400	-1.36414200	-0.86566400
H	-1.62549900	-1.36414600	0.86565700
H	-1.79196700	2.08491000	-0.00000500
H	0.04508200	2.29972300	-0.00000500

TS at α'

C	-3.23648700	-0.11928100	0.07318300
C	-1.82717000	-0.70412200	0.01022200
C	-0.70080000	0.30339500	-0.01445400
C	0.65781200	-0.31088700	-0.07136200
O	1.66378600	0.61458600	-0.12289600
O	0.86744300	-1.49857800	-0.07894900
C	2.97414600	0.13124700	-0.13505700
H	3.63493500	0.91673500	-0.49032300
H	3.07994000	-0.83690500	-0.61917000
H	3.35573300	-0.08849400	1.10685100
C	-0.85204800	1.63059100	0.01590500

H	-3.97624200	-0.92285400	0.08492500
H	-3.45079600	0.51449600	-0.79202700
H	-3.38581400	0.48030700	0.97556000
H	-1.72688500	-1.34718700	-0.87129100
H	-1.66105300	-1.37617400	0.85935600
H	-1.83306700	2.08683300	0.06046800
H	0.00339600	2.29177100	-0.00083400
H	3.61730100	-0.23225500	2.03063200

TS at β

C	-3.14010400	-0.07093600	-0.22083400
C	-1.74131700	-0.61872700	-0.00042900
C	-0.61052500	0.35072000	0.01871000
C	0.74736700	-0.28174600	-0.03999200
O	1.75587700	0.61091500	0.03944100
O	0.92862300	-1.47224100	-0.14936100
C	3.08095300	0.05590300	-0.01730500
H	3.75533200	0.90603100	0.05804000
H	3.23415100	-0.47452800	-0.95845500
H	3.24139000	-0.63677800	0.81029200
C	-0.74396500	1.68167700	0.09944800
H	-3.87200100	-0.88109600	-0.19784200
H	-3.21957100	0.42620800	-1.19301400
H	-3.42290700	0.65102500	0.54979600
H	-1.50920300	-1.46432900	-0.64974100
H	-1.75137400	-1.16032200	1.08011100
H	-1.71859300	2.15248700	0.13715800
H	0.12308800	2.32713800	0.12369200
H	-1.89076600	-1.65657700	2.08173900

TS at γ

C	3.08565700	0.05018100	0.00004200
C	1.71940200	-0.58659200	-0.00000300
C	0.54984500	0.37951200	-0.00003100
C	-0.78715400	-0.29446300	-0.00002700
O	-1.82422100	0.56952800	0.00008600
O	-0.93014000	-1.49549900	-0.00011200
C	-3.13068400	-0.03046600	0.00005900
H	-3.83213300	0.80090300	-0.00004800
H	-3.26815900	-0.64939500	0.88812300
H	-3.26805900	-0.64955300	-0.88790600
C	0.64929100	1.71073700	-0.00007800
H	3.98460300	-0.98529200	0.00017400
H	3.36801900	0.58463300	0.90632300
H	3.36814400	0.58451000	-0.90627300
H	1.61092700	-1.24684200	0.86755400
H	1.61097600	-1.24684100	-0.86756600
H	1.61239000	2.20720200	-0.00010000

H	-0.23441800	2.33419600	-0.00009500
H	4.56444700	-1.69921400	0.00024800

TS at δ

C	3.19743600	-0.15464400	-0.00043600
C	1.78691500	-0.73842200	0.00019400
C	0.65011600	0.27411900	0.00007300
C	-0.71202200	-0.35843200	0.00010000
O	-1.71828900	0.53258000	-0.00043200
O	-0.88312300	-1.55560400	0.00054300
C	-3.04321300	-0.02588700	-0.00033800
H	-3.71672200	0.82804600	-0.00049900
H	-3.20005300	-0.63986100	0.88798400
H	-3.20003800	-0.64016400	-0.88845700
C	0.83199800	1.58443300	0.00003200
H	3.93573800	-0.95977300	-0.00040300
H	3.38011400	0.46225500	0.88386700
H	3.37954100	0.46168100	-0.88525700
H	1.64620900	-1.39069400	0.86860300
H	1.64573000	-1.39146100	-0.86755500
H	1.75498100	2.14943800	0.00007300
H	-0.26717000	2.58222000	0.00109800
H	-0.81441600	3.23550600	0.00190900

(9)methyl isopentanoate

C	-2.90755600	-0.85245100	-0.21017900
C	-1.67352000	0.05816000	-0.24984900
C	-0.41194500	-0.73869500	0.11106600
C	0.88639800	-0.01633300	-0.18407500
O	1.01264400	0.96344800	-0.87599600
O	1.92655300	-0.63668200	0.41637900
C	3.22314900	-0.06533300	0.16581900
H	3.92668800	-0.68808200	0.71393400
H	3.44886400	-0.07896100	-0.90169400
H	-3.80884100	-0.30069200	-0.49072600
H	-3.06717600	-1.25767400	0.79505200
H	-2.80505000	-1.69716800	-0.89805400
H	-0.37838700	-1.67687900	-0.45641900
H	-0.41362900	-1.03095000	1.16637000
C	-1.85345300	1.27593700	0.66684500
H	-1.54379900	0.42495000	-1.27350600
H	-0.99644900	1.94909500	0.60310000
H	-1.97273700	0.96500300	1.71105600
H	-2.74484700	1.84454100	0.38723500
H	3.26334900	0.96497900	0.52281600

TS at α'

C	2.94008500	-0.92224700	0.19901200

C	1.73306000	0.02186500	0.27144800
C	0.45762600	-0.71140800	-0.16847200
C	-0.82152000	0.03015000	0.14269500
O	-0.94999800	0.96048700	0.89271400
O	-1.86905100	-0.52176500	-0.54530100
C	-3.14252100	0.00601000	-0.30744000
H	-3.80213700	-0.28457800	-1.11979300
H	-3.65072500	-0.58463800	0.76259200
H	3.84960600	-0.41684900	0.53449800
H	3.11194500	-1.26579600	-0.82689100
H	2.79745700	-1.80585600	0.82812800
H	0.37971000	-1.68160500	0.33791300
H	0.47549000	-0.93799600	-1.23966100
C	1.97062400	1.28930400	-0.56106400
H	1.59050100	0.32517800	1.31395700
H	1.13437600	1.98565100	-0.47343400
H	2.10509200	1.04129200	-1.61999800
H	2.87223000	1.80912300	-0.22583100
H	-3.13779100	1.06235200	-0.04863100
H	-3.99748800	-1.03809600	1.54077100

TS at α

C	2.90349400	-0.81631400	0.07817000
C	1.67101200	0.08389900	0.23616500
C	0.40481300	-0.64257100	-0.19294400
C	-0.89292800	0.00320900	0.17541900
O	-1.03660700	0.85664500	1.01912000
O	-1.91594400	-0.52486100	-0.53270400
C	-3.22356000	-0.02089200	-0.20695900
H	-3.91283800	-0.56260400	-0.85073200
H	-3.45368800	-0.20419300	0.84377600
H	3.80585500	-0.29493600	0.40771100
H	3.05003800	-1.10421600	-0.96837600
H	2.81008500	-1.73208000	0.66785900
H	0.36891700	-1.73170300	0.43225700
H	0.40786700	-0.98703900	-1.22888800
C	1.83975600	1.39572200	-0.55306500
H	1.55430400	0.34464200	1.29297000
H	0.99109400	2.06335800	-0.39426000
H	1.93286200	1.19850500	-1.62631500
H	2.74446300	1.91879300	-0.23038100
H	-3.27983000	1.05158700	-0.40027400
H	0.38576400	-2.63271400	0.94261100

TS at β

C	2.85329500	-0.96552600	0.14523900
C	1.66305200	-0.02031600	0.15661100
C	0.36366100	-0.72742400	-0.20009100

C	-0.91753800	0.04540800	0.05469400
O	-1.01400200	1.17687600	0.45682900
O	-1.98575600	-0.72964800	-0.23785000
C	-3.27349800	-0.11765000	-0.04123900
H	-4.00130800	-0.87413600	-0.32591700
H	-3.40536700	0.16885700	1.00319300
H	3.75430900	-0.46281000	0.50605700
H	3.05892700	-1.32163800	-0.87249600
H	2.67920100	-1.84242400	0.77533100
H	0.27995900	-1.67366900	0.34420700
H	0.36484500	-1.00713300	-1.26359000
C	1.91696300	1.28859600	-0.57058400
H	1.53781100	0.29863400	1.39702700
H	1.09217000	1.98692100	-0.43347100
H	2.04233300	1.10821000	-1.64723200
H	2.83515700	1.75864200	-0.20849700
H	-3.37593400	0.76949400	-0.66817900
H	1.50035200	0.49470200	2.37396200

TS at γ

C	2.88187500	-0.72128700	-0.00177100
C	1.63357500	0.10968800	0.20358300
C	0.38843400	-0.65442900	-0.26971300
C	-0.92052700	-0.02500800	0.16017200
O	-1.05237900	0.84187800	0.98845400
O	-1.95829100	-0.58719100	-0.49600000
C	-3.26386200	-0.10186000	-0.13309400
H	-3.96386800	-0.66159300	-0.74928700
H	-3.45741900	-0.27881100	0.92601200
H	3.80236700	-0.28279100	0.38231900
H	3.01177700	-1.14882400	-0.99736800
H	2.76360700	-1.84495200	0.78197300
H	0.39095400	-1.67336300	0.13397200
H	0.37941200	-0.76483500	-1.35903200
C	1.76719900	1.47283000	-0.50533500
H	1.51387400	0.30635500	1.27428400
H	0.88874900	2.09185500	-0.31165200
H	1.87283100	1.34211200	-1.58731400
H	2.64586100	2.01392600	-0.14542000
H	-3.34445300	0.96744200	-0.33451000
H	2.66150300	-2.58362900	1.32333300

TS at δ

C	-2.80873700	-1.01239000	-0.21233300
C	-1.61565300	-0.04743600	-0.24289800
C	-0.31423900	-0.79688000	0.10799800
C	0.94867900	-0.00560800	-0.16380900
O	1.01935400	1.02517300	-0.78587200

O	2.02325300	-0.62515700	0.36996500
C	3.29205100	0.01504200	0.14013800
H	4.02967800	-0.61757000	0.62867200
H	3.49603900	0.08836900	-0.92918000
H	-3.73227100	-0.49795500	-0.48757200
H	-2.94755300	-1.43521100	0.78841300
H	-2.66509000	-1.84280100	-0.90944300
H	-0.24239400	-1.71771100	-0.48409700
H	-0.30686900	-1.11533700	1.15511400
C	-1.83111700	1.13477500	0.67890500
H	-1.49669200	0.33724200	-1.26149700
H	-1.06860300	1.90900100	0.63498900
H	-2.13739500	0.88793100	1.69696900
H	-2.93075000	1.81105700	0.20809700
H	3.29860800	1.01698100	0.57194600
H	-3.66346000	2.25086100	-0.13315300

(10)methyl senecioate

C	-2.86926200	-1.03325600	0.00000000
C	-1.66913000	-0.12338900	0.00000000
C	-0.43213600	-0.65097300	0.00000100
C	0.84329600	0.09176100	0.00000200
O	1.01794500	1.29096900	0.00000400
O	1.87780800	-0.78962600	-0.00000100
C	3.18856500	-0.20489900	-0.00000200
H	3.88213500	-1.04319400	-0.00000200
H	3.33470800	0.41378900	-0.88732300
H	-3.49578000	-0.83947800	-0.87790100
H	-3.49577800	-0.83947800	0.87790300
H	-2.58934200	-2.08755500	0.00000000
C	-1.98498800	1.34637600	-0.00000300
H	-1.09027100	1.96117600	-0.00000200
H	-2.59441300	1.59259300	0.87735800
H	-2.59440900	1.59259000	-0.87736700
H	-0.31565200	-1.72868800	0.00000200
H	3.33471000	0.41379000	0.88731800

TS at α'

C	2.91860400	-1.04641200	0.06923800
C	1.72845400	-0.12605500	0.01869800
C	0.48684900	-0.64445200	-0.02454200
C	-0.77378700	0.11037300	-0.07441500
O	-0.95038200	1.30536300	-0.08721500
O	-1.82413600	-0.78050700	-0.11555600
C	-3.11165400	-0.24481200	-0.13026200
H	-3.80535800	-1.00309000	-0.48266200
H	-3.48537200	-0.00436500	1.10334800

H	3.51351700	-0.85150900	0.96852600
H	3.57891600	-0.86344200	-0.78582500
H	2.62971400	-2.09814200	0.06572100
C	2.05616900	1.34041000	0.02245700
H	1.16925200	1.96511100	-0.01564700
H	2.70200800	1.57547100	-0.83150500
H	2.63310000	1.58603100	0.92154800
H	0.35980800	-1.72060300	-0.02069600
H	-3.17845000	0.72516600	-0.61833800
H	-3.74879500	0.15621500	2.03066100

TS at α

C	2.86416300	-1.00334300	-0.00011000
C	1.67823600	-0.07092400	0.00001500
C	0.42989000	-0.53381300	-0.00011900
C	-0.86995600	0.14573100	-0.00014000
O	-1.04511100	1.34642000	-0.00041800
O	-1.88399200	-0.74328700	0.00016900
C	-3.20559000	-0.17812500	0.00015800
H	-3.88375300	-1.02841800	0.00039500
H	-3.35987200	0.43719300	0.88812600
H	3.49007100	-0.81423400	0.87871800
H	3.49014400	-0.81390000	-0.87881400
H	2.56786200	-2.05100700	-0.00032200
C	2.02424200	1.40214300	0.00032000
H	1.13764400	2.02933700	0.00040200
H	2.63536400	1.63387100	-0.87923700
H	2.63532400	1.63353100	0.87999400
H	0.29017200	-1.99869400	0.00001900
H	-3.36001700	0.43681700	-0.88804600
H	0.26397400	-2.85957200	0.00001800

TS at γ

C	2.79492700	-0.96290900	-0.16592500
C	1.61302200	-0.07693500	-0.10894800
C	0.37834000	-0.62689000	-0.08667500
C	-0.90585700	0.09324300	-0.00744600
O	-1.09498700	1.28871800	0.05660200
O	-1.92603000	-0.80358500	-0.01659200
C	-3.24500100	-0.24151500	0.05796200
H	-3.92519000	-1.09035200	0.03840600
H	-3.36893600	0.32842900	0.98054500
H	3.31351500	-0.98480200	0.95143100
H	3.61097000	-0.58329700	-0.78307100
H	2.57939000	-2.00888900	-0.38008800
C	1.90823800	1.39595600	-0.03304200
H	1.00479000	1.99318300	0.04015100
H	2.47754200	1.70630200	-0.91623500

H	2.54695700	1.59575000	0.83543800
H	0.28002900	-1.70519000	-0.13721000
H	-3.43058300	0.41890200	-0.79101100
H	3.81763200	-1.03680400	1.90600800

TS at δ

C	2.81253800	-1.12026500	-0.00433500
C	1.62515100	-0.19557600	-0.07426400
C	0.37485500	-0.69949200	0.02285600
C	-0.88007500	0.07138600	-0.01861600
O	-1.01681800	1.27254600	-0.11221900
O	-1.93799100	-0.77585200	0.06602400
C	-3.23205900	-0.15465100	0.03961300
H	-3.94836000	-0.96965300	0.11886700
H	-3.34394400	0.53755600	0.87607300
H	3.46492500	-0.83604900	0.82926500
H	3.41542500	-1.04250400	-0.91542700
H	2.51649200	-2.16156300	0.12810300
C	1.94178600	1.24165100	-0.20040800
H	1.10379300	1.87584100	-0.46979900
H	2.83733600	1.43670300	-0.79262500
H	2.27150700	1.64527500	0.90576600
H	0.24111300	-1.76965900	0.12814300
H	-3.37671400	0.39406100	-0.89277600
H	2.60371900	2.05811900	1.86489800

(11)methyl 3-methylbut-3-enoate

C	2.92057800	-0.75377500	-0.14858700
C	1.67412100	0.09130700	-0.08770600
C	0.53661800	-0.54759300	0.69943000
C	-0.82694600	0.05402200	0.44107500
O	-1.19962200	1.13575800	0.82230400
O	-1.59665500	-0.78037200	-0.29084600
C	-2.91134000	-0.29076600	-0.61271000
H	-3.38554700	-1.08512700	-1.18467400
H	-3.47505200	-0.08145200	0.29764100
H	3.72977700	-0.23566700	-0.66560500
H	2.72942700	-1.69977700	-0.66784600
H	3.26790800	-1.01210400	0.85876800
C	1.59830800	1.29505400	-0.65173300
H	0.74611000	-0.44140900	1.77028200
H	0.49841100	-1.61650100	0.47787700
H	2.44487500	1.70721600	-1.18983100
H	0.71016200	1.90987000	-0.58079000
H	-2.84388800	0.62237500	-1.20609900

TS at α'

C	2.96037600	-0.79622600	-0.11461700
C	1.73235200	0.07569900	-0.07328800

C	0.58359200	-0.51444300	0.73743500
C	-0.76216600	0.10278000	0.44544300
O	-1.16080700	1.16184900	0.85050600
O	-1.49327400	-0.70329600	-0.38298400
C	-2.76543800	-0.25401900	-0.75269900
H	-3.09275400	-0.80608400	-1.62863800
H	-3.62353600	-0.59304400	0.19618400
H	3.77795800	-0.30925200	-0.64824200
H	2.74723200	-1.75157700	-0.60735900
H	3.30592100	-1.03395600	0.89827200
C	1.67630200	1.26478200	-0.66940900
H	0.79004000	-0.36996300	1.80365600
H	0.52577600	-1.58962800	0.55396800
H	2.52723900	1.64767200	-1.22167000
H	0.80016900	1.89879500	-0.61402700
H	-2.84902100	0.82886500	-0.80885900
H	-4.22646900	-0.86170000	0.89934300

TS at α

C	2.96037600	-0.79622600	-0.11461700
C	1.73235200	0.07569900	-0.07328800
C	0.58359200	-0.51444300	0.73743500
C	-0.76216600	0.10278000	0.44544300
O	-1.16080700	1.16184900	0.85050600
O	-1.49327400	-0.70329600	-0.38298400
C	-2.76543800	-0.25401900	-0.75269900
H	-3.09275400	-0.80608400	-1.62863800
H	-3.62353600	-0.59304400	0.19618400
H	3.77795800	-0.30925200	-0.64824200
H	2.74723200	-1.75157700	-0.60735900
H	3.30592100	-1.03395600	0.89827200
C	1.67630200	1.26478200	-0.66940900
H	0.79004000	-0.36996300	1.80365600
H	0.52577600	-1.58962800	0.55396800
H	2.52723900	1.64767200	-1.22167000
H	0.80016900	1.89879500	-0.61402700
H	-2.84902100	0.82886500	-0.80885900
H	-4.22646900	-0.86170000	0.89934300

TS at γ

C	2.91543100	0.64931000	-0.06088300
C	1.67973200	-0.15998200	0.00253600
C	0.46843900	0.51540700	-0.62323000
C	-0.88004900	-0.10672600	-0.32642100
O	-1.18495300	-1.25812300	-0.51561400
O	-1.73563700	0.81423600	0.16493300
C	-3.06445100	0.33959200	0.45220400
H	-3.60710600	1.20487000	0.82575000

H	-3.53456300	-0.04997300	-0.45196100
H	2.83484100	1.58198100	0.76353200
H	3.05740700	1.19494300	-0.99619900
C	1.65773400	-1.36518200	0.58547400
H	0.58908700	0.50696700	-1.71451000
H	0.44211200	1.56475800	-0.32046500
H	2.56156800	-1.77952400	1.01831500
H	0.76182700	-1.96934900	0.62225400
H	-3.03288800	-0.44952200	1.20475400
H	3.81965500	0.11769300	0.23230300
H	2.81176300	2.39374400	1.44360200

TS at δ

C	2.85447700	-1.01795400	0.08732000
C	1.69136400	-0.05452500	0.00293300
C	0.37186100	-0.74174000	-0.34210600
C	-0.90037000	0.06795800	-0.20113100
O	-1.03928900	1.24164300	-0.43768200
O	-1.91428800	-0.72858400	0.20190700
C	-3.20114100	-0.09178800	0.31271000
H	-3.88536400	-0.87433000	0.63242700
H	-3.16610500	0.71311300	1.04817000
H	3.79011200	-0.49799900	0.28860900
H	2.96315500	-1.57499300	-0.85018300
H	2.69014000	-1.75642800	0.87978300
C	1.82023300	1.24343600	0.19149300
H	0.26615200	-1.65250400	0.25300100
H	0.41791000	-1.07498600	-1.38840800
H	3.17739300	1.75982900	0.51666600
H	1.10446600	2.05037500	0.14605000
H	-3.50862200	0.31947700	-0.64993400
H	3.96084200	2.05165500	0.70270400

Vibrational frequenices at the B3LYP/6-311G(2d,d,p) level

(1)methyl valerate

33.1872	67.3186	106.6800
122.4525	125.5725	175.9897
241.4982	259.0597	305.9342
348.8763	489.6772	584.5917
702.4483	736.8760	809.9110
882.2713	923.6456	942.6787
996.0374	1041.0676	1071.6687
1129.5914	1133.3974	1173.2054
1191.4609	1212.9713	1235.7660
1298.8391	1313.8993	1332.3125
1376.2133	1408.8269	1417.6213
1464.3539	1472.7020	1483.4338

1491.1056 1499.5726 1500.9794
1501.1445 1514.0218 1807.0767
3004.3185 3021.2813 3026.4662
3026.8652 3036.2575 3047.1769
3050.3415 3073.4597 3084.8881
3087.7171 3117.0069 3154.0752

TS: α'

-1295.1844 37.1323 63.6568
95.0501 113.9932 123.5241
152.4828 243.9199 265.2109
300.8729 328.9761 367.5490
492.7480 547.8557 578.9751
701.9300 736.3727 807.9900
872.7391 921.8864 941.4955
1016.1472 1058.7564 1074.2605
1110.2920 1132.6932 1136.7174
1165.4119 1200.8676 1235.7681
1277.0711 1289.5072 1296.8328
1313.5978 1332.8312 1375.0732
1408.9550 1418.0988 1453.0426
1461.9976 1491.1699 1495.0413
1499.7352 1501.6527 1513.9387
1820.4328 3005.1530 3022.1155
3026.6615 3027.6746 3036.5897
3050.5326 3074.0237 3085.7882
3089.2287 3092.0413 3200.0411

TS: α

-1184.3094 41.4131 62.2713
100.2161 113.0204 119.2041
172.3464 244.9652 253.4120
303.1079 320.1353 339.2224
347.9687 500.4964 688.6847
714.0583 738.7642 831.0345
885.8146 926.5480 953.6265
999.1196 1045.2904 1077.6884
1113.4262 1132.8825 1172.3251
1188.7652 1210.9496 1212.4971
1271.2389 1294.6091 1308.9856
1321.7445 1343.1910 1377.8157
1408.2283 1416.5873 1472.2031
1480.9478 1482.3063 1495.4515
1499.7843 1501.7549 1510.8339
1786.3196 2998.2734 3011.6162
3022.5049 3037.4470 3047.4208
3064.7341 3084.7917 3090.3005
3103.3404 3117.6763 3155.6943

TS: β

-1173.9213	32.9720	73.4852
94.7822	119.7425	126.1169
179.4293	232.0661	256.9639
299.3939	324.0425	345.7586
368.1871	488.5280	595.5507
708.7092	770.5368	851.2737
883.9125	927.2001	954.6728
998.5969	1039.4348	1095.3359
1103.6061	1132.4922	1173.1566
1195.0851	1204.4555	1214.7082
1243.2202	1256.4304	1283.2530
1296.3319	1374.0672	1410.2563
1417.5413	1453.8495	1472.7755
1483.2400	1483.4703	1499.9933
1500.4247	1507.1982	1514.0402
1808.5980	2975.3473	2989.1805
3021.2182	3027.7652	3049.0504
3065.8434	3089.2271	3095.8464
3104.5791	3120.3969	3156.6818

TS: γ

-1151.3110	22.2245	62.1550
105.5474	109.6299	117.4777
173.5160	200.4107	252.7006
286.2186	340.6532	349.8635
359.8440	490.4307	583.8586
703.0117	768.4635	849.0930
884.7724	927.5619	956.3375
997.5870	1046.1303	1092.9733
1103.7548	1132.2698	1172.9387
1186.7513	1201.6108	1213.9778
1242.9131	1266.9941	1293.3118
1311.2551	1373.9679	1411.5908
1412.2020	1464.0722	1472.5289
1477.3522	1483.0878	1483.2466
1493.1018	1500.4280	1508.4492
1805.8970	3001.9878	3007.3221
3032.8369	3044.6703	3047.3481
3057.9563	3066.4000	3072.5104
3094.9011	3117.5933	3154.8029

TS: δ

-1178.5096	25.8384	64.9030
100.7092	110.5300	112.2322
154.0532	182.7596	249.9428
294.0358	319.2896	364.2865
488.8695	579.7139	588.9042

703.5674	737.0209	827.4884
883.0248	923.5283	947.1695
998.9737	1045.5277	1072.4479
1100.5616	1129.2605	1172.7836
1185.8782	1191.9563	1207.5770
1212.1052	1219.6243	1289.6359
1301.5804	1330.1826	1375.9157
1410.7236	1458.3017	1465.2839
1471.9423	1479.6123	1482.4071
1500.3013	1504.3876	1684.2309
1807.4043	2968.0406	3019.0856
3025.5169	3041.9650	3047.4638
3056.3053	3075.2376	3082.3836
3117.7475	3154.3893	3154.5729

(2) methyl-2-pentenoate

48.7455	97.3390	114.3752
124.4214	144.3960	220.2054
238.5439	309.4100	352.1053
395.1359	482.1826	725.0058
729.4871	795.8750	884.7299
902.0985	940.9437	1006.5262
1021.6414	1049.0270	1096.3706
1144.5754	1172.5472	1199.9191
1214.0116	1276.6512	1311.9057
1337.7502	1366.8819	1411.8395
1470.6595	1480.9780	1483.2236
1499.1070	1499.7692	1507.8080
1708.9607	1785.0713	3006.2357
3029.3655	3045.4736	3055.9508
3095.5326	3099.3912	3114.4511
3135.4090	3152.7076	3175.7779

TS: α'

-1297.0389	47.0278	81.9601
115.5800	123.9903	144.9828
199.6672	235.7805	317.6253
336.8376	364.4350	397.5997
487.0685	550.6224	720.7949
725.0045	795.0020	881.4636
898.8857	938.6426	1013.7156
1022.3726	1079.2036	1096.4022
1116.3263	1146.3003	1182.6923
1204.5497	1270.7083	1286.0391
1296.6983	1311.6603	1336.7157
1366.5606	1412.0669	1452.9922
1466.8498	1483.2917	1499.1083
1507.6532	1704.1920	1794.7108

3007.4408 3030.1699 3057.8818
3090.8718 3096.7043 3100.6347
3137.0193 3180.0464 3197.7043
TS: α
-922.8453 35.3339 90.6701
93.1095 119.5878 131.1380
174.1277 230.6095 268.2031
289.3810 310.8495 348.8997
391.5034 479.7031 710.5263
740.9678 793.7298 883.0580
902.8868 909.3731 951.4683
1002.6837 1034.2788 1068.7991
1094.6747 1147.5549 1172.4941
1210.3389 1244.7417 1270.9557
1301.2691 1354.7926 1411.9722
1471.2745 1482.6719 1484.7497
1498.5018 1498.9018 1507.5431
1698.0408 1759.3477 2247.7185
3013.0187 3029.6344 3048.0078
3058.7614 3078.5588 3098.7849
3102.0774 3118.4399 3158.0955
TS: β
-1033.8335 43.5731 92.7169
96.7324 113.5101 135.4886
182.9537 234.2572 250.9083
301.7124 311.9137 352.9634
399.0332 497.8440 716.0564
726.8521 792.8355 866.9222
890.1845 929.5300 991.5156
1001.7736 1035.8945 1073.8851
1094.2700 1108.1766 1172.9094
1173.1265 1210.4123 1267.2537
1313.5701 1342.7813 1411.4039
1467.3505 1470.6599 1481.0853
1498.7316 1499.3661 1506.7576
1700.8209 1794.8868 2046.5243
2990.5671 3030.0762 3035.9273
3045.7345 3095.9877 3104.5297
3106.4906 3115.0528 3153.3161
TS: γ
-847.8711 52.0433 98.3021
110.5942 124.0171 147.5881
218.8807 227.8699 272.4704
279.9377 343.7541 364.7951
397.5321 502.5042 725.9158
731.2199 834.7255 884.9512

912.8792 947.0059 1011.2319
1024.8458 1067.7044 1096.2261
1147.0369 1172.2716 1201.8093
1215.1389 1246.2831 1295.7536
1330.5046 1358.4637 1380.8527
1413.7199 1470.6795 1480.8260
1494.7267 1499.2964 1499.4479
1538.8571 1699.1793 1781.5427
3027.3664 3045.9717 3065.7064
3089.3429 3102.4402 3115.2959
3139.2668 3153.9589 3178.8859
TS: δ
-1174.5033 50.5804 93.5937
101.5591 116.5507 120.7734
166.6374 227.7027 281.6212
307.3125 346.3819 417.1840
483.6792 571.2086 727.2664
730.8232 807.9801 887.5790
924.8475 949.2959 1004.7583
1022.7799 1047.6650 1061.2677
1130.1415 1172.6213 1192.2236
1199.4017 1206.6168 1216.4942
1280.4777 1300.3222 1330.5506
1354.9672 1461.7532 1471.2228
1481.4150 1485.3084 1499.3211
1686.3607 1702.2542 1784.7074
3014.6972 3046.0775 3066.8803
3081.4513 3115.4916 3145.2792
3153.8777 3163.7528 3177.2326
(3) methyl-3-pentenoate
32.0611 67.2929 119.8152
127.1646 175.0541 207.5362
263.2725 270.9333 336.5749
373.5947 531.2067 593.2002
705.5366 779.1656 892.5822
933.0984 965.9796 1002.3412
1007.1446 1069.3315 1088.7022
1137.2684 1173.4974 1181.4350
1210.7257 1232.9979 1308.4858
1332.3785 1381.6440 1416.6497
1455.7466 1472.4102 1481.7804
1483.4763 1494.1989 1500.4552
1741.9445 1808.8959 2995.5245
3012.6089 3048.4907 3054.8609
3089.9889 3093.1369 3113.3742
3119.4340 3149.5216 3155.6914

TS: α'

-1296.6869	27.9940	61.1095
95.7755	125.6002	147.0426
206.9624	262.9409	274.8773
323.5376	342.5072	386.9681
539.2930	548.3947	578.3714
699.3739	776.0609	882.9840
928.8774	964.5634	999.4906
1045.5442	1069.8154	1091.4176
1110.8552	1142.8366	1159.6734
1200.7715	1222.0941	1276.7815
1288.8818	1308.5944	1334.5453
1379.4816	1416.8555	1450.6730
1452.8760	1482.0336	1493.7566
1498.8084	1742.7964	1822.6746
2997.4583	3013.8291	3056.7198
3083.4865	3093.4975	3093.5631
3113.3333	3148.9595	3201.7138

TS: α

-721.7026	39.3140	79.9099
114.3248	116.8522	166.5318
195.7585	206.3890	253.0215
269.4529	332.0861	346.5160
390.2099	527.5878	649.9659
714.8385	788.9225	900.9981
938.2366	971.9388	1003.7107
1010.7860	1066.7208	1098.0029
1144.7511	1172.8601	1177.4391
1206.4794	1216.2637	1300.3177
1329.8032	1356.7396	1391.4058
1415.0377	1472.3087	1480.2288
1482.6940	1490.4219	1499.7915
1656.1117	1760.8409	1804.4756
3012.1880	3049.0923	3054.2445
3094.7217	3101.7290	3116.7236
3120.3960	3152.8403	3157.0704

TS: β

-984.9429	25.9093	60.5748
105.6532	114.8282	168.9539
178.5960	230.6347	247.5306
269.9078	293.0702	359.1067
366.6289	529.8648	597.9877
696.5927	796.0752	875.6894
904.7902	943.5967	956.4566
1006.6964	1064.7870	1076.0824
1102.4289	1142.4464	1172.9802

1186.2216 1205.6113 1212.5866
1298.8643 1355.9992 1411.7544
1436.6442 1471.8017 1482.5953
1484.4484 1490.3879 1499.9761
1744.7728 1819.0631 2075.8990
2995.4145 3020.3991 3028.6322
3048.4098 3049.7271 3065.1478
3118.8687 3119.7309 3156.3755

TS: γ

-1032.1237 30.8899 60.0516
105.9542 112.2290 157.9937
173.3516 244.7408 251.6451
284.8671 297.7521 342.0402
373.9919 517.6621 586.0480
704.4423 789.1353 887.4671
935.0847 967.1153 979.2658
1007.3382 1057.1922 1062.2621
1108.0317 1152.2109 1172.7893
1185.3143 1209.3715 1227.5530
1282.0029 1373.1847 1403.0806
1455.8405 1464.5429 1471.9041
1481.9190 1482.7255 1499.6194
1737.6353 1807.8577 1961.9387
3002.2540 3003.7179 3049.0846
3064.2157 3069.2166 3071.6806
3109.8427 3120.3303 3156.9025

TS: δ

-1138.1893 32.3402 58.7734
101.7578 126.6522 168.1034
180.9114 240.3446 267.3972
314.3404 371.9023 385.0908
512.8762 567.4222 594.0168
710.7632 794.9239 898.0662
944.7736 972.7474 994.2255
1009.4975 1061.8657 1104.6994
1142.2369 1173.3594 1183.3137
1210.9677 1229.9956 1283.5777
1306.2880 1330.9127 1347.4543
1384.0196 1398.9423 1453.3379
1470.6581 1473.1281 1483.8118
1500.0905 1702.6529 1809.2190
2992.2498 3049.5363 3066.1344
3091.4384 3115.8270 3121.1110
3139.5498 3154.4166 3157.4075

(4) methyl-4-pentenoate

16.6670 57.2557 92.7146

112.5576 147.5622 174.6019
291.1352 308.2240 387.1814
467.6997 584.5712 641.3662
711.8789 795.1370 892.5982
945.5993 950.5851 996.1722
1002.2071 1034.8376 1071.8296
1133.5347 1172.6229 1189.1236
1211.0972 1223.1553 1299.4606
1313.2820 1329.2831 1393.8013
1454.2629 1462.5675 1472.3457
1482.7523 1488.0588 1500.0339
1709.4824 1806.4934 3028.4503
3035.9902 3047.6778 3062.4104
3081.8066 3112.1156 3118.0367
3126.4770 3155.1506 3208.7911

TS: α'

-1297.2307 23.9857 54.9672
88.6951 106.7226 141.0743
158.3861 294.4513 313.7652
330.0471 395.9082 471.5088
548.1752 578.7906 642.0722
710.9218 792.7383 882.1913
946.8492 951.7208 996.2921
1031.4640 1034.4925 1083.3070
1113.1853 1133.4188 1164.2528
1201.0485 1222.1322 1275.5088
1288.1354 1298.5006 1312.6318
1329.5882 1393.0994 1452.9437
1455.1371 1460.5109 1488.3687
1498.8570 1710.0211 1819.3880
3028.9167 3036.4593 3062.1122
3082.2152 3093.0070 3113.4383
3127.1372 3201.5356 3209.7275

TS: α

-1213.9068 52.4273 61.1985
88.0102 117.1022 144.2082
175.0311 273.7750 307.3528
319.6131 341.9662 395.7074
474.2364 642.9753 695.5115
720.9481 828.4542 898.2221
948.2652 952.8456 1001.6443
1004.8282 1035.8452 1081.9008
1119.1779 1172.0285 1183.8368
1201.9341 1212.6930 1262.3959
1298.8749 1307.4655 1328.1855
1343.6412 1396.2750 1453.5582

1472.1964 1477.0339 1482.3474
1499.5265 1709.8010 1785.1615
3017.3937 3048.1790 3056.5192
3115.7846 3118.8968 3120.9673
3128.6757 3156.8968 3210.3966

TS: β

-979.8031 40.5021 66.1501
115.3663 118.9891 134.5722
188.5248 279.1264 291.3040
296.2511 334.9722 381.6613
506.7881 584.5449 663.2916
716.0314 841.7748 896.1069
943.7753 949.1456 1008.1786
1017.6646 1041.6050 1083.6995
1138.0075 1173.2637 1195.2347
1202.5149 1216.3143 1280.1995
1292.8624 1327.0208 1355.7350
1391.5954 1399.4683 1460.2083
1464.0317 1473.1374 1483.3058
1500.0491 1686.2812 1808.2976
3017.0335 3049.6896 3077.3265
3101.6439 3120.1517 3121.1777
3131.4601 3157.4586 3215.8931

TS: γ

-1044.6045 28.8186 56.2219
89.9516 110.8206 123.6024
173.8668 224.9730 284.5834
305.3528 359.2970 380.5052
461.3709 585.5307 627.2350
708.7454 788.4186 887.4829
916.3366 935.1872 983.7144
1000.0645 1004.3494 1069.1931
1088.2742 1158.8406 1172.1142
1190.1193 1193.1518 1212.8183
1300.7896 1305.3141 1391.3162
1427.1388 1461.1726 1471.7335
1473.4474 1482.6957 1499.7615
1706.0923 1805.7599 1930.2983
3007.5555 3046.6566 3049.0447
3052.8450 3078.8819 3083.1873
3119.7623 3157.0758 3173.3549

TS: δ

-895.7584 29.6438 55.2837
89.7630 113.5008 133.6718
173.8802 191.4669 233.0085
302.7364 319.8266 403.5363

478.6293	584.7816	675.7161
715.0897	792.7181	891.8140
917.9174	918.3431	928.8947
994.5431	1000.4571	1069.1321
1094.1759	1107.7701	1172.6005
1186.8533	1193.8312	1212.2883
1287.1023	1305.4898	1322.1568
1393.1442	1463.2136	1472.5078
1483.0982	1486.4888	1499.9032
1660.3101	1806.1577	2291.3912
3032.9281	3040.4841	3048.6081
3066.3242	3085.2325	3099.0183
3119.4285	3156.4715	3191.3881

(5) methyl 2-methylbutanoate

23.0374	76.5175	114.1620
135.7321	168.2767	216.6165
239.2333	277.1149	311.5122
346.4196	361.5736	471.3024
680.6869	756.3588	780.2239
839.2820	876.4828	974.1048
987.3074	1006.7875	1040.3657
1109.2253	1142.1213	1172.6015
1173.4111	1203.4977	1212.9534
1292.5305	1333.4846	1347.4499
1396.7006	1403.1858	1417.3002
1470.6458	1482.1107	1488.4988
1498.5181	1500.5734	1503.6822
1510.5400	1513.6124	1802.0141
3023.0730	3024.8111	3033.3818
3038.6665	3047.2190	3063.7776
3086.7161	3094.0630	3101.4402
3114.6121	3117.3704	3153.8385

TS: α'

-1295.2492	31.5699	67.5324
99.4640	125.3316	170.4162
220.4814	230.5180	277.7140
304.5705	340.0811	364.3552
371.0091	473.4399	549.0526
673.7127	751.0292	778.5228
835.0647	870.4512	975.1080
988.4419	1026.6934	1060.4434
1104.6621	1114.7452	1145.8403
1157.3905	1197.9202	1200.9367
1277.7699	1289.3533	1292.8495
1329.7662	1345.1628	1395.2792
1407.4530	1418.4347	1452.1156

1487.6400 1494.5544 1499.5356
1504.0942 1510.5585 1515.3362
1814.5528 3020.8527 3024.6984
3035.2306 3039.4948 3064.7444
3088.2644 3091.4580 3094.9645
3104.2523 3119.1715 3199.5740

TS: α

-889.0634 35.5832 72.6517
115.5523 144.1810 167.7848
196.0213 231.0734 279.2881
299.6088 303.5620 340.8775
353.9966 400.7601 471.0715
648.5411 760.6452 783.6352
841.1707 884.4342 990.3824
999.2574 1011.4772 1048.3228
1108.4204 1167.8402 1172.5793
1175.3828 1207.4783 1215.4455
1275.4527 1299.2154 1313.9638
1375.6218 1397.4707 1409.2944
1416.2829 1471.0483 1481.4545
1481.7091 1495.2425 1499.1693
1500.3224 1505.5278 1512.0981
1784.3380 3007.9785 3025.6764
3028.7657 3048.4774 3077.4708
3091.4232 3094.5468 3101.6371
3119.5795 3134.1429 3155.8503

TS: δ

-1193.4355 36.7726 78.4455
110.0364 125.7165 130.2537
200.1096 235.0882 236.8498
257.2940 325.8803 347.5433
394.6791 487.6365 569.5491
685.1967 753.1187 783.4884
854.8526 887.8552 978.9696
982.9401 1019.7938 1037.6602
1088.2853 1112.3691 1153.3745
1173.3794 1191.5753 1201.2525
1214.0773 1219.1967 1278.3469
1329.1411 1355.5381 1389.4961
1414.9991 1441.3017 1472.1235
1483.1667 1494.0168 1499.3865
1500.0821 1508.5236 1685.9107
1804.4726 3025.7825 3027.6766
3040.0758 3049.3168 3063.1475
3089.8831 3095.3480 3101.0580
3120.8429 3156.7365 3184.8146

TS: β

-1175.2662	27.5271	78.7767
116.8620	135.3316	176.5335
202.0244	234.4962	240.8072
277.0055	317.7384	322.3013
353.2970	397.4679	487.9969
700.7100	767.2990	833.9107
856.5072	882.2278	972.5203
996.8404	1016.0560	1063.4125
1098.1692	1113.7042	1166.9739
1173.3319	1192.8532	1214.6176
1242.9590	1256.5241	1308.5381
1339.6025	1398.5605	1405.0068
1412.9547	1471.6755	1474.7070
1482.5692	1492.4994	1499.8136
1501.2373	1504.3920	1507.1637
1803.5731	3013.0656	3034.2274
3048.9442	3050.0241	3064.9913
3088.1153	3101.7955	3106.2203
3112.1926	3121.3332	3156.8815

TS: γ

-1199.1214	30.0404	88.0639
109.2801	116.6855	124.4092
195.3078	212.5742	233.9611
300.8975	315.9753	348.2311
379.2211	487.0857	580.8317
673.2740	756.1226	793.4719
848.2119	882.9253	976.6052
984.7237	1016.5925	1045.0681
1085.0156	1120.6031	1169.1761
1172.4963	1199.4510	1210.9327
1212.4405	1218.7918	1288.8640
1320.3108	1349.1643	1380.2849
1417.0873	1467.4265	1470.8962
1482.5013	1492.8825	1495.3614
1500.3270	1504.4839	1661.2017
1802.3949	3024.1772	3039.2119
3042.2473	3048.2017	3072.7803
3077.6505	3107.6678	3112.7415
3118.9907	3155.6704	3159.2099

(6) methyl tiglate

59.0100	116.3642	123.5275
141.2081	154.3364	177.7685
239.0375	297.6463	348.5556
403.0483	433.9764	490.3682
664.2402	753.4215	820.3017

914.4588 925.0127 1013.2859
1027.6060 1065.3481 1072.0355
1101.8136 1173.7210 1178.3163
1213.3910 1275.4246 1376.4412
1413.3248 1427.1312 1470.3595
1479.8098 1481.5177 1483.8344
1484.1826 1495.6767 1500.7143
1706.7524 1781.7655 3017.2316
3039.1433 3046.8217 3055.2529
3084.7063 3112.7895 3116.6804
3126.7474 3152.1231 3153.1083

TS: α'

-1294.8331 56.6566 92.9424
122.3749 138.2356 147.8569
183.0515 223.9793 301.4924
327.0495 368.2109 407.6134
436.0664 492.6816 550.5074
666.3094 745.6412 809.4664
911.6811 922.7534 1024.3463
1045.1663 1065.7788 1071.7507
1099.0518 1130.1183 1167.6798
1202.8690 1255.2713 1287.3562
1293.9278 1378.5529 1413.6371
1427.9211 1451.3581 1477.0229
1479.5392 1483.4078 1484.5579
1495.7973 1702.1314 1790.1609
3018.2074 3040.6878 3056.4649
3086.9153 3091.4664 3115.5012
3129.7315 3154.6356 3198.4311

TS: δ

-1177.6527 57.0356 109.8426
117.8938 118.7472 144.1438
179.3415 232.8623 290.6546
301.8147 356.3717 401.0052
473.6431 507.7969 543.9777
674.3800 763.6789 829.9614
900.5581 925.8608 1012.4089
1041.2800 1057.8271 1064.0344
1105.5512 1173.8932 1182.2800
1214.7732 1273.1768 1297.3446
1337.1995 1359.0604 1401.7871
1416.5641 1466.4836 1472.7204
1480.2100 1481.9978 1488.5087
1500.1873 1671.7563 1782.2208
3016.3221 3048.8132 3054.0955
3098.7112 3117.6545 3119.7527

3155.2748 3160.2767 3171.8056

TS: β

-1054.8900 37.0690 102.2937
110.5406 125.3772 160.3425
163.8880 174.4253 249.6367
281.1099 333.4216 356.8353
391.9343 447.0368 474.6266
641.6336 767.6159 811.9897
919.0193 965.2914 996.8168
1016.0963 1038.1440 1055.2714
1074.7007 1118.2497 1150.2575
1174.0548 1211.3796 1258.6351
1396.1856 1413.4050 1464.5324
1470.2181 1472.8393 1479.7890
1481.7741 1491.0827 1500.6890
1698.1449 1790.8589 2067.4272
3010.4206 3040.8049 3047.2858
3064.9298 3074.6167 3093.7795
3117.3749 3125.0056 3152.8889

TS: γ

-1073.8432 56.4268 100.7748
116.0064 132.4078 149.0312
181.7040 203.9260 298.9592
344.6572 348.8087 405.6988
447.5596 487.9285 524.9141
672.5927 756.2456 823.8964
926.8634 943.1949 1014.8937
1037.9998 1058.8138 1064.0951
1113.0747 1173.5591 1181.5533
1214.1640 1274.6216 1281.9265
1355.4663 1381.8217 1425.7804
1460.0082 1470.5870 1479.7846
1481.5914 1481.6767 1499.8118
1504.7033 1678.8155 1775.9460
3037.8593 3047.5859 3077.1087
3083.3096 3117.9444 3124.5841
3141.4516 3153.7183 3163.4309

(7) methyl 2-methylbut-3-enoate

16.7405 83.7991 117.3694
147.8525 203.2646 232.4962
262.9459 288.1961 319.0628
405.6259 456.4853 648.0422
722.1882 789.9714 853.3587
890.6612 951.0345 985.3236
1001.7206 1035.5652 1067.3087
1103.2568 1172.9354 1180.6547

1193.0408 1213.6666 1310.9145
1323.7765 1363.4252 1405.4204
1452.5168 1470.6186 1482.5250
1496.4333 1499.0743 1502.6219
1703.6151 1800.6849 3034.7834
3049.6180 3075.6825 3101.9586
3117.5187 3121.4090 3126.5942
3140.4675 3157.0098 3211.5360

TS: α'

-1304.3730 19.9452 73.6927
102.1112 134.6403 212.9816
227.9564 235.5095 286.2062
329.0879 350.7728 407.5414
463.5207 551.2788 645.8911
709.6284 783.7144 846.5468
886.5892 954.3066 988.7275
1029.2807 1034.9602 1077.7253
1105.9348 1111.8901 1158.1510
1188.3484 1201.0798 1274.4957
1287.5463 1310.1816 1323.4607
1360.6556 1408.7906 1451.1890
1452.9821 1496.1578 1502.5310
1503.7801 1702.1698 1811.8456
3038.0333 3074.6782 3094.0287
3104.8618 3120.4234 3128.0562
3138.6466 3202.6109 3213.9245

TS: α

-711.3260 53.1917 70.6658
118.1879 131.5763 189.6558
202.4618 247.7871 267.7599
280.9664 329.9657 344.2616
431.2459 511.1292 597.4773
679.7265 795.9168 844.7005
904.3119 949.1064 994.7592
1021.0716 1045.6751 1063.6521
1120.5828 1156.5703 1173.3804
1195.7777 1217.1730 1267.7258
1317.6925 1362.0420 1413.6384
1450.1057 1472.3662 1483.2472
1489.0517 1494.8080 1500.6213
1620.7638 1711.2068 1799.2837
3041.4622 3050.3004 3108.7339
3117.9289 3121.9429 3126.7807
3149.0833 3158.6912 3232.5641

TS: δ

-1189.7941 27.3053 84.0669

114.9104 129.3592 144.3107
204.0880 230.3452 264.1617
317.1947 362.2460 399.6141
454.0543 569.8266 650.7965
718.6814 787.4032 863.8345
909.8477 949.9722 983.9508
994.2347 1032.6824 1061.9908
1090.6751 1147.1981 1172.8695
1186.0309 1200.9904 1214.5288
1217.2620 1296.8639 1318.5059
1367.3855 1439.0542 1447.3798
1471.4656 1482.9481 1498.4660
1681.1611 1693.0532 1802.8724
3051.0217 3074.7724 3093.3707
3123.6628 3128.6537 3146.6588
3159.4479 3182.4791 3213.8496

TS: β

-1031.7004 17.9311 59.3876
108.5799 124.6819 184.3624
209.2162 211.8697 252.4771
313.7754 320.7279 370.8959
389.5802 485.0607 630.6866
665.0669 781.3720 838.8063
886.5906 918.7617 976.1418
983.9040 996.2006 1059.1176
1108.1565 1134.3576 1142.1387
1172.0949 1189.6047 1216.3791
1287.1421 1338.1164 1412.9199
1423.8489 1470.7495 1482.6578
1493.7321 1498.3200 1500.0983
1699.0447 1809.5869 1990.4858
3001.8988 3045.8874 3049.6353
3083.9179 3112.8563 3121.5540
3128.8867 3158.2948 3176.0897

TS: γ

-909.3531 15.3164 81.5306
116.2808 137.0599 170.3778
188.7538 223.1792 247.7554
278.2798 309.1328 335.9063
415.2395 469.7464 675.0335
721.8585 783.5298 853.1601
886.8303 920.5902 945.0601
951.2290 997.9998 1056.0571
1092.6201 1108.1788 1138.9246
1171.8587 1184.7334 1214.2072
1276.7570 1330.5676 1359.1080

1406.5992 1470.5182 1482.4278
1495.4267 1498.7360 1502.9963
1650.9831 1800.4199 2269.9481
3036.5376 3050.6478 3082.8849
3103.5297 3116.2531 3122.2722
3122.9179 3158.7367 3194.7250

(8) methyl 2-methylenebutyrate

53.5869 72.4042 121.6173
152.3081 175.9337 274.6625
300.9423 352.7617 371.7356
398.5545 496.4607 637.8169
663.2528 803.2883 833.2489
840.0102 891.5441 971.7447
1010.2641 1025.6231 1083.7296
1113.4902 1169.0284 1173.4542
1211.6001 1289.8435 1304.1440
1393.3212 1414.4592 1438.2249
1472.8765 1475.6960 1482.2884
1500.8464 1505.1238 1511.9061
1692.7481 1777.4147 3026.7812
3029.7748 3045.4423 3046.9167
3089.3348 3096.5302 3116.7291
3153.5079 3158.9625 3246.9498

TS: α'

-1300.7232 53.5026 71.3347
100.8327 136.7972 180.4799
273.5550 308.4067 315.0634
355.8930 385.9843 406.8423
498.1589 549.4621 633.9479
665.8942 803.7532 826.6805
833.8549 884.7160 975.5286
1021.0417 1046.5189 1090.9372
1113.0963 1114.2710 1159.5612
1202.7059 1276.6703 1291.8455
1294.2789 1299.0847 1393.5040
1415.2620 1439.1906 1453.9921
1474.6303 1476.4753 1505.4329
1511.8514 1690.6902 1786.5173
3027.3239 3030.3549 3046.3584
3090.3864 3091.9918 3098.1330
3161.5267 3199.0119 3249.8305

TS: δ

-952.5448 31.5358 69.3822
124.2257 138.2087 155.4799
169.1969 269.0660 276.5251
325.5943 356.0743 379.5930

395.5086	518.6742	656.7353
678.8261	792.6283	820.0488
832.6971	879.2463	928.4040
954.8712	1019.9754	1082.5871
1095.9187	1097.5848	1143.0118
1173.1812	1212.6709	1283.7612
1293.3682	1359.6440	1417.8341
1466.1948	1473.0995	1483.1781
1499.6473	1504.5546	1509.2216
1641.9224	1774.2076	2305.8499
3028.3961	3032.6454	3048.0399
3053.9621	3091.6054	3097.7022
3118.2806	3157.1597	3207.5301

TS: β

-954.6166	53.2560	75.2791
121.5731	149.3252	174.6204
238.3169	271.5981	297.1401
308.7239	359.3762	379.0207
458.0691	500.3220	660.3846
670.2544	828.8389	838.8355
854.2814	901.8759	962.0031
1009.3405	1044.2146	1085.1464
1108.9962	1172.8803	1173.3241
1212.2576	1244.7852	1299.0105
1346.3987	1390.1943	1411.6224
1436.7625	1470.4188	1474.7671
1482.2785	1499.1410	1500.5910
1506.8323	1670.1057	1779.7371
3025.6530	3048.3699	3080.9124
3093.6295	3106.0621	3119.1311
3155.5543	3159.6752	3250.3336

TS: γ

-1188.1874	50.8019	64.1551
120.4446	125.8268	152.6880
159.7000	258.8936	333.7609
351.2095	371.2393	390.6368
508.2943	579.9494	637.4526
673.3722	809.5319	838.5162
845.8078	900.9498	973.4104
1000.6606	1010.1163	1061.8749
1106.4531	1162.7487	1173.3078
1198.4001	1200.7801	1212.0027
1293.3873	1295.1106	1367.6477
1434.7158	1468.6571	1471.5814
1474.8092	1482.6935	1500.6654
1692.6538	1709.1472	1777.8110

3028.6234 3048.0503 3052.2443
3078.1521 3118.5107 3153.4628
3155.3600 3157.9568 3244.9026

(9) methyl isopentanoate

29.5059 79.5629 114.8391
142.9859 179.1433 226.3020
250.3679 288.2246 320.2340
360.2140 420.7520 460.0668
594.2665 712.3608 832.9150
895.1930 902.5448 935.3552
961.9888 971.0983 1024.3480
1127.4730 1142.4920 1172.4589
1188.2430 1203.4580 1216.3329
1258.3841 1325.0577 1368.1415
1397.2491 1403.4672 1423.1173
1458.7608 1471.5318 1482.6950
1491.2764 1496.0017 1499.9460
1506.7180 1515.8843 1802.4118
3014.2473 3017.2659 3024.2547
3033.6700 3047.6283 3061.9711
3073.7042 3081.6624 3087.7843
3105.9976 3117.7676 3154.7660

TS: α'

-1296.3808 37.6183 76.7286
99.5987 146.4830 158.0866
231.8223 255.9378 293.0018
317.1145 338.0741 369.5161
422.0131 464.1367 548.8464
588.1275 711.0464 833.3468
885.6479 898.4792 937.6410
968.5348 970.0364 1059.2210
1110.3493 1126.6792 1146.0080
1173.1492 1198.3544 1203.6871
1254.7593 1277.3954 1289.8850
1321.8548 1367.4326 1396.6275
1404.2412 1423.6658 1453.0230
1457.6819 1491.1594 1495.4784
1498.1123 1507.3540 1516.3365
1815.9224 3015.5885 3018.3873
3023.5602 3034.3977 3062.5954
3075.8313 3083.6639 3089.8617
3092.7343 3105.8349 3200.8706

TS: α

-1192.5066 49.8823 73.7206
113.2997 137.8659 174.3464
232.0381 237.3623 259.5571

308.5088	325.6180	328.6861
397.1976	451.5700	460.9887
686.5262	719.8432	838.4899
902.5072	920.3793	936.0928
967.2082	972.4011	1034.5614
1115.8214	1140.1801	1172.1948
1185.4221	1200.5437	1212.3878
1215.6088	1305.3090	1311.8390
1334.8587	1350.3794	1394.5699
1405.3643	1420.1890	1472.2617
1482.0255	1489.3588	1495.9828
1499.8631	1505.1659	1515.2902
1782.2909	3018.5792	3021.8341
3040.3135	3047.5837	3078.7287
3085.1322	3094.8719	3096.2491
3108.7427	3117.9264	3156.0448
TS: β		
-1121.5861	31.6562	85.1617
121.4235	151.1744	169.5463
203.1702	218.7186	279.9236
309.5318	320.4251	338.4599
354.9477	414.5863	467.0272
590.4880	715.7125	822.0434
897.0220	911.7320	949.5356
975.7546	990.9319	1027.9435
1096.6149	1143.3619	1173.4101
1192.6807	1199.7834	1212.3839
1218.8483	1276.7732	1317.2305
1379.7988	1400.3011	1407.8653
1420.9764	1447.6836	1472.2895
1482.0140	1483.5107	1489.2977
1499.5377	1500.6516	1516.6701
1808.5825	2994.4012	2997.0117
3004.9180	3048.6777	3057.4338
3065.4300	3072.2100	3094.1528
3119.5349	3130.6218	3156.0730
TS: δ		
-1168.0508	38.7225	81.7228
116.8562	123.5543	156.8192
177.9083	239.7272	260.7745
297.8900	321.8415	369.1222
413.8640	490.6085	593.1798
594.1299	711.1036	841.7154
896.5410	906.6495	935.3047
958.3935	974.3529	1022.0558
1099.3188	1138.6631	1172.3519

1174.0321	1192.8779	1201.6109
1206.7716	1220.0328	1243.8221
1320.2470	1365.8733	1386.4109
1414.7609	1453.8064	1458.3857
1472.1986	1483.3286	1499.7972
1500.1717	1505.1435	1710.4094
1802.7091	3019.2537	3022.9251
3033.6643	3048.9851	3066.3326
3072.6681	3082.8575	3098.1476
3119.8343	3156.5652	3168.1285

TS: γ

-1168.0146	34.9793	78.8980
120.1856	131.7135	143.9577
177.9720	233.5188	253.8328
289.6395	344.0014	369.9465
433.7924	451.4705	578.8135
597.7770	714.7107	840.2156
896.3272	903.5772	937.4975
961.0389	974.4256	1022.1939
1105.4985	1136.4779	1156.0018
1173.0859	1194.6251	1201.7684
1208.9014	1219.6427	1259.0573
1323.2365	1349.9778	1396.9712
1403.9939	1458.6772	1461.4200
1472.6916	1483.3024	1496.5510
1500.2571	1506.9164	1703.6113
1802.2489	3021.6725	3031.1192
3036.9622	3048.5557	3065.9023
3069.4069	3087.9531	3106.0247
3119.3127	3148.4053	3156.1166

(10) methyl senecioate

54.3915	81.0587	110.0089
135.4095	171.9516	175.0597
248.8208	321.3054	344.9043
384.6610	472.3652	479.3493
747.0179	751.7201	837.6217
877.4493	936.7353	961.2700
1005.6713	1028.1689	1106.8465
1107.8258	1171.5462	1173.1376
1210.0456	1251.5964	1380.6746
1411.2884	1416.0328	1470.2212
1472.5083	1475.7512	1481.8887
1490.6310	1500.4916	1505.2672
1699.3277	1772.2040	3011.5570
3018.2101	3044.3988	3052.4739
3061.1359	3111.8044	3112.3830

3151.0512 3168.7368 3174.9969

TS: α'

-1290.1444 52.8270 79.0158
89.7302 124.3803 165.0217
177.4848 227.8811 324.0823
332.8046 363.0649 391.9396
474.2629 483.2626 550.6818
739.9130 744.5288 839.9919
874.5130 929.5026 961.0920
1003.6929 1059.4013 1104.7248
1106.2077 1129.6029 1155.7219
1202.3514 1240.7174 1289.8314
1299.3998 1380.5470 1411.3958
1416.0303 1451.2158 1457.6593
1471.9981 1474.9275 1489.8707
1504.2192 1693.4897 1783.1542
3012.9567 3019.5771 3054.2500
3062.6581 3088.9789 3113.5117
3170.3069 3179.7722 3194.8720

TS: α

-951.7987 15.9760 95.0409
103.0906 129.9597 159.8408
162.2977 184.1135 252.1167
300.4865 336.5266 359.8129
375.7472 473.6589 478.5928
721.0519 758.3316 817.5978
911.5554 939.2064 958.5051
968.8958 1019.0629 1071.3533
1098.7635 1127.3116 1172.8239
1208.7271 1216.3418 1266.2445
1391.7371 1409.4161 1470.1440
1471.2761 1479.0351 1483.0104
1484.1414 1499.1355 1502.8450
1690.7830 1741.7366 2212.1652
3014.5035 3022.5158 3047.1740
3059.9216 3066.9563 3116.7777
3134.9270 3156.4015 3165.7388

TS: δ

-1118.5845 58.8551 97.2395
111.2156 130.0190 170.8168
176.8644 238.2905 283.3645
323.7326 347.9658 382.0167
476.3450 536.9655 551.5034
744.0747 750.9984 854.7959
870.6720 938.2425 983.9227
1011.8732 1027.7611 1095.8658

1107.3711 1172.5809 1174.5747
1209.3254 1251.9999 1290.6732
1336.4800 1374.6786 1413.1349
1429.9033 1466.6178 1470.6808
1481.0809 1482.8204 1492.0252
1500.0892 1667.7351 1765.5600
3016.8015 3044.8601 3062.8759
3078.8854 3113.2791 3114.8140
3152.2083 3180.0809 3188.3503

TS: γ

-1173.5057 56.3723 101.5045
108.5128 130.2050 143.6151
174.0667 219.6848 309.0281
319.7485 346.6458 382.1774
480.9119 523.5405 557.5437
744.0629 752.5953 844.7642
880.5562 938.4426 982.2084
1011.7099 1028.1849 1096.2673
1106.5990 1172.6949 1172.9968
1210.2808 1256.7508 1291.2142
1330.8933 1382.9189 1393.1208
1416.3277 1468.3677 1471.3397
1480.9045 1481.9503 1500.0357
1504.2195 1665.1035 1767.3335
3016.3959 3045.0697 3057.9441
3071.8193 3113.4769 3147.2694
3152.3996 3171.0505 3176.3769

(11) methyl 3-methylbut-3-enoate

25.4764 40.6895 114.0408
142.6498 192.3735 230.0431
285.4762 328.3932 402.2869
424.4993 472.7772 632.8373
709.2190 760.5961 859.3615
890.6651 936.3749 952.3651
977.7592 1030.7006 1041.5826
1070.8963 1171.8525 1178.5765
1208.1558 1245.5594 1281.0683
1367.7573 1411.5392 1446.0443
1466.3401 1476.1882 1481.6207
1482.5182 1495.4709 1499.2904
1717.4968 1803.8652 3009.8058
3029.3658 3048.7904 3052.8379
3084.2308 3107.3087 3119.8720
3140.8884 3156.2637 3228.0791

TS: α'

-1300.7773 29.6982 38.1545

90.4954 136.2218 191.9454
203.3548 299.9208 320.9816
346.1392 417.5423 424.4833
470.6143 549.7785 634.3797
705.1065 757.0856 852.6019
878.2940 934.5520 953.9901
977.0045 1033.5796 1064.4661
1082.7029 1117.9955 1162.3728
1199.1344 1245.8725 1261.4943
1281.1941 1291.0471 1360.2990
1412.3723 1446.4324 1453.4612
1473.6069 1481.7406 1495.4217
1496.8681 1717.4712 1816.2183
3011.2009 3035.7704 3054.6497
3087.2296 3093.6119 3108.8096
3141.1448 3202.1789 3225.2667

TS: α

-815.3075 36.0039 55.8482
122.1428 156.4715 188.0833
192.8689 250.8771 269.2858
317.5355 339.7894 380.8001
482.5969 499.8053 655.0239
714.5105 749.1318 872.7689
908.0113 950.2221 961.7653
984.1638 1034.8235 1042.6734
1070.9016 1172.5961 1176.4376
1209.4876 1219.8865 1268.7018
1333.7558 1409.9130 1412.0552
1441.7473 1472.7774 1482.3693
1482.9086 1495.0333 1499.2810
1600.0949 1711.1193 1799.0851
3010.4694 3049.4188 3053.9924
3090.5623 3109.9882 3120.7351
3144.1879 3157.6752 3248.1831

TS: δ

-900.3008 18.6036 45.6854
121.7333 152.3675 167.1807
182.1687 203.9310 266.2551
309.6555 325.9865 377.6512
422.0823 520.9038 601.5391
729.7774 744.7001 846.7004
899.8041 924.7512 927.4725
932.9010 1014.5481 1033.0197
1063.2772 1123.3838 1167.4358
1173.2655 1200.2988 1213.0392
1237.5922 1372.7087 1409.9846

1453.7510	1473.1719	1483.2069
1486.1203	1486.4338	1499.5719
1679.0616	1805.6117	2287.1232
3005.8577	3015.4225	3050.0191
3058.3318	3072.9656	3121.6802
3129.5539	3158.1668	3240.6103

TS: γ

-1196.2367	20.9711	34.2089
122.4701	142.5451	158.3211
224.8363	266.9558	294.3958
342.4002	386.1113	459.3174
496.8162	568.7773	622.6694
705.3063	760.4153	865.2770
900.1566	931.4137	960.8026
987.4464	1031.5241	1043.2167
1057.6513	1173.3087	1180.9490
1210.3083	1243.4854	1276.6209
1297.1679	1328.6240	1358.4796
1388.1885	1438.9646	1463.2286
1474.7055	1477.3655	1483.5607
1499.3795	1674.2170	1803.4994
3015.8889	3050.1968	3064.3284
3080.9132	3121.8792	3142.2263
3146.2791	3158.4868	3241.8435